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Numerical Models to Forecast Water Quality

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Abstract. The depth-averaged hydrodynamic equations were numerically investigated. Numerical solutions of the equations were obtained using Chebyshev polynomials for a given number of operations and various ratios of the number of layers and the number of polynomials.
Numerical solutions were compared with analytical ones using, as an example, the heat conduction equation. The performed numerical studies demonstrated the tendency of the numerical solution to the exact one over time in all cases considered. The best ratio of the number of layers and the number of polynomials was revealed.
Comparison of finite-difference solutions with the analytical one for the same number of operations showed the advantage of the polynomial method.

INTRODUCTION

The beginning of the use of numerical models based on the method of finite differences, designed to solve hydrodynamic problems, including for predicting transport processes in open watercourses and reservoirs, is associated with the development of computer technology [1 - 15]. The essence of the finite difference method lies in the discretization of time and space variables (grid construction) and the required functions (introduction of grid functions) from derivatives and integrals of these functions (construction of a difference scheme on a grid). As a result, the systems of differential or integral equations in each discrete structure (cell) of the region under consideration are replaced by systems of algebraic equations, the solution of which allows finding numerical values of the sought functions.

METHODS

According to [17 – 11], the general equations of hydrodynamics can be written in the following form:

$$\begin{aligned} &\frac{\partial u_i \rho}{\partial t} + \frac{\partial u_i u_j \rho}{\partial x_j} + \frac{\partial \rho}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + g_i \rho \\ &\frac{\partial \rho}{\partial t} + \frac{\partial u_i \rho}{\partial x_i} = 0; \quad \frac{\partial S_r}{\partial t} + \frac{\partial S_r u_j}{\partial x_j} = q_{Sr} \\ &\rho = f(S_r); \quad i = 1,2,3\,, \end{aligned} \tag{1}$$

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where u_i is projection of the current velocity vector onto the axis x_i, p is hydrodynamic pressure, τ_i is shear stress tensor component, ρ is density, g_i is component of the gravity acceleration vector, q_{Sr} are internal sources of substance for Newtonian fluid,

$$\tau_{ij} = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \nu\rho, \tag{2}$$

ν is kinematic fluid viscosity, S_r is some substance that determines the density, for example, temperature, salinity. In the case of an incompressible fluid, when considering water bodies, the planned dimensions of which are much greater than the depth and introducing the scale of consideration:

$$M_L = L_n^2 T, \tag{3}$$

here L_n is linear scale with $L_n >> h$, here h is flow depth; $T = L_n / U$, U is intrinsic velocity in the case when

$$\frac{\rho_{\max} - \rho_{\min}}{\rho_{\max} + \rho_{\min}} << 1 \tag{4}$$

the system of equations (1) could be converted in the following system of equations:

$$\begin{cases} \dfrac{\partial u_i}{\partial t} + \dfrac{\partial u_i u_j}{\partial x_j} + \dfrac{\partial u_i w}{\partial z} + g\left(\dfrac{\partial z_\Gamma}{\partial x_i} + \dfrac{1}{\rho} \displaystyle\int_z^{z_\Gamma} \dfrac{\partial \rho}{\partial x_i} \partial z \right) = \dfrac{\partial}{\partial z} \nu_T \dfrac{\partial u_i}{\partial z} + \dfrac{\partial}{\partial z} \mu \dfrac{\partial u_i}{\partial z} \dfrac{1}{\rho} \\ \dfrac{\partial u_i}{\partial x_i} + \dfrac{\partial w}{\partial z} = 0 \\ \dfrac{\partial S_r}{\partial t} + \dfrac{\partial S_r u_j}{\partial x_j} + \dfrac{\partial S_r w}{\partial z} = \dfrac{\partial}{\partial z} D \dfrac{\partial S_r}{\partial z} + q_{Sz} \\ \rho = \rho(S_r) \end{cases} \tag{5}$$

RESULTS AND DISCUSSION

Basic requirements for numerical models

All processes could be considered in time layers (discrete time):

$$t_n = \sum_{m=1}^{n} \tau_m \tag{6}$$

Denote by f_c is a grid function that is a solution to an algebraic system of equations obtained by discretization, and by f_n is the projection of the solution of the system of initial equations onto the selected grid. From the point of view of the accuracy of the method, the only requirement for the numerical model is the requirement for convergence:

$$\left(f_e - f_n \right(= \varepsilon\left(R_i, \tau \right) \to 0, \text{ for } R_i \to 0;\ \tau \to 0, \tag{7}$$

here R_i is the size of i- cell, $\varepsilon\left(R_i,\tau\right)$ is a function describing the error with which the desired value is determined. At present, the theory of difference schemes does not allow to find the function $\varepsilon\left(R_i,\tau\right)$ and a priori estimate the error of the numerical method for complex nonlinear systems.

