UDC 519.6 10.23947/2587-8999-2019-1-1-1-16

Improvement of numerical solution smoothness for the hydrodynamics problems modeling on rectangular grids *

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The article has been devoted to the problem of improvement real numerical modeling accuracy for the viscous fluid flow between two coaxial half-cylinders on rectangular grids taking into account the filling of cells are used to solve this problem. Approximation of the problem with respect to time is performed on the basis of splitting schemes for physical processes. Difference schemes for solving the hydrodynamic problem are proposed. Analytic solution describing the Taylor-Couette flow is used as a standard to evaluate the numerical solution accuracy of hydrodynamics problems. The simulation was performed on a sequence of condensing computed grids of sizes 11 × 21, 21 × 41, 41 × 81, and 81 × 161 nodes for the areas of smooth and piecewise rectangular boundaries. The grids taking into account the filling of cells are used to improve the smoothness of the solution. In the case of piecewise rectangular approximation the numerical solution error reaches 70%. The grids taking into account the filling of cells reduce the numerical solution error to 6% for the test problem. The test problem shows that using the grid condenced in each spatial direction by 8 times does not lead to increasing the accuracy solutions whereas the solutions accuracy obtained on the basis proposed approach has significant advantage in accuracy.

Keywords: Navier-Stokes equation, splitting schemes for physical processes, the Taylor-Couette flow, the error of numerical solution.

Introduction. Difference schemes taking into account the degree the filling of cells for solving two-dimensional problems of wave hydrodynamics with dynamically varied geometry of the computational domain were proposed in [1]. The solutions obtained on the basis of these schemes are devoid of defects associated with graded approximation of the boundary. Tree-dimensional mathematical model of the movement of the water medium in the Azov Sea was developed on the basis of these schemes [2], the total water depth was 14.2 meters, free surface elevation may be reach 4 meters or more. The dynamic recalculation of the filling of cells is used as a mechanism for reconstructing the geometry of the reservoir. The model possesses high accuracy and a large margin

* The work was supported by the RSF (project No. 17-11-01286).
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of stability. During calculating the storm surge that occurred in September 2014, in Taganrog bay of Azov sea (wind speed reached 40 *m/s*), the simulation error was 20 *cm* with a total over travel of more than 4 meters, the model showed a time lag of about 15 minutes with a total storm interval of about 1000 minutes [3]. The σ-coordinate system is traditionally used in modeling the hydrodynamics of shallow water bodies [4-6]. The solutions obtained on these grids have a large error and poorly describe the influence of the bottom relief on nowadays the structure of the currents. The optimal curvilinear grids that approximate the boundary ear used as an alternative to rectangular grids, which have low accuracy in the case of direct piecewise rectangular approximation of the boundary [7-8].

The constructing problem of optimal three-dimensional computational grids remains open nowadays for the 3D regions of common configurations in computational fluid dynamics [9]. One can say without reducing the significant value of optimal curvilinear grids for computational fluid dynamics, that using rectangular grids with filling cell functions has attractive features, for example in parallel computational fluid dynamics. Difference schemes accuracy comparison has been discussed in this paper in cases of direct rectangular grids usage and additional involvement of the cell filling function for the Taylor-Couette flow numerical modeling. The proposed method is likely close to Volume Of Fluid (VOF) method [10, 11].

Statement of the problem. The viscous incompressible fluid motion in a two-dimensional region between two infinitely long coaxial circular cylinders is considered. We introduce the Cartesian coordinate system *xOy* perpendicular to the axis of the cylinders. The coordinate system origin coincides with the cylinders' axis. In the section of the cylinder by the plane $x = 0$ defines the field of velocity. It is required to determine the liquid motion. The initial equations for the mathematical description of the fluid dynamics problem are [12, 13]:

– Navier-Stokes equation:

$$u_t' + uu_x' + vu_y' = -\frac{P_x'}{\rho} + (\mu u_x')_x' + (\mu u_y')_y', \quad (1)$$

$$v_t' + uv_x' + vv_y' = -\frac{P_y'}{\rho} + (\mu v_x')_x' + (\mu v_y')_y'; \quad (2)$$

– the continuity equation for incompressible fluid:

$$u_x' + v_y' = 0. \quad (3)$$

Equations (1)-(3) are considered under the following boundary conditions:

– the flows are defined on the input and output boundaries:

$$u(x,y,t) = U(x,y),\ v(x,y,t) = V(x,y),\ P_n'(x,y,t) = 0, \quad (4)$$

– the frictionless and slip conditions are set on the lateral surfaces (in the case $|\boldsymbol{\tau}| = 0$, that is, without friction):

$$P_n'(x,y,t) = 0,\ \mathbf{u}_n(x,y,t) = 0,\ \rho\mu u_y'(x,y,t) = -\tau_x(t),\ \rho\mu v_x'(x,y,t) = -\tau_y(t) \quad (5)$$

or sticking condition:

$$P_n'(x,y,t) = 0,\ u(x,y,t) = 0,\ v(x,y,t) = 0, \quad (6)$$

where $\mathbf{u} = \{u, v\}$ is the water medium velocity vector; (*x*, *y*) is Cartesian coordinates, *t* is time, P is pressure; μ is the turbulent exchange coefficient; ρ is the liquid density; n is the normal vector;

τ_x, τ_y are the tangential stress components at the bottom of the liquid.

The wind stress according to the Van Dorn law, is calculated by the formulas [6]:

$$\boldsymbol{\tau} \equiv \{\tau_x, \tau_y\} = \rho_v C_p\left(|\mathbf{u}|\right)\mathbf{u}|\mathbf{u}|,\ C_p\left(|\mathbf{u}|\right) = \begin{cases} 0.0088, & |\mathbf{u}| < 6,6\ м/с, \\ 0.0026, & |\mathbf{u}| \geq 6,6\ м/с, \end{cases} \tag{7}$$

where ρ_v is the external environment density.

Discrete model of hydrodynamics. The computational domain inscribed in a rectangle. For numerical realization of the discrete mathematical model of the formulated wave hydrodynamics problem, uniform grid is introduced:

$$w_h = \{t^n = n\tau, x_i = ih_x,\ y_j = jh_y;\ n = \overline{0,\ldots,N_t},\ i = \overline{0,\ldots,N_x},\ j = \overline{0,\ldots,N_y};$$
$$N_t\tau = T,\ N_x h_x = l_x,\ N_y h_y = l_y\},$$

where τ is the time step, h_x, h_y are steps in space, N_t is the step number on the time coordinate, N_x, N_y are spacing steps on the spatial coordinates x and y, respectively.

We use the splitting schemes for physical processes [14, 15]. In this case, the solution of the problem (1)-(3) reduces to solving the following system of equations:

$$\frac{u^{n+\sigma} - u^n}{\tau} + uu'_x + vu'_y = (\mu u'_x)'_x + (\mu u'_y)'_y, \tag{8}$$

$$\frac{v^{n+\sigma} - v^n}{\tau} + uv'_x + vv'_y = (\mu v'_x)'_x + (\mu v'_y)'_y, \tag{9}$$

$$P''_{xx} + P''_{yy} = \frac{\rho}{\tau}\left(\left(u^{n+\sigma}\right)'_x + \left(v^{n+\sigma}\right)'_y\right), \tag{10}$$

$$\frac{u^{n+1} - u^{n+\sigma}}{\tau} = -\frac{P'_x}{\rho}, \frac{v^{n+1} - v^{n+\sigma}}{\tau} = -\frac{P'_y}{\rho}. \tag{11}$$

The calculated cells are rectangles, which may be filled, partially filled, or empty. The cell centers and nodes are separated apart $h_x/2$ and $h_y/2$ on the coordinates x and y, respectively. Fig. 1 shows that the velocity field and pressure are calculated at the tops of the cells. The cells' vertices (i, j) are nodes (i, j), $(i-1, j)$, $(i, j-1)$, $(i-1, j-1)$.

Let us introduce grid value $o_{i,j}$ for the notation of the cell filling. The filling of cells means the value of cell part volume (area) which has been filled with a liquid medium. Fig. 2 shows that in the neighborhood of the node are cells (i, j), $(i+1, j)$, $(i, j+1)$, $(i+1, j+1)$.

