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Simulation of spreading of non-conservative passive substances in water bodies

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Abstract. Numerical modeling has become an indispensable tool for solving various physical problems. In this context, two fundamentally different approaches to the derivation of equations describing the motion of a liquid and the transfer of both conservative and non-conservative substances that have or do not affect the flow structure. In addition to the classical approach, in which the hydrodynamic equations of the baroclinic fluid are obtained from the Reynolds equations by introducing the assumption that the turbulent viscosity between jets is neglected, there is another approach, which is to introduce a certain scale of consideration, as well as the use of hypotheses about the magnitude of turbulent viscosity and small changes of flow characteristics along with horizontal coordinates as compared with the changes along with vertical one. Thus, there is the option to obtain similar equations allowing to numerically simulating unsteady flows with fixed boundary conditions (fluctuating streams). Also, the article discusses an approach to numerical simulation of biogenic substances as well as the chemical and biological processes in reservoirs.

1. Introduction

Currently, restrictions arising from the practical use of hydrodynamic equations do not allow to find their solutions in the complete formulation. Therefore, simplifying hypotheses are used in the practice of research and calculations. It is known that applied hypotheses lead to three-dimensional equations of baroclinic fluid, two-dimensional Saint-Venant equations, one-dimensional and zero-dimensional equations.

It turned out that in addition to the classical approach when hydrodynamic equations of the baroclinic fluid are obtained from the Reynolds equations by introducing the assumption that the planar turbulent viscosity between jets is neglected, there is another approach. The similar equations could be established by introducing a certain scale of consideration, using hypotheses about the magnitude of turbulent viscosity and the smallness of changes in all flow characteristics along the horizontal coordinate compared with the change along with the vertical one. This approach allows to numerically simulating unsteady (fluctuating) flows with fixed boundary conditions [1, 2].

The mathematical models described in [3–5] make it possible to predict the concentrations of various water-polluting substances in water bodies with varying degrees of accuracy and details.



2. Method

Therewith, the higher accuracy the more complex the algorithms and all models are built on the principle of dimension in space starting with three-dimensional which give the best possible details (concentration distribution both in depth and in the area of the water body) and ending with zero-dimensional ones which allowing to determine only average concentration over the volume of the entire water body. In this sense, there is a hierarchy of mathematical models.

3. Discussion

The next question is: in what cases, which model should be used? This is connected, first of all, with the limits of applicability of each model and with the scale and details of the forecast. According to [5], the following hypothesizes:

if the horizontal dimensions of water bodies are much greater than their depth, and the scope of consideration:

$$M_L = L_n^2 T, \quad (1)$$

here: L_n is linear planar scale (and, and, $L_n \gg h$, where h is the depth of the stream); $T = L_n/U$, where U is the representative speed of the stream, and

$$\frac{\rho_{\max} - \rho_{\min}}{\rho_{\max} + \rho_{\min}} \ll 1$$

when changes of all flow characteristics along horizontal coordinates are much smaller than along vertical one, and

the turbulent viscosity hypothesis is used:

$$\tau_i = \nu_T \frac{\partial u_i}{\partial z} \quad (2)$$

here: ν_T is determined either using the Karman model or “κ-ε” model, and to determine the pulsations of density and pressure, it is assumed that

$$\nu_T = \nu_T^{(0)} f(Ri) \quad (3)$$

here: $Ri = g \frac{\partial \bar{\rho}}{\partial z} / \left(\frac{\partial u}{\partial z} \right)^2$ is Richardson number [7], $\nu_T^{(0)}$ is turbulent viscosity (i.e. with $Ri = 0$

there is a single-density flow).

The following equations could be used for the water bodies whose horizontal dimensions are much greater than their depths:

$$\begin{cases} \frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} + \frac{\partial u_i w}{\partial z} + g \left(\frac{\partial z}{\partial x_i} + \frac{1}{\rho} \int_z^z \frac{\partial \rho}{\partial x_i} \partial z \right) = \frac{\partial}{\partial z} \nu_T \frac{\partial u_i}{\partial z} + \frac{\partial}{\partial z} \mu \frac{\partial u_i}{\partial z} \frac{1}{\rho} \\ \frac{\partial u_i}{\partial x_i} + \frac{\partial w}{\partial z} = 0 \\ \frac{\partial S_r}{\partial t} + \frac{\partial S_r u_j}{\partial x_j} + \frac{\partial S_r w}{\partial z} = \frac{\partial}{\partial z} D \frac{\partial S_r}{\partial z} + q_{S_z} \\ \rho = \rho(S_r) \end{cases} \quad (4)$$

It should be emphasized here that all dependent variables u_i , q_i and h_i in (4) have different meanings depending on, these equations are obtained from the Reynolds equations or directly from the conservation laws. In the first case, these variables are averaged first by probability and then by a large scale. In the second case, these are actual variables averaged over the same scale.

