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DIFFUSION INTERACTION OF IMPURITIES IN AQUEOUS MEDIUM

Abstract

In this work the mathematical model of the water discharge to a clearance is viewed for drawing a picture, demonstrating the setting of the water output polluters cloud. At the first moment a cloud of small particles, being included in $V_0 \subset V$, is directed into the fluid volume. At the given primary distribution of the mixture speed, that allows to forsee the concentration of polluting substances in the river in accordance with a fixed scheme of the flow and a given discharge of the polluters and to control the technological process at the clearing station

1. Introduction. Analysis of mass transfer processes has a great importance while planning and developing water protection systems. However exact analysis of these processes in the space time are impossible in majority of cases because of awkwardness and absence of analytic solution of equation describing distribution of calculated ingredient concentration in water reservoirs or drain sewerage system. Besides, the number of possible variants as a rule, many times exceeds the number of really existing standard objects. Therefore, researchers and designers use the mathematical simulation methods.

Mathematical simulation of ecosystems is an intensively developed scientific field that achieved great successes at present. As direct experiments with natural ecosystems are difficult and very often inadmissible and their possibilities of laboratory simulations are very restricted, mathematical models are one of main instruments of quantitative and practical control of aqueous ecological systems. The problems on impurity propagation are determined by systems of partial equations reflecting physical laws describing liquid motion in water-reservoir and different mass transfer in it [3]. The problems of mass propagation in stationary aqueous flow in general case are described by a system of partial differential equations including the Navier-Stock's equation ("hydrodynamics constituent") and mass transfer equation considering physico-chemical interaction of impurity with media and availability of impurity sources. The availability of effective algorithm and calculation program, as a rule, wholly defines possibility of application of this or other model; absence of appropriate mathematical apparatus often leads to necessity of refusal from the chosen conception of modeling or its simplification. Therefore, the problem of numerical realization of ecological models is very urgent. Their use enables to shorten expensive observation on location and get unique ecological predictions. Behavior of impurity in aqueous medium depends on many factors: chemical (decay, combination with other materials, fall-out); physical (transition between states, adsorption, coagulation); hydrodynamic (transfer by flows and scattering in turbulent diffusion process): biological (accumulation and transfer by sea bodies). In scientific-technical literature [1-6] there is a great number of mathematical models of impurity propagation in aqueous flow, considering the processes of aero oxidation of organic combinations nitrification, denitrification, growth and atrophy of plankton and etc. All these models are intended for investigating concrete objects. Their application to other similar objects is connected with serious difficulties, since the use of traditional methods of identification requires, many experiments. Besides, input effect vectors and output reactions have exclusively great dimension. And as the result, this complicates the use of known models in concrete situation. Application of computing engineering and up-to-date computer technologies opens new possibilities both before scientists researchers and the persons and organizations accepting responsible decisions on rational use of environment for the welfare of mankind. The required information-expert systems will be intended for estimation, control and prediction of ecological states of aqueous ecosystem of basin, and also support of decisions for realization of actions in all types of house-hold and cultural-every-day activity with using water resources and water-catchments basins by means of formation of highly qualified recommendations. Protection of water resources from increasing external affect of anthropogenic character is an actual practical matter and requires urgent measures.

The main cause of impurity of water basins is discharge of insufficiently sewage disposal by industrial enterprises, municipal economy and agriculture. The very important characteristic of the described process is dynamics of concentration of polluters influencing on the structure of water-ecological system. Creation of mathematical prediction model of quality of water is connected with choice of equations that more completely describe regularities of phenomena occurring in water-cources, and also by the definition of parameters characterizing peculiarities of the process. Near a spillway polluting impurity may move several times upstream and downstream. Its permutation process in a great degree is determined by turbulent stirring. Particles of polluters in water reservoir participate in adsorption exchange, alternate ratio of pollutions between phases at the expense of purely hydraulic processes of sedimentation and stirring up o bottom sediments. If for long-term estimation of pollution accumulation in bottom sediments it suffices to give constant coefficient of sedimentation, for seasonal prediction it is necessary to construct models describing temporal dynamics of sedimentation and stirring up flows.

However, up to day, control strategy taking into account assimilating ability of water-cources and dynamics of factors influencing on water quality in water basins has not been elaborated. Water quality control according to scientifically justified system is a part of a general system of rational nature management, whose important part is a mathematical model of hard particles sedimentation and transfer of passive impurities by viscous liquid flow. The given paper is devoted to elaboration of technical method of simulation of water flows that allows to construct adequate mathematical model and solution of the obtained mathematical problem with using applied program complex ANSYS in availability of qualitative and incomplete quantitative information on behavior of the object.