However, the rich empirical material accumulated to date on the application of numerical methods in gas dynamics and hydraulics makes it possible to outline the conditions under which the finite difference method gives an accuracy acceptable for practice. In this case, instead of (2), the requirement is usually imposed on the approximation on the template of the initial equations by the difference scheme and the stability of the linearized equations. In the case of initial linear equations, these requirements are necessary and sufficient for the convergence of the scheme.

For nonlinear circuits, the approximation requirement is natural since otherwise, as the steps tend to zero, they can converge to others and not to the original equations. The requirement of stability of linearized equations is discussed in detail in [17, 18, 21], where it is shown that, in addition to the approximation condition, all requirements for difference schemes should have the meaning of exact observance of some properties of the original equations. It was also shown that not all schemes that satisfy the requirements of approximation and stability give satisfactory results. Additional requirements often need to be set, such as:

- For the scheme to be conservative (divergent), i.e., it is possible to introduce grid functions that are analogues of momentum and mass, which would be exactly preserved when summed on the grid, regardless of the size of the cell. However, it should be borne in mind that the scheme is conservative within the region under natural boundary conditions, i.e. for the Cauchy problem, it can give difference sources of momentum and mass at the boundary, as shown in [12 – 17].
- For the circuit to have a trivial solution on grids that do not change in time, the fulfilment of this requirement is not difficult. If the grid on the real region changes in time, then this requirement leads to the need to introduce additional terms in the difference equations.
- It is necessary that the property of symmetry is fulfilled, i.e. when changing the direction of flow, the solution would be the same as before changing.
- For flows with small Froude numbers ($|U| << \sqrt{gh}$), the difference scheme did not contradict the approximate self-similarity in the Froude number, i.e. when the speed at the boundary changes by α times, the time scale by a factor of $1/\alpha$ the speed inside the region would change by approximately α times.
- If velocity at the boundary changes by α times, the velocities in a stationary flow (or time-averaged velocities in a pulsating flow) should also change α times. The fulfilment of this requirement is necessary so that, using the same scheme, it would be possible to calculate sharply stationary, quasi-stationary, and pulsating flows and, in addition, stationary flows by the "establishment" method.
- Invariance of linearized equations concerning transformation $\hat{U}_i' = U_i' + C$, where C is any constant. This requirement is very important because, otherwise, small perturbations can be masked by the difference effects.
- Such an approximation of two-dimensional equations, in which for straightened channels a one-dimensional scheme, taking into account the real change in the cross-flow area, would be a consequence of a two-dimensional.

For the equation of pollution transfer, as the experience of calculations shows [118 – 23], the following properties should be required:

1. Divergence (the property to accurately preserve the mesh analogue of the impurity mass on the pattern).
2. Invariance of difference equations concerning transformation $\hat{S} = S + C$, here S is admixture concentration, C is constant,
3. Symmetrical.

In addition, it is necessary to comply with the requirements for the independence of the stationary state in time.

Numerical models

Following [18], the complete equations of motion (without the hydrostatic hypothesis) can be written in the form:

$$\frac{\partial \Omega_2}{\partial t} - \left(\Omega_1 \frac{\partial U_2}{\partial x_1} + \Omega_2 \frac{\partial U_2}{\partial x_2} + \Omega_3 \frac{\partial U_2}{\partial z} + \right) = \frac{\partial^2 \tau_1}{\partial z} - \frac{\partial \rho}{\partial x_1} \frac{g}{\rho}$$
$$- \frac{\partial \Omega_1}{\partial t} - \left(\Omega_1 \frac{\partial U_1}{\partial x_1} + \Omega_2 \frac{\partial U_1}{\partial x_1} + \Omega_3 \frac{\partial U_1}{\partial z} + \right) = \frac{\partial^2 \tau_2}{\partial z} - \frac{\partial \rho}{\partial x_2} \frac{g}{\rho}, \quad (8)$$

here $\Omega_1 = \frac{\partial W}{\partial x_2} - \frac{\partial U_2}{\partial z}$; $\Omega_2 = \frac{\partial U_1}{\partial z} - \frac{\partial W}{\partial x_1}$; $\Omega_3 = \frac{\partial U_2}{\partial x_1} - \frac{\partial U_1}{\partial x_2}$.