We introduce the coefficients k_0, k_1, k_2, k_3, k_4, describing the filling of regions located in the neighborhood of the cell. The value k_0 characterizes the filling of the region Ω_0: $x \in (x_{i-1}, x_{i+1})$, $y \in (y_{j-1}, y_{j+1})$, k_1 – Ω_1: $x \in (x_i, x_{i+1})$, $y \in (y_{j-1}, y_{j+1})$, k_2 – Ω_2: $x \in (x_{i-1}, x_i)$, $y \in (y_{j-1}, y_{j+1})$, k_3 – Ω_3: $x \in (x_{i-1}, x_{i+1})$, $y \in (y_j, y_{j+1})$, k_4 – Ω_4: $x \in (x_{i-1}, x_{i+1})$, $y \in (y_{j-1}, y_j)$. The filled parts of the regions Ω_m is called D_m, where $m = \overline{0,\ldots,4}$. The coefficients k_m can be calculated from the

formulas:

$$(k_m)_{i,j} = \frac{S_{D_m}}{S_{\Omega_m}},\ (k_0)_{i,j} = \frac{o_{i,j} + o_{i+1,j} + o_{i+1,j+1} + o_{i,j+1}}{4},\ (k_1)_{i,j} = \frac{o_{i+1,j} + o_{i+1,j+1}}{2},$$

$$(k_2)_{i,j} = \frac{o_{i,j} + o_{i,j+1}}{2},\ (k_3)_{i,j} = \frac{o_{i+1,j+1} + o_{i,j+1}}{2},\ (k_4)_{i,j} = \frac{o_{i,j} + o_{i+1,j}}{2}.$$

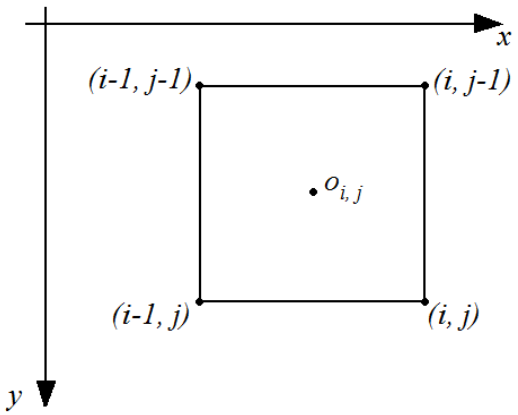

Fig. 1. The cell location of the relative to the adjacent nodes

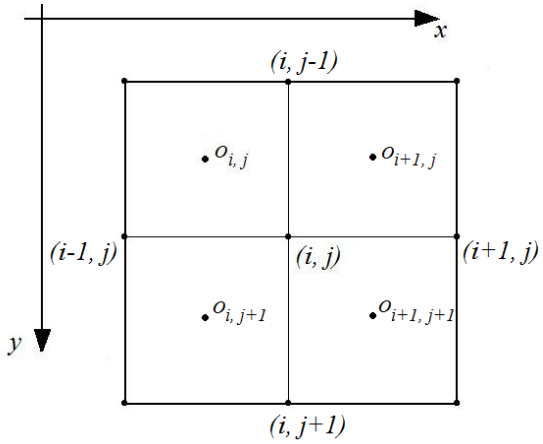

Fig. 2. The arrangement of nodes relative to cells

The boundary conditions for the first subproblem of wave hydrodynamics (8), (9) take form:

$$u'_x(x,y,t) = \alpha_{u,x}u + \beta_{u,x},\quad v'_x(x,y,t) = \alpha_{v,x}v + \beta_{v,x},$$

$$u'_y(x,y,t) = \alpha_{u,y}u + \beta_{u,y},\quad v'_y(x,y,t) = \alpha_{v,y}v + \beta_{v,y}. \qquad (12)$$

We integrate equation (8) over the region D_0 and use the property of linearity of the integral, as a result of which we obtain:

$$\iint_{D_0} \frac{u^{n+\sigma} - u^n}{\tau} dxdy + \iint_{D_0} uu'_x dxdy + \iint_{D_0} vu'_y dxdy = \iint_{D_0} (\mu u'_x)'_x dxdy + \iint_{D_0} (\eta u'_y)'_y dxdy. \qquad (13)$$

After calculating separately each of the integrals we obtain:

$$\iint_{D_0} \frac{u^{n+\sigma} - u^n}{\tau} dxdy \approx (k_0)_{i,j} \iint_{\Omega_0} \frac{u^{n+\sigma} - u^n}{\tau} dxdy = (k_0)_{i,j} \frac{u^{n+\sigma}_{i,j} - u^n_{i,j}}{\tau} h_x h_y. \qquad (14)$$

The second integral in expression (13) may be written in the form:

$$\iint_{D_0} uu'_x dxdy = \iint_{D_1} uu'_x dxdy + \iint_{D_2} uu'_x dxdy \approx (k_1)_{i,j} \iint_{\Omega_1} uu'_x dxdy + (k_2)_{i,j} \iint_{\Omega_2} uu'_x dxdy.$$

Calculating the integrals over the regions Ω_1 and Ω_2, we obtain

$$\iint_{D_0} uu'_x dxdy = \frac{(k_1)_{i,j} u_{i+1/2,j} h_y (u_{i+1,j} - u_{i,j}) + (k_2)_{i,j} u_{i-1/2,j} h_y (u_{i,j} - u_{i-1,j})}{2}. \qquad (15)$$

We calculate the integral on the right-hand side of expression (13):

$$\iint\limits_{D_0} (\mu u'_x)'_x dxdy = \iint\limits_{D_1} (\mu u'_x)'_x dxdy + \iint\limits_{D_2} (\mu u'_x)'_x dxdy .$$

In the last equality, let us assume that $S_{D_1} > S_{D_2}$, where we select from the region D_1 fragment $D_{1,2}$, adjacent to the region D_2, and $S_{D_2} = S_{D_{1,2}}$ (Fig. 3).

$$\iint\limits_{D_0} (\mu u'_x)'_x dxdy = \iint\limits_{D_1 / D_{1,2}} (\mu u'_x)'_x dxdy + \iint\limits_{D_{1,2} \cup D_2} (\mu u'_x)'_x dxdy =$$

$$= \left((k_1)_{i,j} - (k_2)_{i,j}\right) \iint\limits_{\Omega_1} (\mu u'_x)'_x dxdy + (k_2)_{i,j} \iint\limits_{\Omega_0} (\mu u'_x)'_x dxdy .$$

As a result, we get:

$$\iint\limits_{D_0} (\mu u'_x)'_x dxdy = \left((k_1)_{i,j}\, \mu_{i+1/2,j} \frac{u_{i+1,j} - u_{i,j}}{h_x} - (k_2)_{i,j}\, \mu_{i-1/2,j} \frac{u_{i,j} - u_{i-1,j}}{h_x} - \right.$$

$$\left. - \left((k_1)_{i,j} - (k_2)_{i,j}\right) \mu_{i,j} \left(\alpha_{u,x} u_{i,j} + \beta_{u,x}\right) \right) h_y . \qquad (16)$$

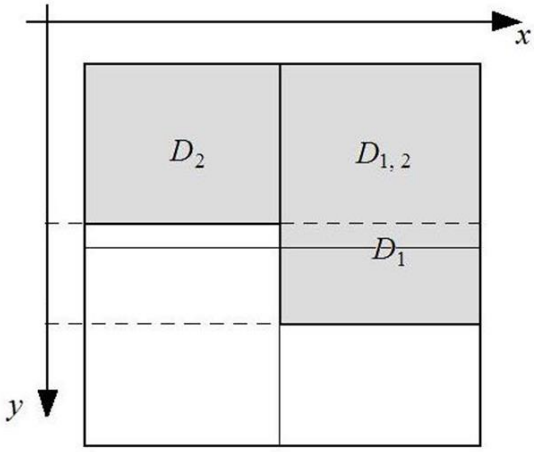

Fig. 3. The scheme of the domain filling

In case, if $S_{D_2} > S_{D_1}$, the result will be similar. Substituting into equation (13), the expressions (14) - (16), we readily obtain:

$$(k_0)_{i,j} \frac{u^{n+\sigma}_{i,j} - u^n_{i,j}}{\tau} h_x h_y + \left((k_1)_{i,j}\, u_{i+1/2,j} h_y \left(u_{i+1,j} - u_{i,j}\right) + (k_2)_{i,j}\, u_{i-1/2,j} h_y \left(u_{i,j} - u_{i-1,j}\right)\right) \Big/ 2 +$$

$$+ \left((k_3)_{i,j}\, v_{i,j+1/2} h_x \left(u_{i,j+1} - u_{i,j}\right) + (k_4)_{i,j}\, v_{i,j-1/2} h_x \left(u_{i,j} - u_{i,j-1}\right)\right) \Big/ 2 =$$

$$= \left((k_1)_{i,j}\, \mu_{i+1/2,j} \frac{u_{i+1,j} - u_{i,j}}{h_x} - (k_2)_{i,j}\, \mu_{i-1/2,j} \frac{u_{i,j} - u_{i-1,j}}{h_x} - \right. \qquad (17)$$

$$\left. - \left((k_1)_{i,j} - (k_2)_{i,j}\right) \mu_{i,j} \left(\alpha_{u,x} u_{i,j} + \beta_{u,x}\right) \right) h_y + \left((k_3)_{i,j}\, \eta_{i,j+1/2} \frac{u_{i,j+1} - u_{i,j}}{h_y} - \right.$$

$$-\left(k_4\right)_{i,j}\eta_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{h_y}-\left(\left(k_3\right)_{i,j}-\left(k_4\right)_{i,j}\right)\eta_{i,j}\left(\alpha_{u,y}u_{i,j}+\beta_{u,y}\right)\Bigg)h_x.$$