2. Problem statement. Let's consider a problem on motion of mixture consisting of a great of fine hard particles in viscous liquid, in a spatial domain. At initial moment (for $t = 0$) clouds of fine particles concentrated in the volume V were discharged into liquid of volume $V_0 \subset V$. In sedimentation process fine particles turn to be weighted in ambient viscous liquid and move together with it as a single whole that reduces to variation of local density of mixture.

By gravity and hydrodynamical interaction forces the particles move translationally and rotate together with ambient liquid. We'll assume that inertial effects of relative motion of liquid and solid phases of suspension are small-dimension of particles are small and specific densities of materials of particles ρ_p and liquid ρ_l are close among themselves. For determining local mean velocity of mixture we suggest the following equation obtained according to some technical assumptions given in [1]:

$$\frac{\partial(\overline{U}\rho)}{\partial t} + (\overline{u}\nabla)(\overline{u}\rho) - 2\mu \sum_{npqr=1}^{3} \frac{\partial}{\partial x_p} \times$$
$$\times \left\{ a_{npqr}(x,t)\varepsilon_{np}[\overline{u}]\overline{e}^q + \nabla p = \overline{f}\rho;\ \operatorname{div}\overline{u} = 0, \right\}, \tag{2.1}$$

where $\overline{u} = \overline{u}(x,t)$ is a mean velocity of the suspension; $p = p(t,x)$ is pressure; $\rho = \rho(t,x)$ is a mean density of mixture; $\rho = \rho(t,x) = \rho_l[1-c(x,t)]+\rho_p c(x,t)$, $c(x,t)$ is a body mean concentration of particles; μ is a dynamic viscosity of carrying liquid; $\overline{f}$ are external forces effecting on suspension;

$$\varepsilon_{np}[\overline{u}] = \frac{1}{2}\left(\frac{\partial u_n}{\partial x_p} + \frac{\partial u_p}{\partial x_n}\right)$$

is a strain tensor of viscous liquid, $\overrightarrow{e}^p$ is a unit vector of the coordinate axis $\overrightarrow{x}^p$ $(p = 1, 2, 3)$; a_{npqr} (x, t) is viscosity tensor.

The system of equations (2.1) is not closed, since it contains additional dynamical variables a_{npqr} (x, t) $(n, p, q, r = 1, 2, 3)$ $u^{\rho(t,x)}$ taking into account presence of a great number of hard weighted particles in viscous liquid. Calculation of viscosity tensor is a difficult problem since it depends on great totality of particles that undergo strong hydrodynamic interaction, as for ass diameter of particles and distances between them have the same order of smallness. If body concentration $c(x, t)$ is small, mean value of the viscosity tensor by the volumes of particles may be approximately calculated by the asymptotic formula given in [1]. But this formula is very complicated for practical applications. Therefore, in weak flow conditions characterized by small gradients of velocity of carrying liquid, Brownian motion will affect on motion of particles with predominant factors. In this case, the mean value of the suspension tensor is an isotropic tensor, and we can take into account influence of particles on liquid by introduction of effective viscosity of suspensions

$$\mu_{ev} = \mu[1 + \gamma c(x, t)], \tag{2.2}$$

where μ is dynamical viscosity of carrying liquid, γ is a coefficient determined by the form of axially symmetric particle. In general case, viscosity tensor depends on mean vector of orientation of particles $\overline{\lambda}(x, t)$ and body mean concentration of particles in liquid $c(x, t)$. From physical reasonings it follows that the function $c(x, t)$ should satisfy the discontinuity condition

$$\frac{\partial c}{\partial t} + (\overline{u}\nabla)c = 0, \tag{2.3}$$

Mean specific density of the suspension

$$\rho(x, t) = \rho_l[1 - c(x, t)] + \rho_p c(x, t), \tag{2.4}$$

satisfies the same equation as well.

According to formulae (2.1)-(2.4) the motion of weakly concentrated suspension of solid particles in viscous incompressible liquid will be described by the following closed system of equations $\left(\rho_p \neq \rho_l\right)$

$$\rho\left[\frac{\partial \overline{u}}{\partial t} + (\overline{u}\nabla)\overline{u}\right] - \sum_{i,k=1}^{3} \frac{\partial}{\partial x_i}\left[\mu_{ev}(\rho)\frac{\partial \overline{u}}{\partial x_i}\right] + \nabla p = \rho\overline{f};\ \operatorname{div}\overline{u} = 0 \tag{2.5}$$

$$\frac{\partial \rho}{\partial t} + (\overline{u}\nabla)\rho = 0 \tag{2.6}$$

where

$$\mu_{ev} = \mu\left[\frac{\rho_p - (1+\gamma)\rho_l}{\rho_p - \rho_l} + \frac{\gamma}{\rho_p - \rho_l}\rho(x, t)\right]. \tag{2.7}$$