When deriving equation (8), it was assumed that the change in stresses along the horizontal coordinates is much less than along the vertical ones. Making this assumption about the flow rates, the following will be obtained from (8):

$$\frac{\partial \sigma_1}{\partial t} - \sigma_1 \frac{\partial U_2}{\partial x_2} + \sigma_2 \frac{\partial U_1}{\partial x_2} = \frac{\partial^2 \tau_1}{\partial z^2} + g \frac{\partial \rho}{\partial x_1}$$
$$\frac{\partial \sigma_2}{\partial t} + \sigma_2 \frac{\partial U_1}{\partial x_1} - \sigma_1 \frac{\partial U_2}{\partial x_1} = \frac{\partial^2 \tau_2}{\partial z^2} + g \frac{\partial \rho}{\partial x_2}, \quad (9)$$

here $\tau_1 = \mu \frac{\partial U_1}{\partial z}$; $\tau_2 = \mu \frac{\partial U_2}{\partial z}$; $\mu = \nu\rho$; $\sigma_i = \frac{\partial U_i}{\partial z}$.

To consider the problem in vertical limits independent of *x*, *y,* a new coordinate system is introduced:

$$\tilde{z} = \frac{z - z_Д}{z_П - z_Д}; \quad \tilde{x} = x; \quad \tilde{y} = y; \quad \tilde{t} = t$$

In which the flow region lies in the range from 0 to 1. In these coordinates, the equations have practically the same form as in the old coordinates, with the replacement W for W_0:

$$W_0 = W - \frac{\partial h}{\partial t}\tilde{z} - \left(\frac{\partial h}{\partial x_1} U_1 + \frac{\partial h}{\partial x_2} U_2 \right) \tilde{z} - \left(\frac{\partial z_Д}{\partial x_1} U_1 + \frac{\partial z_Д}{\partial x_2} U_2 \right).$$

In what follows, the sign "~" over variables is meant.

To consider the fundamental approaches to solving the problem, we will assume that ρ and μ are weakly dependent functions of coordinates and time, and μ - is a given function. In addition, we will neglect the vertical convective transport in comparison with the diffusion. These assumptions do not affect the principled approach. In addition, a large number of problems can be solved with these assumptions. The solution algorithm, taking into account the terms corresponding to them in the equation, will be presented below.

Under the assumptions made above, the equations are as follows:

$$\frac{\partial \tau_1}{\partial t} + U_j \frac{\partial \tau_1}{\partial x_j} - \tau_1 \frac{\partial U_2}{\partial x_2} + \tau_2 \frac{\partial U_1}{\partial x_2} = \frac{\mu}{h^2} \frac{\partial^2 \tau_1}{\partial z^2}$$

$$\frac{\partial \tau_2}{\partial t} + U_j \frac{\partial \tau_2}{\partial x_j} + \tau_2 \frac{\partial U_1}{\partial x_1} - \tau_1 \frac{\partial U_2}{\partial x_1} = \frac{\mu}{h^2} \frac{\partial^2 \tau_2}{\partial z^2}$$

$$\tau_1 = \frac{\mu}{h} \frac{\partial U_1}{\partial z} \tag{10}$$

$$\tau_2 = \frac{\mu}{h} \frac{\partial U_2}{\partial z}$$

$$\frac{\partial U_i}{\partial x_i} + \frac{1}{h} \frac{\partial W}{\partial z} = 0$$

With boundary conditions:

$$U\big|_{z=0} = 0 \vee U\big|_{z=0} = \sqrt{\frac{\tau_b}{\alpha_b}} \tag{11.1}$$

$$\vec{\tau}\big|_{z=1} = \vec{\tau}_n = \lambda W_i |W| \tag{11.2}$$

$$\frac{\partial z_s}{\partial t} + \left(U_s\right)_i \frac{\partial z_s}{\partial x_i} = W_s \tag{11.3}$$