Considering a statistically stationary flow, in the case of an ergodic process averaging over probability is equivalent to averaging over infinite time. Therefore, if equations (4) are the result of the Reynolds equations, then in the case, they can be used to describe constant-property flows only. At the same time, if equations (4) are the result of conservation laws and all dependent variables u_i , q_i and h_i in (4) are actual averaged on the scale (1), then it is possible to even in the case of statistically stationary flows using the equations (4) for considering flows with the time scales greater than L_n/U_{CB} here U_{CB} - disturbances drift velocity. Thus, in the first case, an important class of tasks with pulsating flows under constant boundary conditions is excluded from consideration.

Strictly speaking, all of the above is valid for a border-free flows. Therefore, if the flow is considered near a rough vertical wall then the hydrodynamic variables should not be considered as actual and circuits cannot be considered as the result of flows averaged over probability. It is proposed to consider hydrodynamic variables in (4) as averaged over the scale M_Δ which is much bigger than the scale of roughness but much smaller than (1). In this case, τ_{ij} are similar to Reynolds stresses when averaging is carried out not on probability, but on a scale M_Δ . These stresses are determined by peaks of roughness. Stresses at the bottom $\tau_{n_b x_i}$ could be determined analogically by the bottom roughness.

Tangent force acting on the lateral face $(F_\tau)_B$, is in the order of magnitude:

$$(F_\tau)_B = \bar{\tau}_c \quad (5)$$

here τ_c - shear stress on the wall, and shear force acting on the bottom $(F_\tau)_b$, is in the order of magnitude:

$$(F_\tau)_b = \tau_b \Omega_b \quad (6)$$

here τ_b - shear stress on the bottom, Ω_b - bottom surface area.

From (5,6) it follows that in order to neglect by $(F_\tau)_B$ compare to $(F_\tau)_b$, it is necessary comply with the following condition:

$$\frac{\tau_c}{(\tau_b)} \ll \frac{\Omega_c}{\Omega_b} \quad (7)$$

Since, τ_c and τ_b depend on the bottom and walls roughness and L_n always $\gg L$, then (7) is almost always enforced.

A modified Prandtl [6] model usually used to close the system equations:

$$v_T = L^2 \left| \frac{\partial u}{\partial z} \right| \quad (8)$$

here: $L = L_0 \exp\left(c \frac{\partial \rho}{\partial u} \sqrt{dL}\right)$; $c = 275$, if $\frac{\partial \rho}{\partial z} < 0$

$$\left. \begin{aligned} L_0 &= 0.14 - 0.08\tilde{z} - 0.06\tilde{z}^2 \\ \tilde{z} &= \begin{cases} (z - z_0) / (1 - z_0) & z > z_0 \\ (z - z_0) / z_0 & z < z_0 \end{cases} \\ z_0 &= \frac{\tau_b}{\tau_b + \tau_s} \end{aligned} \right\} \quad (9)$$

if $\frac{\partial \rho}{\partial z} > 0$, then

$$v_T = \sqrt{g \frac{\partial \rho}{\partial z} + \left(\frac{\partial u}{\partial z}\right)^2} \cdot L_0^2 \quad (10)$$

or “k-ε” model [7]:

$$\begin{aligned} \frac{\partial K}{\partial t} + u_i \frac{\partial K}{\partial x_i} + w \frac{\partial K}{\partial z} &= \frac{\partial}{\partial z} \left(\frac{v_T}{\sigma_K} \frac{\partial K}{\partial z} \right) - F_K \\ \frac{\partial \varepsilon}{\partial t} + u_i \frac{\partial \varepsilon}{\partial x_i} + w \frac{\partial \varepsilon}{\partial z} &= \frac{\partial}{\partial z} \left(\frac{v}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial z} \right) - F_\varepsilon \\ F_K &= (P + G) + \varepsilon \\ F_\varepsilon &= c_{1\varepsilon} \frac{\varepsilon}{K} (P + G) (1 + c_{3\varepsilon} Ri_f) - c_{2\varepsilon} \frac{\varepsilon^2}{K} \\ Ri_f &= -\frac{G}{p + G} \\ P &= -v_T \left[\left(\frac{\partial u_1}{\partial z}\right)^2 + \left(\frac{\partial u_2}{\partial z}\right)^2 \right] \\ G &= -g \frac{v_T}{\sigma_t \rho} \frac{\partial \rho}{\partial z}, \end{aligned} \quad (11)$$