In the case $a_{npqr}(x, t) = a_{npqr}(\overline{\lambda}, c)$ for mean vector of orientation it is valid the equation

$$\begin{gathered}\frac{\partial \overline{\lambda}}{\partial t} + (\overline{u}\nabla)\overline{\lambda} - \frac{1}{c(\rho)}\operatorname{div}[c(\rho)\nabla]\overline{\lambda} + D\overline{\lambda} = \\ = \Omega[\overline{u}]\overline{\lambda} + q_1(\left|\overline{\lambda}\right|)E[\overline{u}]\overline{\lambda} - q_2(\left|\overline{\lambda}\right|)E[\overline{u}]\overline{\lambda}, \overline{\lambda})\overline{\lambda},\end{gathered} \tag{2.8}$$

where $c(\rho)$, $q_i(\left|\overline{\lambda}\right|)$ are the known analytic or discrete functions; $k > 0$; $D \geq 0$ are the constants; $\Omega[\overline{u}]$, $E[\overline{u}]$ are antisymmetric and symmetric parts of the tensor of velocity gradient, respectively, i.e. the matrices with elements

$$\{\Omega[\overline{u}]\}_{i.k=1}^{3} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_x} - \frac{\partial \overline{u}_k}{\partial x_i}\right), \quad \{E[\overline{u}]\}_{i.k=1}^{3} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_x} + \frac{\partial \overline{u}_k}{\partial x_i}\right).$$

Thus, the closed system of equations (2.1), (2.6), (2.8) determines dynamics of suspension of solid axially-symmetric particles in viscous incompressible liquid.

3. Solution of the problem. We apply the stated mathematical model of motion of suspension of solid particles in viscous incompressible liquid to calculation of pattern of polluters clouds sedimentation from water outlet of industrials system of purification structures. To this end we consider the system of equations (2.5)-(2.7) in the bounded domain.

$$\Omega = \{x \in R_3 \colon |x_1| \le a;\ 0 \le x_2 \le a,\ |x_3| \le b, \quad b >> a\}.$$

We'll consider that at initial moment ($t = 0$) a cloud of fine particles concentrated in Ω was released into liquid of volume $\Omega_0 \subset \Omega$. Give initial distribution of particles

$$\rho(x,0) = \begin{cases} f_1(x,0), x \in \Omega_0 \\ \rho_l, x \in \Omega \backslash \Omega_0 \end{cases} \tag{2.9}$$

and polluters outlet discharge at initial moment

$$u(x,0) = f_2(x,0)\ . \tag{2.10}$$

The external effect has one constant component $q = 9,8\ m/s^2$ free fall acceleration. For successful application of ANSYS program complex we'll divide the problem into two parts. Part I is devoted to finding velocity field and pressure field in the flow, part II considers the process of propagation of masses for the known velocity field.

By the results of calculations we can construct the pattern of polluters cloud sedimentation ($\rho_p > \rho_l$), mixture density change, velocity field of the mixture. The stated mathematical model allows to predict concentration of polluters in a river for fixed scheme of flow and the given discharge of polluters and to control the technological process at the clearing stations.

4. Conclusion. A shell of information-prediction system is created, mathematical models and numerical algorithms are chosen for determining hydrothermal condition of water cources, calculation of thermal condition of the river with regard to 'heat' discharges, calculation of propagation of impurities in one-dimensional and approximation with regard to lateral diffusion. Modules of finite-element packet ANSYS / FLOTRAN and THERMAL were used for calculations. A new method is suggested for solution of such class of problems when velocity field is in ANSYS / FLOTRAN, and then it is imported to FlexPDE, where impurity transfer problem is solved. We consider a model problem on propagation of impurity in the section of a river or big channel in the case of predominant diffusion and in the case of mild diffusion. We give graphs of concentration change allowing to compare the obtained results. Graphs of impurity propagation at different moments after discharge are obtained. The results of calculations of velocity field are compared with data obtained in [2] by approximation formulae. Because of absence (on different reasons) of calculation data for other water reservoirs, some characteristics of water reservoir 'Khanbulanchay' known from information bulletin of ministry of Agriculture of the Republic is used. Therefore the cited results (in figures 1-3) are of illustrative character.

Fig. 1. Impurity propagation in the mild diffusion case at the moment $\Delta t = 70$ (after Δt time from the beginning of discharge)

Fig. 2. Impurity propagation in the strong diffusion case at the moment $\Delta t = 7$ (after Δt time from the beginning of discharge).

Fig. 3. Variation of velocity filed in longitudinal section of a water reservoir.

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