Obviously, conditions (11) are not enough for the solvability of the equations. There is a need for one more condition. However, there are no physical prerequisites for it. This happened because, having passed to the equations in stresses, the pressure was excluded, i.e. an additional condition is included in the original formulation of the problem. Indeed, integrating the first two equations (5), we obtain the missing condition:

$$\rho\left(\frac{\partial \overline{U}_i h}{\partial t} + \frac{\partial \overline{U}_i \overline{U}_j h}{\partial x_j}\right) + \rho g h \frac{\partial z_П}{\partial x_i} + \frac{\partial R_{ij} h}{\partial x_j} = \left(\tau_П - \tau_Д\right)_i \tag{12}$$

$$i = 1,2$$

here: $R_{ij} = \int_{z_Д}^{z_П} \rho\left(U_i - \overline{U}_i\right)\left(U_j - \overline{U}_j\right) dz$; $\overline{U} = \frac{1}{h} \int_{z_Д}^{z_П} U_i dz$.

With the introduction of depth-averaged equations, the problem is posed as closed. In this case, it turns out to be more convenient, instead of condition (11.3), to use the averaged continuity equation:

$$\frac{\partial h}{\partial t} + \frac{\partial \overline{U}_i h}{\partial x_i} = 0 \tag{13}$$

In [16-20], an algorithm is given for solving equations (9) for flows with high viscosity using Chebyshev polynomials. To study the accuracy of the solution method, the following numerical experiments were carried out:

for a given number of operations $M=nN$ various relations between the number of layers n and the number of polynomials were considered N:

1) n=1, N=21
2) n=7, N=3

Using the example of the heat conduction equation

$$\frac{\partial u}{\partial t} = \mu \frac{\partial^2 U}{\partial z^2} \tag{14}$$

with the initial condition $U\big|_{t=t_0} = \delta(t - t_0)$ in the point z=0, the numerical solution was compared with the analytical one.

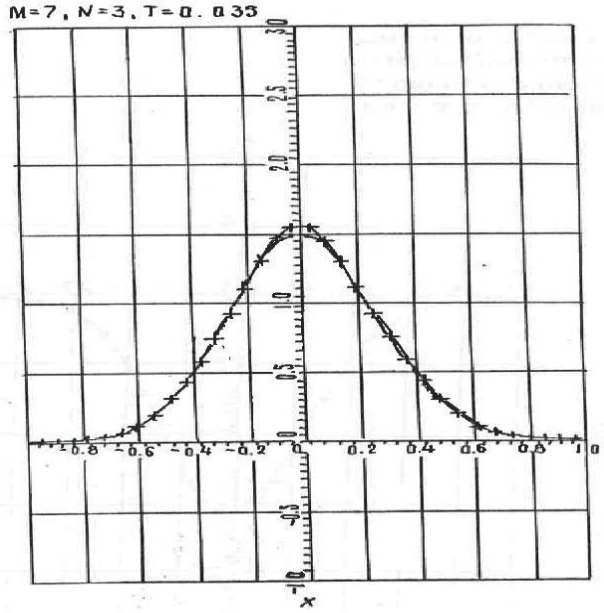
The performed numerical studies showed the tendency in time of the numerical solution to the exact one in all cases. But the obvious advantage of splitting into n=7, N=3 in comparison with other cases. Comparison of the analytical solution with the finite-difference solution with the same number of operations showed the advantage of the polynomial method.

An example of such a time-varying solution of the heat conduction equation is the propagation of the δ - function on the segment (−1.1):

$$U(t) = \frac{e^{-Z^2/4at}}{2\sqrt{\pi a t}} \qquad (a = \mu = 1)$$

serves as a good illustration of the advantage of solving it with the help of polynomials and the expediency of partitioning into layers with the representation of the function by the number of polynomials N=3.

A series of numerical experiments were also carried out for N=3 (n=7) with different variants of equations for determining a_0^j, a_1^j, a_2^j $(j = \overline{1,n})$. It turned out that the best option is to use a quadratic polynomial in combination with Galerkin's method (Fig.1).