If we divide the obtained expression by the area of the cell $h_x h_y$ we are coming to:

$$\left(k_0\right)_{i,j}\frac{u_{i,j}^{n+\sigma}-u_{i,j}^{n}}{\tau}+\left(k_1\right)_{i,j}u_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{2h_x}+\left(k_2\right)_{i,j}u_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{2h_x}+$$

$$+\left(k_3\right)_{i,j}v_{i,j+1/2}\frac{u_{i,j+1}-u_{i,j}}{2h_y}+\left(k_4\right)_{i,j}v_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{2h_y}=\left(k_1\right)_{i,j}\mu_{i+1/2,j}\frac{u_{i+1,j}-u_{i,j}}{h_x^2}-$$

$$-\left(k_2\right)_{i,j}\mu_{i-1/2,j}\frac{u_{i,j}-u_{i-1,j}}{h_x^2}-\left(\left(k_1\right)_{i,j}-\left(k_2\right)_{i,j}\right)\mu_{i,j}\frac{\alpha_{u,x}u_{i,j}+\beta_{u,x}}{h_x}+ \qquad (18)$$

$$+\left(k_3\right)_{i,j}\eta_{i,j+1/2}\frac{u_{i,j+1}-u_{i,j}}{h_y^2}-\left(k_4\right)_{i,j}\eta_{i,j-1/2}\frac{u_{i,j}-u_{i,j-1}}{h_y^2}-\left(\left(k_3\right)_{i,j}-\left(k_4\right)_{i,j}\right)\eta_{i,j}\frac{\alpha_{u,y}u_{i,j}+\beta_{u,y}}{h_y}.$$

In a similar way, one can obtain discrete analogs for equations (9)-(12). In order to simplify the recording of equations, a «mask» of the boundary condition $m_{i,j}$ is introduced. The parameter $m_{i,j}$ takes the value 1 if the node (i, j) belongs to the boundary nodes set located in the border region where slip occurs with friction, otherwise $m_{i,j}=0$. The discrete model of the hydrodynamic problem may be represented by the following grid equations [16]:

– for the component of the velocity vector $u_{i,j}$ under slip condition:

$$\left(k_0\right)_{i,j}\frac{u_{i,j}^{n+\sigma}-u_{i,j}^{n}}{\tau}+\left(k_1\right)_{i,j}u_{i+1/2,j}^{n}\frac{u_{i+1,j}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{2h_x}+\left(k_2\right)_{i,j}u_{i-1/2,j}^{n}\frac{u_{i,j}^{n+\sigma/2}-u_{i-1,j}^{n+\sigma/2}}{2h_x}+$$

$$+\left(k_3\right)_{i,j}v_{i,j+1/2}^{n}\frac{u_{i,j+1}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{2h_y}+\left(k_4\right)_{i,j}v_{i,j-1/2}^{n}\frac{u_{i,j}^{n+\sigma/2}-u_{i,j-1}^{n+\sigma/2}}{2h_y}=$$

$$=\left(k_1\right)_{i,j}\mu_{i+1/2,j}\frac{u_{i+1,j}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{h_x^2}-\left(k_2\right)_{i,j}\mu_{i-1/2,j}\frac{u_{i,j}^{n+\sigma/2}-u_{i-1,j}^{n+\sigma/2}}{h_x^2}+$$

$$+\left(k_3\right)_{i,j}\mu_{i,j+1/2}\frac{u_{i,j+1}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{h_y^2}-\left(k_4\right)_{i,j}\mu_{i,j-1/2}\frac{u_{i,j}^{n+\sigma/2}-u_{i,j-1}^{n+\sigma/2}}{h_y^2}-\left|\left(k_3\right)_{i,j}-\left(k_4\right)_{i,j}\right|\frac{\tau_x}{\rho h_y}m_{i,j};$$

under sticking condition:

$$\frac{u_{i,j}^{n+\sigma}-\left(k_0\right)_{i,j}u_{i,j}^{n}}{\tau}+\left(k_{1,2}\right)_{i,j}u_{i+1/2,j}^{n}\frac{u_{i+1,j}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{2h_x}+\left(k_{1,2}\right)_{i,j}u_{i-1/2,j}^{n}\frac{u_{i,j}^{n+\sigma/2}-u_{i-1,j}^{n+\sigma/2}}{2h_x}+$$

$$+\left(k_{3,4}\right)_{i,j}v_{i,j+1/2}^{n}\frac{u_{i,j+1}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{2h_y}+\left(k_{3,4}\right)_{i,j}v_{i,j-1/2}^{n}\frac{u_{i,j}^{n+\sigma/2}-u_{i,j-1}^{n+\sigma/2}}{2h_y}=$$

$$=\left(k_{1,2}\right)_{i,j}\mu_{i+1/2,j}\frac{u_{i+1,j}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{h_x^2}-\left(k_{1,2}\right)_{i,j}\mu_{i-1/2,j}\frac{u_{i,j}^{n+\sigma/2}-u_{i-1,j}^{n+\sigma/2}}{h_x^2}+$$

$$+\left(k_{3,4}\right)_{i,j}\mu_{i,j+1/2}\frac{u_{i,j+1}^{n+\sigma/2}-u_{i,j}^{n+\sigma/2}}{h_y^2}-\left(k_{3,4}\right)_{i,j}\mu_{i,j-1/2}\frac{u_{i,j}^{n+\sigma/2}-u_{i,j-1}^{n+\sigma/2}}{h_y^2},$$

$$\left(k_{1,2}\right)_{i,j}=\min\left\{\left(k_1\right)_{i,j},\left(k_2\right)_{i,j}\right\},\ \left(k_{3,4}\right)_{i,j}=\min\left\{\left(k_3\right)_{i,j},\left(k_4\right)_{i,j}\right\};$$

– for the velocity vector $v_{i,j}$ component under slip conditions:

$$\left(k_0\right)_{i,j}\frac{v_{i,j}^{n+\sigma}-v_{i,j}^{n}}{\tau}+\left(k_1\right)_{i,j}u_{i+1/2,j}^{n}\frac{v_{i+1,j}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{2h_x}+\left(k_2\right)_{i,j}u_{i-1/2,j}^{n}\frac{v_{i,j}^{n+\sigma/2}-v_{i-1,j}^{n+\sigma/2}}{2h_x}+$$

$$+\left(k_3\right)_{i,j}v_{i,j+1/2}^{n}\frac{v_{i,j+1}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{2h_y}+\left(k_4\right)_{i,j}v_{i,j-1/2}^{n}\frac{v_{i,j}^{n+\sigma/2}-v_{i,j-1}^{n+\sigma/2}}{2h_y}=$$

$$=\left(k_1\right)_{i,j}\mu_{i+1/2,j}\frac{v_{i+1,j}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{h_x^2}-\left(k_2\right)_{i,j}\mu_{i-1/2,j}\frac{v_{i,j}^{n+\sigma/2}-v_{i-1,j}^{n+\sigma/2}}{h_x^2}+$$

$$+\left(k_3\right)_{i,j}\mu_{i,j+1/2}\frac{v_{i,j+1}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{h_y^2}-\left(k_4\right)_{i,j}\mu_{i,j-1/2}\frac{v_{i,j}^{n+\sigma/2}-v_{i,j-1}^{n+\sigma/2}}{h_y^2}-\left|\left(k_1\right)_{i,j}-\left(k_2\right)_{i,j}\right|\frac{\tau_y}{\rho h_x}m_{i,j};$$

under sticking condition:

$$\frac{v_{i,j}^{n+\sigma}-\left(k_0\right)_{i,j}v_{i,j}^{n}}{\tau}+\left(k_{1,2}\right)_{i,j}u_{i+1/2,j}^{n}\frac{v_{i+1,j}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{2h_x}+\left(k_{1,2}\right)_{i,j}u_{i-1/2,j}^{n}\frac{v_{i,j}^{n+\sigma/2}-v_{i-1,j}^{n+\sigma/2}}{2h_x}+$$

$$+\left(k_{3,4}\right)_{i,j}v_{i,j+1/2}^{n}\frac{v_{i,j+1}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{2h_y}+\left(k_{3,4}\right)_{i,j}v_{i,j-1/2}^{n}\frac{v_{i,j}^{n+\sigma/2}-v_{i,j-1}^{n+\sigma/2}}{2h_y}=$$

$$=\left(k_{1,2}\right)_{i,j}\mu_{i+1/2,j}\frac{v_{i+1,j}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{h_x^2}-\left(k_{1,2}\right)_{i,j}\mu_{i-1/2,j}\frac{v_{i,j}^{n+\sigma/2}-v_{i-1,j}^{n+\sigma/2}}{h_x^2}+$$

$$+\left(k_{3,4}\right)_{i,j}\mu_{i,j+1/2}\frac{v_{i,j+1}^{n+\sigma/2}-v_{i,j}^{n+\sigma/2}}{h_y^2}-\left(k_{3,4}\right)_{i,j}\mu_{i,j-1/2}\frac{v_{i,j}^{n+\sigma/2}-v_{i,j-1}^{n+\sigma/2}}{h_y^2};$$