here: K - energy of turbulence, ε - turbulence dissipation rate, P – element describing the generation of turbulence energy, G – element which indicates the the change in turbulence energy due to Archimedean forces, β - volume expansion coefficient, Ri_f - modified Richardson number [7], $c_\mu, c_{1\varepsilon}, c_{2\varepsilon}, c_{3\varepsilon}, c_k, c_\varepsilon, c_t$ - empirical constants, in shear flows they are as follows:

$$c_\mu = 0.09, c_{1\varepsilon} = 1.44, c_{2\varepsilon} = 1.92, c_{3\varepsilon} = 0.8, c_k = 1.0, c_\varepsilon = 1.3, c_t = 0.9.$$

Hereinafter, an active substance is understood as a component affecting the flow, and passive substance which is not affecting. The substance S_i in (4) is an active one. This for example, mineralization or water temperature. Mineralization and temperature may be a passive substance if [8].

$$Ri = \frac{\partial \rho / \partial z \cdot g}{(\partial u / \partial z)^2} < 0.1 \quad (12)$$

$$\frac{\partial z_s}{\partial x} \gg H \frac{\partial \bar{\rho}}{\partial x} \quad (13)$$

here: H is total flow depth, $\bar{\rho}$ is depth average density.

Other examples of passive substances are various contaminants: dissolved and suspended phosphorus and nitrogen compounds, herbicides, pesticides, BOD, etc.

If the substances interact with each other, then the equations of their distribution should characterize both their transport and the decomposition reaction and production and have the following form [9]:

$$\begin{aligned} \frac{\partial S_r}{\partial t} + \frac{\partial u_i S_r}{\partial x_i} + \frac{\partial w S_r}{\partial z} &= a_{rj} S_j = F_r \\ r &= 1, 2, \dots, n \\ j &= 1, 2, \dots, n \end{aligned} \quad (14)$$

here: r and j are the numbers of substances, a_{rj} is interaction matrix elements:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdot & \cdot & \cdot & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

In general, a_{rj} could depend on S_r , coordinates, and time.

An important negative consequence of anthropogenic impact which significantly affects the aquatic environment is eutrophication. The main reason for this is the discharge of agricultural fertilizers and untreated wastewater from the food industry or municipal wastewater. This leads to the enrichment of water with biogenic elements (phosphorus and nitrogen mainly) and in turn to a significant increase in the torpidity of water bodies. Large masses of phytoplankton, especially blue-green algae, leading to a deterioration in water quality, negative impacts on fisheries, and possibly a complete change in ecosystems.

Biogenic substances entering water bodies as well as those resulting from chemical and biological processes are carried by flows without affecting its movement because their concentration is very small. Thus, the motion of any component of the biosystem (S_k) can be described by equation (14) while biological processes are determined by the right side of this equation.

A large number of bio species involved in the eutrophication process does not allow each of them to be considered individually. Recently, some works [10, 11] have appeared that are based on the grouping of different types of biota by signs of consumption and excretion of the main nutrients - phosphorus and nitrogen. With this approach (S_k) denotes not bio species but the concentration of nutrient in the group of bio species.

Blue-green algae are an important adverse factor affecting water quality. It is well known [11] that phosphorus is the limiting factor for the development of these algae. Thus, the right side (14) should describe the circuit of phosphorus compounds, and S_k - various phosphorus compounds. In this case, the right side of equation (14) can be written as:

$$F_k = A_k - K_k + C_k$$

here: A_k is the growth rate of this component of the phosphorus system due to intra-water processes, C_k is the speed of its inflow from external sources, K_k is its decreased rate due to intra-water processes.