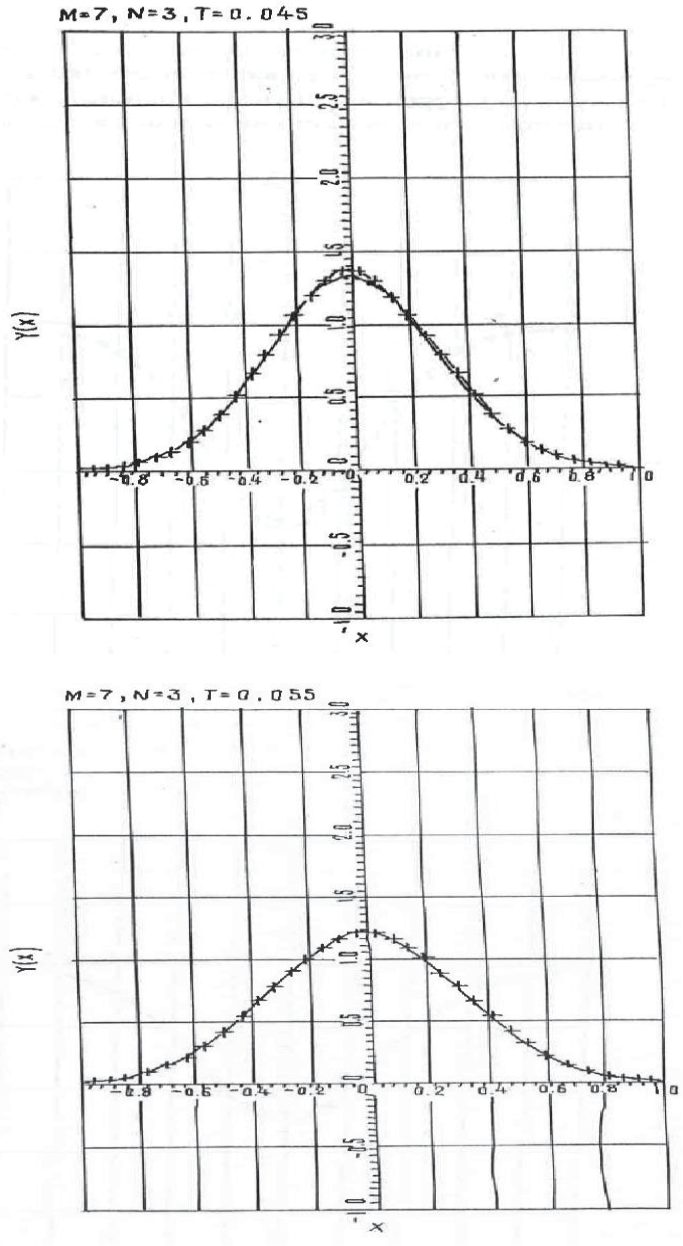


FIGURE 1. Comparison of the numerical and analytical solutions of the heat conduction equation for the moments of time T = 0.035; T = 0.045; T = 0.055. Polynomial method: number of layers M = 7, number of polynomials N = 3. Legend: --- - analytical solution; x x – numerical solution.

CONCLUSIONS

The accumulated practical experience in using finite-difference schemes in solving dynamic problems made it possible to find the necessary conditions under which numerical methods can be used for engineering calculations and research of hydrodynamic processes.

To solve practical problems related to predicting the spread of pollutants in water bodies and watercourses, a grid-spectral method was developed, which showed high efficiency in the case of studying stratified currents. It turned out that this method requires strong restrictions on the time steps.

Especially for solving problems related to the calculation of stratified flows, an algorithm was developed based on integro-interpolation methods, characterized by the ability to perform calculations with large time steps.