– for calculation the pressure field:

$$\left(k_1\right)_{i,j}\frac{P_{i+1,j}-P_{i,j}}{h_x^2}-\left(k_2\right)_{i,j}\frac{P_{i,j}-P_{i-1,j}}{h_x^2}+\left(k_3\right)_{i,j}\frac{P_{i,j+1}-P_{i,j}}{h_y^2}-\left(k_4\right)_{i,j}\frac{P_{i,j}-P_{i,j-1}}{h_y^2}=$$

$$=\frac{\rho}{\tau}\left(\frac{\left(k_1\right)_{i,j}u_{i+1/2,j}^{n+\sigma}-\left(k_2\right)_{i,j}u_{i-1/2,j}^{n+\sigma}}{h_x}+\frac{\left(k_2\right)_{i,j}-\left(k_1\right)_{i,j}}{h_x}U_{i,j}+\right.$$

$$\left.+\frac{\left(k_3\right)_{i,j}v_{i,j+1/2}^{n+\sigma}-\left(k_4\right)_{i,j}v_{i,j-1/2}^{n+\sigma}}{h_y}+\frac{\left(k_4\right)_{i,j}-\left(k_3\right)_{i,j}}{h_y}V_{i,j}\right);$$

– equations to refine the velocity field by pressure:

$$\left(k_0\right)_{i,j}\frac{u_{i,j}^{n+1}-u_{i,j}^{n+\sigma}}{\tau}=-\left(\left(k_1\right)_{i,j}\frac{P_{i+1,j}^{n+1}-P_{i,j}^{n+1}}{2h_x\rho}+\left(k_2\right)_{i,j}\frac{P_{i,j}^{n+1}-P_{i-1,j}^{n+1}}{2h_x\rho}\right),$$

$$\left(k_0\right)_{i,j}\frac{v_{i,j}^{n+1}-v_{i,j}^{n+\sigma}}{\tau}=-\left(\left(k_3\right)_{i,j}\frac{P_{i,j+1}^{n+1}-P_{i,j}^{n+1}}{2h_y\rho}+\left(k_4\right)_{i,j}\frac{P_{i,j}^{n+1}-P_{i,j-1}^{n+1}}{2h_y\rho}\right).$$

It is shown that the order of approximation of the system of equations is $O\left(\tau+h_x^2+h_y^2\right)$. The sufficient condition for the stability of the scheme for the method of «corrections to pressure» is

determined on the basis of the grid maximum principle [17] with spacing values restrictions: $h_x < \left|\frac{2\mu}{u}\right|$, $h_y < \left|\frac{2\mu}{v}\right|$ or $\mathrm{Re} \le 2N$, where $\mathrm{Re} = u \cdot l / \mu$ is the Reynolds number, u is the velocity of the aquatic environment, l is the characteristic size of the region, μ is the turbulent exchange coefficient.

To solve the grid equations obtained, an adaptive modified alternating-triangular method of variational type was applied, which is advanced variant of SSOR method.

Taylor-Couette flow. Let us consider the steady flow of fluid between two infinitely long coaxial circular cylinders

$$uu'_x + vu'_y = -\rho^{-1}P'_x + \mu\Delta u,\ uv'_x + vv'_y = -\rho^{-1}P'_y + \mu\Delta v,\ r_1 \le r \le r_2,\ r = \sqrt{x^2 + y^2}.$$

Suppose, on the internal side, the rotation speed is $\|\mathbf{u}\|_{r=r_1} = u_1$, on the external side, the rotation speed is $\|\mathbf{u}\|_{r=r_2} = u_2$. The polar coordinate system was introduced to solve the problem ($x = r\cos\theta,\ y = r\sin\theta$)

$$u_r\frac{\partial u_r}{\partial r} + \frac{u_\theta}{r}\frac{\partial u_r}{\partial \theta} - \frac{u_\theta^2}{r} = -\frac{1}{\rho}\frac{\partial P}{\partial r} + \mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial(ru_r)}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u_r}{\partial \theta^2} - \frac{2}{r^2}\frac{\partial u_\theta}{\partial \theta}\right),$$

$$u_r\frac{\partial u_\theta}{\partial r} + \frac{u_\theta}{r}\frac{\partial u_\theta}{\partial \theta} + \frac{u_\theta u_r}{r} = -\frac{1}{r\rho}\frac{\partial P}{\partial \theta} + \mu\left(\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial(ru_\theta)}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 u_\theta}{\partial \theta^2} + \frac{2}{r^2}\frac{\partial u_r}{\partial \theta}\right).$$

Taking into account that $v_r = 0$, $v_\theta = v_\theta(r)$ and $P = P(r)$, we obtain:

$$\frac{1}{\rho}\frac{\partial P}{\partial r} = \frac{u_\theta^2}{r},\ \frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial(ru_\theta)}{\partial r}\right) = 0.$$

The analytical solution of this system of equations is:

$$u_\theta(r) = c_1 r + c_2 / r,\ P(r) = P(r_1) + \rho\int_{r_1}^{r}\left(u_\theta^2 / r\right)dr.$$

To compare the results of numerical calculations with the analytical solution, we take

$r_1 = 5\ m,\ r_2 = 10\ m,\ u_1 = 1\ m/s,\ u_2 = 0.5\ m/s.$

In this case, the analytical solution takes the form

$$u_\theta(r) = 5/r,\ P(r) = P(r_1) - 12.5\rho/r^2 + \rho/2.$$

The analytical solution in the Cartesian coordinate system takes the form

$$u(x,y) = -\frac{5y}{x^2+y^2},\ v(x,y) = \frac{5x}{x^2+y^2},\ P(x,y) = P(r_1) - \frac{12.5\rho}{x^2+y^2} + \rho/2.$$

Results of numerical experiments. The problem of finding the numerical flow of a viscous fluid between two coaxial cylinders ($x \ge 0$) is considered. The inside cylinder radius is $r_1 = 5\ m$. The outside cylinder radius is $r_2 = 10\ м$. The calculated domain is inscribed in a rectangle with dimensions $10 \times 20\ m$ ($0 \le x \le 10,\ -10 \le y \le 10$). In the section of the cylinder by the plane $x = 0$ sets the velocity

field $u(0,y)=-5/y$ *m/s*, $v(0,y)=0$ *m/s*. In all other grid nodes, the velocity field is calculated. On the inside and outside walls of the cylinder, the conditions for slip and non-flow are specified.

Defects of numerical solutions are most clearly visible on coarse grids. We describe the parameters of a coarse grid. The steps in the spatial directions are 1 *m*, the time step is 0.1 *s*, the mesh size is 21 × 11 knots, the length of the counting interval is 10 *s*, the density is $\rho=1000$ *kg/m*^{3}, the turbulent exchange coefficient is $\mu=1$ *m*^{2}*/s*. Fig. 4 shows the contents of an array describing the degree of filling of cells in the case of using the grid of 21 × 11 nodes.