The general scheme of the phosphorus cycle is as follows (fig. 1):

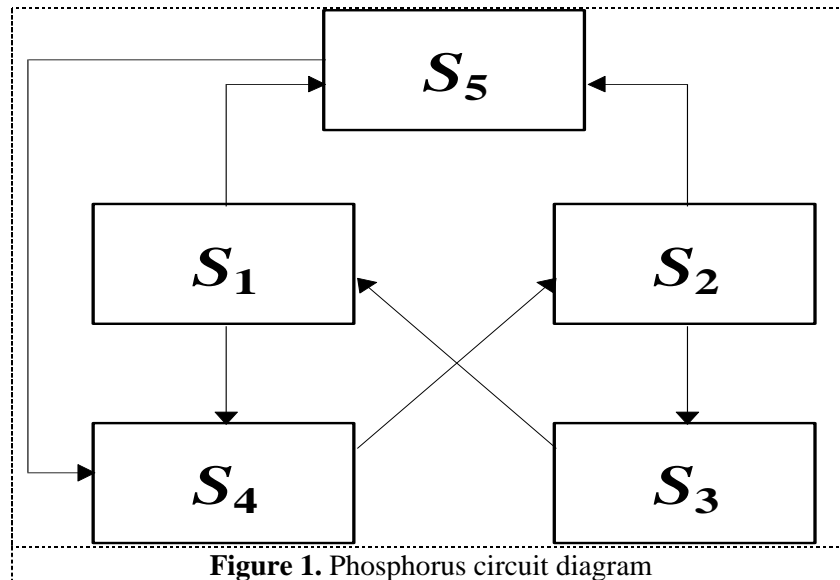


Figure 1. Phosphorus circuit diagram

S_1 is phosphorus concentration in phytoplankton; S_2 is phosphorus concentration in bacteria; S_3 is the concentration of dissolved inorganic phosphorus S_4 is the concentration of dissolved organic phosphorus; S_5 is a detrital phosphorus concentration.

Based on the phosphorus circuit model proposed in [10] expressions for A_k , K_k and C_k are as follows:

$$A_1 = B_1 S_1; \quad K_1 = B_1 r_1 S_1 + v_1 \frac{S_1^2}{B_1}$$

$$A_2 = B_2 S_2; \quad K_2 = B_2 r_2 S_2 + v_2 \frac{S_2^2}{B_2}$$

$$A_3 = r_2 B_2 S_2; \quad K_3 = B_1 S_1$$

$$A_4 = r_1 B_1 S_1 + \alpha_D S_5; \quad K_4 = B_2 S_2$$

$$A_5 = v_1 S_1^2 / B_1 + v_2 S_2^2 / B_2; \quad K_5 = \alpha_D S_5 + D_r$$

here:

$$B_i = \frac{K_i R_T^{(i)} R_i^{(i)}}{1 + \alpha_i S_i / S_{i+2}};$$

$$r_i = \frac{(a_i / b_i) B_i}{1 / b_i + B_i} + (1 - a_i / b_i);$$

$a_i, b_i, K_i, v_i, \alpha_i$ - dimensional constants according to [10]:

$$K_1 = 2.3 \text{ day}^{-1};$$

$$v_1 = 1 \text{ (mg/l)}^{-1}(\text{day})^{-2}; v_2 = 0.005 \text{ day}^{-1}; v_3 = 0.5 \text{ (mg/l)}^{-1}(\text{day})^{-2};$$

$$a_1 = 0.057 \text{ day}; a_2 = 0.075 \text{ day};$$

$$b_1 = 0.3 \text{ day}; b_2 = 0.45 \text{ day};$$

$$\alpha_1 = 0.6; \alpha_2 = 1.$$

$$R_T^{(1)} = 0.2 + \frac{2.2 \cdot 10^{-3} (\exp(0.21T) - 1)}{1 + 2.8 \cdot 10^{-3} \exp(0.21T)}$$

$$R_T^{(1)} = 0.2 + \frac{2.2 \cdot 10^{-3} (\exp(0.21T) - 1)}{1 + 2.8 \cdot 10^{-3} \exp(0.21T)}$$

here: T is the temperature of the water, °C;

$R_T^{(i)}$ is a light factor.

$$R_T^{(1)} = (e / K_e h) [\exp(-r_x) - \exp(-r_e)];$$

here $r_e = I / I_0$; $r_x = r_e \exp(-K_e h)$; $K_e = K_a + \alpha_s S_1$.