REFERENCES

1. Militeyev A.N. Solution of problems of hydraulics of shallow reservoirs and ponds of waterworks using numerical methods, M. (1982). Pp. 43.
2. Militeyev A.N. Numerical modelling of pulsation currents and heat and mass transfer in small non-stratified water bodies // Hydraulic research in energy and water management, M. (1983). Pp.8 – 22.
3. Obidov, B., Vokhidov, O., Shodiev, B., Ashirov, B., Sapaeva, M.: Hydrodynamic loads on a water drain with cavitation quenchers. IOP Conf. Ser. Mater. Sci. Eng. 883, 012011 (2020). https://doi.org/10.1088/1757-899x/883/1/012011.
4. Vasiliev O. F., Gladyshev M. T. On the calculation of discontinuous waves in open channels // Izvestiya AN SSSR, ser. Mechanics of liquid and gas, 1966. No. 6, p. 184 - 189.
5. Bazarov, D., Markova, I., Raimova, I., Sultanov, S.: Water flow motion in the vehicle of main channels. IOP Conf. Ser. Mater. Sci. Eng. 883, 012001 (2020). https://doi.org/10.1088/1757-899x/883/1/012001.
6. Vasiliev, O.F., Temnoeva, T.A., Shugrin, S.M., A numerical method for calculating tireless flows in open channels, Izd. USSR Academy of Sciences ser. mechanics 2, (1965).
7. Bazarov, D., Shaazizov, F., Erjigitov, S.: Transfer of Amudarya flowing part to increase the supportability of the Uzbekistan southern regions. IOP Conf. Ser. Mater. Sci. Eng. 883, 012068 (2020). https://doi.org/10.1088/1757-899x/883/1/012068.
8. Kwon D.V., Mathematical modelling of hydrothermal processes in the Lake Tel-etskoye. Thesis of dissertation. Barnaul. 1998. P. 21.
9. Vasiliev O. F., Gladyshev M. T. On the calculation of discontinuous waves in open channels//Izvestiya AN SSSR, ser. Mechanics of liquid and gas, 6, (1966). Pp. 184 - 189.
10. Khidirov, S., Norkulov, B., Ishankulov, Z., Nurmatov, P., Gayur, A.: Linked pools culverts facilities. In: IOP Conference Series: Materials Science and Engineering (2020). https://doi.org/10.1088/1757-899X/883/1/012004.
11. Militeyev A.N., Bazarov D.R., Krutov A.N. Three-dimensional mathematical model for flows with a washed-out bottom. Messages on applied mathematics. Moscow, Computing Centre RAS, 1997, pp. 45.
12. Vasiliev O.F., Voevodin A.F., Atavin A.A. Methods for calculating unsteady flows in systems of open channels and canals // Numerical methods of mechanics of a continuous medium, 6, 4 (1975). Pp. 21-30.
13. Bazarov, D.R., Vokhidov, O.F., Lutsenko, L.A., Sultanov, S.: Restrictions Applied When Solving One-Dimensional Hydrodynamic Equations. In: Proceedings of EECE 2019, Lecture Notes in Civil Engineering 70. pp. 299–305 (2019). https://doi.org/10.1007/978-3-030-42351-3_26.
14. Krutov A.N. Prospects for the application of numerical modelling of channel pro-cesses // Actual problems of water management and reclamation of irrigated lands, Materials of the Republican Scientific and Practical Conference, Tashkent, Uzbekistan, 2011, p. 124-129.
15. Kwon D.V., Mathematical modelling of hydrothermal processes in the Lake Teletskoye. Barnaul. (1998). Pp. 21.
16. Bazarov, D.R., Mavlyanova, D.A.: Numerical studies of long-wave processes in the reaches of hydrosystems and reservoirs. Mag. Civ. Eng. 87, 123–135 (2019). https://doi.org/10.18720/MCE.87.10.
17. Loytsyansky L.G. Mechanics of liquid and gas.- Moscow: Nauka. (1970). Pp. 904.
18. Krutov A.N. Development of the theory and methods of forecasting the spread of pollutants in the surface waters of arid zones. M. (1997). Pp.162.
19. Bazarov, D., Norkulov, B., Vokhidov, O., Uljaev, F., Ishankulov, Z.: Two-dimensional flow movement in the area of protective regulatory structures. In: IOP Conference Series: Materials Science and Engineering. Institute of Physics Publishing (2020). https://doi.org/10.1088/1757-899X/890/1/012162.
20. Krutov, A., Bazarov, D., Norkulov, B., Obidov, B., Nazarov, B. Experience of employment of computational models for water quality modelling. E3S Web of Conferences. (2019). 97. DOI:10.1051/e3sconf/20199705030.
21. Obidov, B., Choriev, R., Vokhidov, O., Rajabov, M.: Experimental studies of horizontal flow effects in the presence of cavitation on erosion – free dampers. IOP Conf. Ser. Mater. Sci. Eng. 883, 012051 (2020). https://doi.org/10.1088/1757-899x/883/1/012051.