	0	1	2	3	4	5	6	7	8	9
0	0.983	0.883	0.678	0.362	0.03	0	0	0	0	0
1	1	1	1	1	0.894	0.344	0	0	0	0
2	1	1	1	1	1	1	0.59	0.01	0	0
3	1	1	1	1	1	1	1	0.59	0	0
4	1	1	1	1	1	1	1	1	0.344	0
5	0.034	0.24	0.683	1	1	1	1	1	0.894	0.03
6	0	0	0	0.453	1	1	1	1	1	0.362
7	0	0	0	0	0.683	1	1	1	1	0.678
8	0	0	0	0	0.24	1	1	1	1	0.883
9	0	0	0	0	0.034	1	1	1	1	0.983
10	0	0	0	0	0.034	1	1	1	1	0.983
11	0	0	0	0	0.24	1	1	1	1	0.883
12	0	0	0	0	0.683	1	1	1	1	0.678
13	0	0	0	0.453	1	1	1	1	1	0.362
14	0.034	0.24	0.683	1	1	1	1	1	0.894	0.03
15	1	1	1	1	1	1	1	1	0.344	0
16	1	1	1	1	1	1	1	0.59	0	0
17	1	1	1	1	1	1	0.59	0.01	0	0
18	1	1	1	1	0.894	0.344	0	0	0	0
19	0.983	0.883	0.678	0.362	0.03	0	0	0	0	0

Fig. 4. The values of the filling of cells for the grid of 21 × 11 nodes

Fig. 5 shows the numerical solution of the problem of fluid flow between two coaxial cylinders. The color shows the flow of fluid $|k_0\mathbf{u}|$.

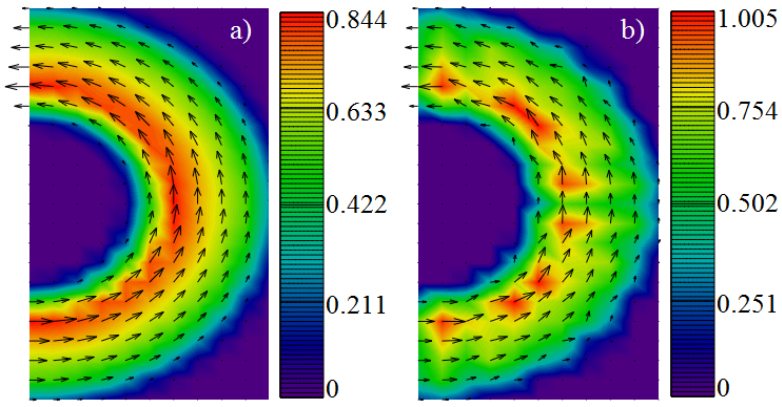

Fig. 5. Numerical solution of the problem: a) in case of partial filling of cells, b) in case of piecewise rectangular interface between two media

Fig. 6. a) shows that the solution of the problem of fluid flow between two coaxial cylinders, obtained on grids that take into account the filling of the cells, is sufficiently smooth. Fig. 6. b) shows

the solution with defects associated with piecewise rectangular approximation of the interface between two media.

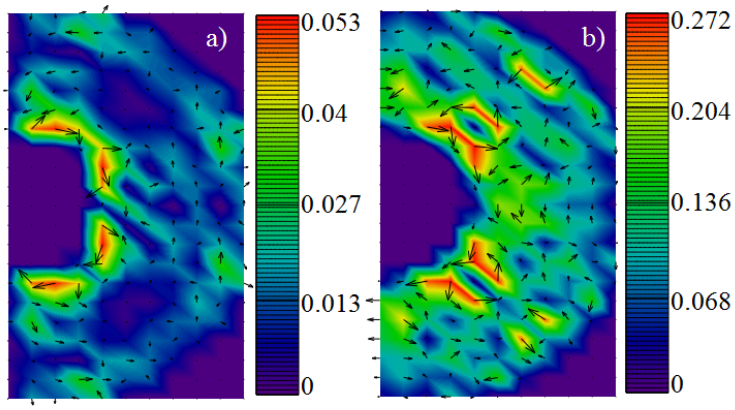

Fig. 6. The error distribution obtained as the difference between the numerical and analytical solutions of the problem: a) in case of a smooth boundary, b) in case of a step boundary

Fig. 7 and 8 show the errors in the numerical solution of the problem of fluid flow between two coaxial cylinders on grids taking into account the filling of the cells (in case of a smooth boundary) and on grids with piecewise rectangular approximation of the boundary. For numerical investigation of the accuracy of the proposed schemes, a solution is found on a sequence of condensing grids. Fig. 8 presents the numerical solution of the initial problem of fluid flow between two coaxial cylinders on more detailed grids of sizes 21 × 41 and 41 × 81 knots.

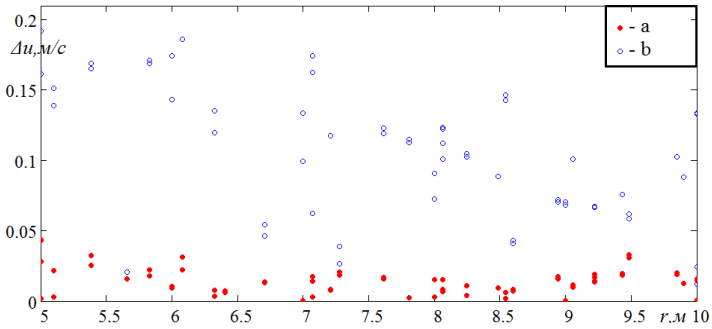

Fig. 7. The dependence of the error from the radius: a) in case of smooth boundary, b) in case of step boundary

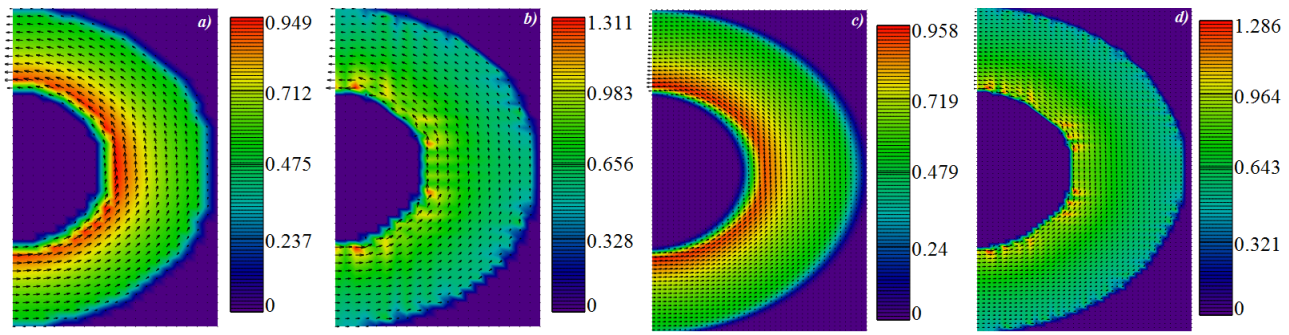

Fig. 8. The numerical solution of the problem: a), c) in case of using partial filling of cells; b), d) in case of stepped interface between two media; a), b) dimensions of the computational grid 21 × 41 knots; c), d) dimensions of the computational grid 41 × 81 knots

Fig. 9 shows the error values of the numerical solution of the fluid flow problem, depending on the radius (circles indicate the error in case of a smooth boundary, circles indicate the error in the case of a step boundary).

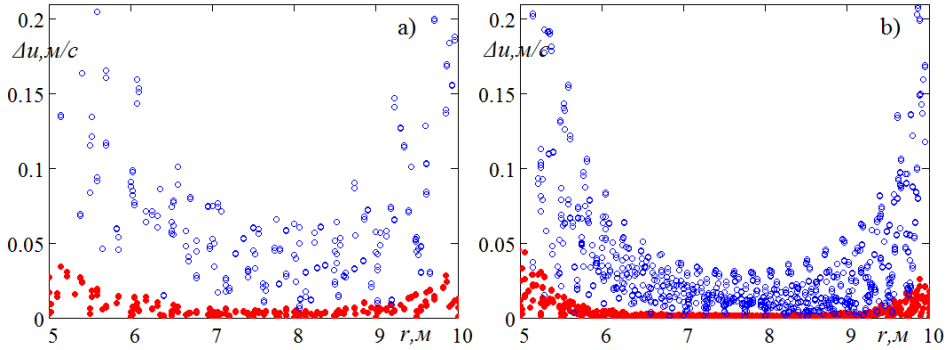

Fig. 9. The dependence of the error in the solution of the problem of fluid flow between two cylinders from the radius on a grid of dimensions: a) 21 × 41 knots, b) 41 × 81 knots

Fig. 7, 9 show that the increase in the size of the calculated grids for the problem of flow of the aqueous medium does not lead to an increase in the accuracy in case of piecewise rectangular approximation of the boundary, but to a decrease in the linear dimensions of the border region where the solutions of the solution associated with rough approximation of the boundary are manifested. It should also be noted that when using grids taking into account the filling of cells, the error in the numerical solution of model hydrodynamic problems caused by the approximation of the boundary does not exceed 6% of the solution of the problem.