(I - daily average light, $I_0 = 350 \text{ calories/sm}^2 \times \text{day}$, h - depth, K_a and α_s - constants; for clear water $K_a = 1.7 \text{ m}^{-1}$; $\alpha_s = 19 \text{ m}^{-1}(\text{mgP/l})^{-1}$; α_D - factor of decomposition of detritus to dissolved organic

phosphorus: $\alpha_D = \frac{1.2 \cdot 10^{-4} (\exp(0.35T) - 1)}{1 + 3 \cdot 10^{-4} \exp(0.35T)}$ D is detritus precipitation rate.

4. Conclusions

Equations allowing numerical simulation of pulsation flows i.e., modelling of unsteady flows under stationary boundary conditions can be obtained by introduction of a particular scale of consideration of flows, using relevant hypotheses about the value of turbulent viscosity, small changes of flows characteristics along the horizontal coordinate compared to a change along the vertical one.

Grouping of different types of biota by signs of consumption and excretion of the main nutrients - phosphorus and nitrogen allows to simulate concentration of nutrients in a group of bio species, including dynamics of the development of blue-green algae.

Application of the proposed models allows to predict the spread of pollution as well as eutrophication of water bodies with sufficient accuracy.

References

- [1] Militeev A N **1983** Numerical modeling of pulsation flows and heat and mass transfer in shallow non-stratified reservoirs *Hydraulic research in the energy and water sectors* pp 8 – 22 (Russia).
- [2] Alberto S, Ugo P **2001** Numerical simulation of pulsating turbulent channel flow. *Physics of Fluids* 2001 Vol. **3(5)** pp 1367-1384
- [3] Bazarov D R and Mavlyanova D A **2019** Numerical studies of long-wave processes in the reaches of hydrosystems and reservoirs *Mag Civ Eng* **87** 123 doi: 10.18720/MCE.87.10
- [4] Safia Meddah, Abdelkader Saidane, Mohamed Hadjel, Omar Hireche 2015 Pollutant Dispersion Modeling in Natural Streams Using the Transmission Line Matrix Method. *Water* **7** pp 4932-4950
- [5] Bazarov D, Shodiev B, Norkulov B, Kurbanova U and Ashirov B **2019** Aspects of the extension of forty exploitation of bulk reservoirs for irrigation and hydropower purposes *E3S Web Conf.* **97**
- [6] Klas Persson, Georgia Destouni **2009** Propagation of water pollution uncertainty and risk from the subsurface to the surface water system of a catchment. *Journal of Hydrology*. Vol **377(3-4)** pp 434-444.
- [7] Krutov A, Bazarov D, Norkulov B, Obidov B and Nazarov B **2019** Experience of employment of computational models for water quality modelling *E3S Web Conf.* **97**

- [8] Krutov A N **1979** Development of the theory and methods for predicting the spread of pollutants in the surface water bodies of arid zones p 21 (Russia).
- [9] Mamajonov M, Bazarov D, Uralov B, Djumabaeva G and Rahmatov N **2019** The impact of hydro-wear parts of pumps for operational efficiency of the pumping station *J Phys Conf Ser* **1425** 012123 doi: 10.1088/1742-6596/1425/1/012123
- [10] Shlihting G Sh **1974** Boundary layer theory. (Mocow, Scinece) p 742 (Russia)
- [11] Rodi W **1984** *Environmental Turbulence Models. Methods for calculating turbulent flows* p 275 (Russia)
- [12] Militeev A N and Bazarov D R **1999** A two-dimensional mathematical model of the horizontal deformations of river channels *Water Resour* **26** 17
- [13] Bazarov D R, Vokhidov O F, Lutsenko L A and Sultanov Sh **2019** Restrictions Applied When Solving One-Dimensional Hydrodynamic Equations *Proc. EECE 2019, Lect. Notes Civ. Eng.* **70** pp 299–305
- [14] Lyatcher V M **1964** Conditions for the formation of density flow in water bodies // Proceedings of the coordination meeting on hydraulic engineering pp 100-117 (Russia).
- [15] Militeev A N **1982** p Solving the problems of hydraulics in shallow reservoirs by numerical methods p 43 (Russia)
- [16] Leonov A V **1986** Mathematical modeling of the transformation of phosphorus compounds in freshwater ecosystems in the Lake Balaton p 152 (Russia)
- [17] Strashkraba M and Gnauk A **1989** *Freshwater ecosystems (mathematical modeling)* p 373