Table 1 presents the error values of the numerical solution of the fluid flow problem between two coaxial cylinders obtained from a sequence of condensing computed grids 11 × 21, 21 × 41, 41 × 81, and 81 × 161 nodes in case of a smooth and stepped boundary.

Table 1. The error in the solution of the problem of fluid flow between two cylinders

Grid dimensions	*11×21*	*21×41*	*41×81*	*81×161*
The maximum error value in the case of a smooth boundary, m / s	*0.053*	*0.052*	*0.058*	*0.056*
The average error value in the case of a smooth boundary, m / s	*0.023*	*0.012*	*0.006*	*0.003*
The maximum error value in the case of a stepped boundary, m / s	*0.272*	*0.731*	*0.717*	*0.75*
The average error value in the case of a stepped boundary, m / s	*0.165*	*0.132*	*0.069*	*0.056*

The analysis of the error calculating results of the numerical solution of the problem of fluid flow between two cylinders on the sequence of condensing grids presented in Table 1 allows us to conclude that the use of difference schemes taking into account the filling of cells is effective. The grid splitting by 8 times in each of the spatial directions does not lead to an increase in the accuracy that solutions obtained on grids taking into account the filling of the cells possess.

Conclusion. The paper considers the problem of searching the numerical flow of a viscous fluid between two coaxial half-cylinders. Analytic solution describing the Taylor-Couette flow is used as a standard to evaluate the accuracy of the numerical solution of hydrodynamic problems. The simulation was performed on a sequence of condensing computed grids of sizes 11 × 21, 21 × 41, 41

× 81, and 81 × 161 nodes in cases of smooth and piecewise rectangular boundaries. To improve the solution smoothness we used grids taking into account the filling of the cells.

In the case of piecewise rectangular approximation the error of numerical solution reaches 70%. The grids taking into account the filling of cells reduce the numerical solution error to 6%. It is shown that crushing the grid by 8 times in each spatial direction does not lead to increasing the accuracy solutions whereas the solutions accuracy obtained on grids taking into account the filling of cells significantly increases.

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УДК 519.6 10.23947/2587-8999-2019-1-1-1-16

Повышение гладкости численного решения моделирования задач гидродинамики на прямоугольных сетках *

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В работе рассматривается развитие и применение метода учета заполненности прямоугольных ячеек материальной средой, в частности, жидкостью для повышения гладкости и точности конечноразностного решения задач гидродинамики со сложной формой граничной поверхности. Для исследования возможностей предлагаемого метода рассмотрены две задачи вычислительной гидродинамики – пространственно-двумерного течения вязкой жидкости между двумя соосными полуцилиндрами и пространственно-трехмерная задача волновой гидродинамики – распространения волны в прибрежной зоне и ее выхода на сушу. Для решения поставленных задач используются прямоугольные сетки, учитывающие заполненность ячеек. Аппроксимация задач по времени выполнена на основе схем расщепления по физическим процессам, а по пространственным переменным – на основе интегро-интерполяционного метода с учетом заполненности ячеек и без ее учета. Для оценки точности численного решения первой задачи в качестве эталона используется аналитическое решение, описывающее течение Куэтта-Тейлора. Моделирование производилось на последовательности сгущающихся расчетных сеток размерами: 11×21, 21×41, 41×81 и 81×161 узлов в случае применения метода и без его использования. В случае непосредственного использования прямоугольных сеток (ступенчатой аппроксимации границ) относительная погрешность расчетов достигает 70%; при тех же условиях использование предлагаемого метода позволяет уменьшить погрешность до 6%. Показано, что дробление прямоугольной сетки в 2-8 раз по каждому из пространственных направлений не приводит к такому же повышению точности, которой обладают численные решения, полученные с учетом заполненности ячеек..

Ключевые слова: схемы расщепления по физическим процессам, течение Куэтта-Тейлора, погрешность численного решения.

* Работа выполнена при поддержке РНФ (проект № 17-11–01286).
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UDC 51-77 10.23947/2587-8999-2019-1-1-17-28

Online Political Flashmob: the Case of 632305222316434

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This paper considers the case of online flashmob 63230522231643, which was intended to show the indignation of Russian opposition to the contested parliamentary elections in 2011. The expression of indignation lasted for 47 days. The organizers called on all who believed that the elections had been rigged to enter the aforementioned number anywhere on the internet so that it could be indexed by search engines. The assumption was that the number could hardly be expected to appear in any context other than the flashmob. Thus, using the Google search engine and counting its appearances, anyone would be able to estimate the extent or severity of indignation, which was the political opposition members thought was as very widespread. However, the flashmob mobilized only a small number of participants and failed to achieve its political goals. At the same time, it turned out to be a rare example of the spread of information in a world that was sparse, that is, considering only those individuals whose political attitudes and dispositions to online activity made them available for participation, we get a social network with relatively few edges, which is a sub-network of a denser and larger network of users.

Methods. The paper presents empirical data on the daily number of flashmob-related tweets and presents a mathematical model to describe the dynamics of a flashmob on Twitter and compare the results of modeling with empirical data for flashmob 63230522231643.

Results. The model correctly represents and explains some important features of the dynamics of a flashmob. To explain the other features would require more a more complex model and building and verifying such a model would call for more abundant empirical data.

Keywords: online flashmob, sparse world, twitter, political protest, mathematical modeling, rumor models.

Introduction. In the aftermath of the parliamentary elections that were held on December 4, 2011, the code number or the string of digits, 632305222316434 was published on the Russian segment of Twitter for those who wished to participate in the Flashmob (written as beginning with capital F to indicate the specific Flashmob that is the subject of this paper, when used in other contexts such as discussing mathematical theory propagation, the word is not capitalized.). The results of the elections, when announced, were strongly contested. Masses of people were seething and one of the attempted actions of protest was the call [1] by an otherwise unremarkable Livejournal user «spichechka» (which means «little match» referring to a matchstick and its potential to cause a fire)

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for those who believed that the elections had been rigged to publish the number 632305222316434 in their blogs, websites or anywhere on the internet so that it could be indexed by search engines. The idea was that this number could hardly appear in any other context. When typed into the Google search engine, the engine would instantly show the number of times it appears. This would indicate to the searcher the extent of indignation, which the opposition thought to be extremely wide. However, the Flashmob did not get support from any major opposition web resource, newspaper or prominent politicians. As it failed to mobilize the expected huge number of participants, the attempt failed to achieve its political goals.

One more probable reason for the failure is that some participants posted the code number of the Flashmob without making any accompanying comment such as «I post this number to express my indignation...». It is possible that some sympathizers came across this 15-digital number but did not realize what it implied. They may have thought that «Maybe, the string of random digits appeared simply because the sender's cat walked over the keyboard...». We mention this possibility to point out that when recipients come across a post with the code number, they do not necessarily recognize the significance of the post and recognize it as a signal of a protestors' Flashmob. Though this may not be the major reason for Flashmob's failure, this possible reason needs to be pointed out because in the mathematical model below there is a parameter describing the probability of coming across a certain post and recognizing it as a part of a flashmob and thus learning about the flashmob from it.

However, the failure of the Flashmob is not very apparent. Google search engine finds 20000 to 32000 results for the query «632305222316434» (it is not clear why this count is so variable). That would lead to the conclusion [2] that there were 20-30 thousand participants, so when planning this study an abundance of statistics was expected to be available. However, a kind of political fraud (or trick) aimed at exaggerating the number of participants was discovered instead.

That fraud utilized the online database of smart questions that have been used in a popular TV show and an intellectual game called «What? Where? When?». Any user may upload a question into the database, and the question creates a new webpage.

The fraud was that the webpage designer inserted the number 632305222316434 into the footer of the page template of this database. As a result, 20000 (for instance) questions resulted in the creation of 20000 pages containing the number in the footer. The Google search, as expected, counted these 20000 pages as if 20000 people had supported the protest against the results of the Parliamentary election. (And even today in 2019 the number of fake protesters has continued to rise as users continue to upload new questions to the website). The number 632305222316434 can easily be seen at the bottom of the screenshot of the webpage given in Appendix 1. The scale of the fraud is not clear because the database claims it has more than 337 thousand game tasks. That number is ten times more the count that the Google search shows, though each page of that database contains the said code number. Probably, not all the pages are indexed by Google. Anyway, the webpages of this database [3] account for the overwhelming majority of mentions of the number 632305222316434.

The motivation behind this fraud seems obvious. The whole idea of the Flashmob was to show a very huge number of people did not accept the results of the parliamentary election. Therefore, the opponents were keen to exaggerate the number of participants.

After eliminating the numbers that were added as a result of the fraud, we were left with a small number of genuine citations of 632305222316434, the vast majority of them being from Livejournal and Twitter.

As for the number of the Flashmob-related posts in Livejournal, the Google search for the number 632305222316434 on livejournal.com yields 1920 pages (accessed 18 June 2019). This presumably means several hundred participants of the Flashmob, because each post in Livejournal appears in several layouts (single post, feed, month, tag1-related feed, tag2-related feed, etc.) and thus generates substantially more than one results in Google search. For example, the search query "632305222316434 on podmoskovnik.livejournal.com gives 16 results (Appendix 2) though they all relate to a single participant of the Flashmob.

Future flashmobs are more likely to appear in Twitter than in Livejournal as the latter seems to have been losing its popularity. For this reason, this study turned to the spread of the Flashmob on Twitter, where 211 participants of the Flashmob were found over 47 days.

This duration far longer than a day (or even a few hours) that a political message requires to reach nearly everyone who may be interested in it. The probable reason for the difference is that the Flashmob is a very rare instance of the spread of information in a sparse world. That is, considering only individuals whose political attitudes and dispositions to online activity made them available for participation in the Flashmob. This resulted in a social network with a relatively small number of edges, embedded in a denser and greater network of users. Also taking into account that people were not so much involved in using social media in 2011 as they are today and watched their feeds less often than they do nowadays, it's not surprising that the Flashmob had only a few participants and that, too, over an unusually long duration.

Introductory Notes and Some Connections to the Literature. It follows from the last paragraph of Section 1 that the network density is pivotal for the speed of propagation of the Flashmob. However, this does not necessarily mean that the mathematical model of the Flashmob must have a design that explicitly accounts for the participants' network, its structure, and density. (It should be noted that the empirical part of this research was conducted several years after the Flashmob. Therefore, it was not possible to separate the connections between users that existed before the time of the Flashmob from those that were established later).

The model below deals with macro-variables such as the number of flashmob-related posts or number of persons aware of the flashmob. This approach is in line with classical models of rumor propagation by Daley & Kendall [4] and Maki & Thompson [5] as well as the recent models [6-13] (see [14] for a very brief review).

Note that spichechka's call to publish «632305222316434» (which we refer to as seeding post) was never published on TV or newspaper. Thus, the information about the Flashmob was transmitted exclusively by the participants of it, making an example of rumor transmission.

Other approaches to mathematical modeling of rumors and propaganda wars include emphasis on position selection, opinion dynamics, social networks, and agent-based and game theory-based models [14-21]. Related empirical studies usually focus on the content of the posts or search queries (see, for example, [22-24]). Broader contexts include Internet security, cyberwars and cybersecurity [25-27].

Mathematical Model. Let us start with numbering days: $t = 0,1,2,3,...$ where $t = 0$ is the day the seeding post was published. Let N_0 be the number of potential participants, that is the number of individuals whose political attitudes and network positions make them available for participation. Each of them is not supposed to post the number 63230522231643 more than once. We categorize all of the individuals into three groups:

– $n(t)$ is the current number of participants, that is, persons who have already published their posts by the start of the day t (obviously, $n(t)$ is also the number of posts);

– $c(t)$ is the number of cunctators, that is, persons who are aware of the Flashmob but have not posted yet by the start of the day t;

– $g(t)$ is the number of ignorants, that is, persons who are not aware of the Flashmob by the start of the day t.

At any moment of time we have $n(t)+c(t)+g(t)=N_0$.

An ignorant can turn into a cunctator or a participant. Also, a cunctator can turn into the participant. Denote $\Delta_{g\to c}(t)$ the number of ignorants turned into cunctators on day t, that is the number of persons who belong among the ignorants at the start of the day t and will belong to cunctators at the start of the day *t+1*. Similarly, $\Delta_{g\to n}(t), \Delta_{c\to n}(t)$ are the numbers of ignorants and cunctators turned into participants. Thus, we have

$$g(t+1)=g(t)-\Delta_{g\to c}-\Delta_{g\to n} \quad (1)$$

$$c(t+1)=c(t)+\Delta_{g\to c}-\Delta_{c\to n} \quad (2)$$

$$n(t+1)=n(t)+\Delta_{g\to n}+\Delta_{c\to n} \quad (3)$$

Let q denote the probability that the average individual uses their account on day t so that they learn about the Flashmob (if they are ignorant) or/and make their post on that day. This probability is supposed to be unaffected by the individual's group. Hence, the total number of persons using their account on day t is $N_0 q(t)$, and among these persons are:

– $qn(t)$ participants,

– $qc(t)$ cunctators, and

– $qg(t)$ ignorants.

Consider an individual using their account on day t and seeing a certain post that has been published at the start of that day. Let p denote the probability that they come across this post and recognize it as a part of the flashmob, thus learning about the flashmob. Then the probability that this individual learns about the Flashmob from at least one of the $n(t)$ posts of the Flashmob is

$$P=1-(1-p)^{n(t)}.$$

Therefore, the number of ignorants who learned about the Flashmob on day t, that is the number of persons who turned from being ignorants into being either cunctators or participants is

$$\Delta_{g\to c}(t)+\Delta_{g\to n}(t)=qg(t)P(t)=qg(t)\left[1-(1-p)^{n(t)}\right]. \quad (4)$$

Let w denote the probability that a person who uses their account on day t, and is aware of the Flashmob (no matter whether they learned about it on this very day or any day earlier), will make their post on day t.

Using this, we can split the number $\Delta_{g\to c}(t)+\Delta_{g\to n}(t)$ of persons leaving the ignorant group as $\Delta_{g\to c}=(1-w)\left(\Delta_{g\to c}(t)+\Delta_{g\to n}(t)\right)$, $\Delta_{g\to n}=w\left(\Delta_{g\to c}(t)+\Delta_{g\to n}(t)\right)$, that is

$$\Delta_{g\to c}=(1-w)qg(t)\left[1-(1-p)^{n(t)}\right], \tag{5}$$

$$\Delta_{g\to n}=wqg(t)\left[1-(1-p)^{n(t)}\right]. \tag{6}$$

The number of cunctators turning into participants is

$$\Delta_{c\to n}=wqc(t) \tag{7}$$

Putting (5)-(7) into (1)-(3), we obtain

$$g(t+1)=g(t)-qg(t)\left[1-(1-p)^{n(t)}\right], \tag{8}$$

$$c(t+1)=c(t)+(1-w)qg(t)\left[1-(1-p)^{n(t)}\right]-wqc(t), \tag{9}$$

$$n(t+1)=n(t)+wqg(t)\left[1-(1-p)^{n(t)}\right]+wqc(t), \tag{10}$$

Equations (8)-(10) present the model of an online flashmob. Obviously, given $n(t)+s(t)+g(t)=N_0$, one of the equations (8)-(10) can be omitted.

(A situation can be easily imagined where flashmob-related political views become increasingly popular, and the pool of persons attitudinally available for participation increases over time. This case of a continuous increase would give rise to a term $g(t)(1+r)$ instead of $g(t)$ in equation (8); in this case N_0 is not constant).

Consider now the realistic case of $p<<1$. That is, the probability that an average ignorant will learn about the flashmob from a certain post is low. This is the case of the sparse net of sympathizers embedded into a dense net of other users. Suppose, for example, that an ignorant follows 500 Twitter accounts, only one of them has published their post inviting support for the flashmob. In this case, the probability must be relatively low that the ignorant will come across this post and pay enough attention to it so as to learn about the flashmob.

As $p<<1$, we can take the following approximation:

$$1-(1-p)^{n(t)}\approx 1-\left[1-pn(t)\right]=pn(t) \tag{11}$$

Putting this into (8)-(10), we obtain the model in the case of a sparse net of sympathizers:

$$g(t+1)=g(t)-pqn(t)g(t), \tag{12}$$

$$c(t+1)=c(t)+(1-w)pqn(t)g(t)-wqc(t), \tag{13}$$

$$n(t+1)=n(t)+wpqn(t)g(t)+wqc(t). \tag{14}$$

Model (12)-(14) must be considered for $t \geq 1$ and supplemented with initial conditions for the number of posts published during day $t = 0$ (which is an observable value) and the number of cunctators at the start of the day $t = 1$ (not observable), that is $n(1)$ and $s(1)$.

As $n(1)$ posts of the day $t = 0$ comprises the seeding post and $n(1)-1$ succeeding posts, we assume that the number of cunctators is $s(1) = (n(1)-1)(1-w)/w$. This completes the construction of the model.

Discussion and Application of the Model to the Case of 632305222316434. The daily number of tweets with code number 63230522231643 is presented in Appendix 3. By applying ordinary least squares to this model the following estimates are obtained: $N_0 = 239$, $q = 0.16$, $p = 0.02$, $w = 0.69$.

Both empirical and model curves are shown in Fig. 1. As the daily number of posts is relatively small, we rounded the numbers on each iteration when calculating the «theoretical» (predicted by the model (12)–(14)) results.

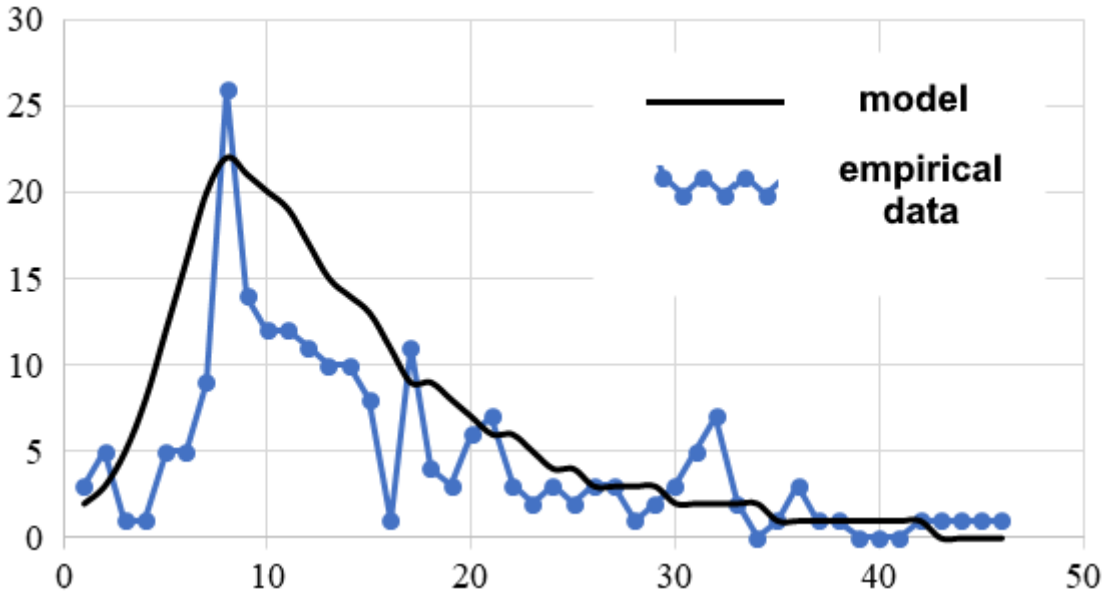

Fig. 1. Empirical data and model curve. Horizontal and vertical axes represent days t and daily number of posts $n(t)-n(t-1)$, respectively.

The obvious problem with matching is the fluctuation of the empirical data. As we said earlier, the statistics were expected to be much more abundant. The paucity of data naturally implies high fluctuation.

The second problem is that the model failed to describe the sharp empirical peak at $t = 8$. We conducted massive numerical experiments with the model (including those with and without direct relation to empirical data) and found that the result yielded by the model clearly tended to show relatively broad and low peak. The cause for this is probably that the model assumes individuals to be psychologically identical. It is pertinent here to refer to the study of public attention to one-time

political events such as referendums, elections or coups [28]. That study dealt with empirics and mathematical modeling of the dynamics of the number of search queries about the event. The empirical curve (the number of search queries as a function of time) was very sharp, having the double-exponential shape such as $\exp\left[3.94+2.91\exp\left(-0.19t\right)\right]$ (Russia's public attention to Brexit) or $\exp\left[3.16+3.73\exp\left(-0.23t\right)\right]$ (Russia's public attention to the US Presidential Elections of 2016). Mathematical models that assume psychological sameness of the individuals (which are close in their philosophy to models employing the concept of «representative individual» of «representative household») are unable to describe this double-exponential empirical regularity. Accordingly, paper [28] builds on the assumption that individuals are differentially predisposed towards being interested in a given event (for example, because the individuals are not equally interested in politics) and constructs the model to explain the sharp double-exponential decrease of public attention as a result of this differential predisposition. Thus, it looks highly probable that in explaining the sharpness of the peak in Fig. 1, the notion of differential predisposition towards online political activity would be crucial. Though, the examination of this hypothesis requires richer empirical data.

What is clear even with sparse statistics is that model (12)-(14) successfully explains the asymmetry of the curve: the increase of the daily number of posts before the peak is obviously steeper than the decrease of it after the peak. The reason is that some people procrastinate before posting, that is, they are cunctators. Removing the class of cunctators (that is, assuming $w=1$) from the model would lead to a much more symmetrical solution. The smaller is w, the longer and more gradual is the decrease of the daily number of posts, the greater is asymmetry.

To summarize, the model correctly represents and explains some important features of the process. Explaining other features requires more abundant empirical data to build and verify a more complex model.

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APPENDIX 1.

The screenshot of https://db.chgk.info/question/belch16.2/1 which represents the evidence of the fraud aimed at exaggerating the number of participants. The Flashmob number can be seen at the footer. Other websites of the online database of smart questions employ the same template with 632305222316434 in the footer.

APPENDIX 2

This list of URLs illustrates that a single user can generate as many as 16 results on the Google search (query: 632305222316434 site: podmoskovnik.livejournal.com)

1. https://podmoskovnik.livejournal.com/133050.html
2. https://podmoskovnik.livejournal.com/tag/
3. https://podmoskovnik.livejournal.com/133289.html
4. https://podmoskovnik.livejournal.com/tag/%D1%82%D0%BE%D1%88%D0%BD%D0%BE%D1%82%D0%B2%D0%BE%D1%80%D0%BD%D1%8B%D0%B5%20%D0%B4%D0%B5%D0%B1%D0%B8%D0%BB%D1%8B
5. https://podmoskovnik.livejournal.com/tag/%D0%A7%D1%83%D1%80%D0%BE%D0%B2%20%D1%81%D0%BC%D0%BE%D1%82%D1%80%D0%B8%D1%82%20%D0%BD%D0%B0%20%D0%B2%D0%B0%D1%81
6. https://podmoskovnik.livejournal.com/tag/%D1%81%D1%82%D1%80%D0%B0%D0%BD%D0%BD%D0%BE%D0%B5
7. https://podmoskovnik.livejournal.com/tag/%D0%B2%D0%B5%D0%BD%D1%82%D0%B8%D0%BB%D1%8F%D1%82%D0%BE%D1%80
8. https://podmoskovnik.livejournal.com/tag/ %D0%B1%D1%80%D0%B5%D0%B4
9. https://podmoskovnik.livejournal.com/tag/ %D0%BF%D0%B5%D0%B0%D1%80
10. https://podmoskovnik.livejournal.com/tag/%D0%B2%D1%81%D0%B5%20%D1%83%D0%B6%D0%B5%20%D1%83%D0%BA%D1%80%D0%B0%D0%B4%D0%B5%D0%BD%D0%BE%20%D0%B4%D0%BE%20%D0%BD%D0%B0%D1%81
11. https://podmoskovnik.livejournal.com/tag/ %D1%81%D1%83%D0%BA%D0%B8
12. https://podmoskovnik.livejournal.com/tag/politics
13. https://podmoskovnik.livejournal.com/tag/ %D1%8F%D0%B2%D0%BA%D0%B0
14. https://podmoskovnik.livejournal.com/tag/%D0%A2%D1%80%D0%BE%D0%B8%D1%86%D0%BA%D0%B8%D0%B9%20%D0%92%D0%B0%D1%80%D0%B8%D0%B0%D0%BD%D1%82
15. https://podmoskovnik.livejournal.com/tag/%D0%BF%D0%B0%D0%BC%D1%8F%D1%82%D1%8C
16. https://podmoskovnik.livejournal.com/tag/%D0%B3%D0%BE%D1%81%D1%83%D0%B4%D0%B0%D1%80%D1%81%D1%82%D0%B2%D0%B5%D0%BD%D0%BD%D0%B0%D1%8F%20%D0%B4%D1%83%D0%BC%D0%B0

APPENDIX 3

Empirical data: the daily number of tweets with 63230522231643. The seeding post was made on December 6, 2011; thus $t = 1$ refers to December 7.

Day (t)	1	2	3	4	5	6	7	8	9	10
Number of tweets	3	5	1	1	5	5	9	26	14	12

Day (t)	11	12	13	14	15	16	17	18	19	20
Number of tweets	12	11	10	10	8	1	11	4	3	6

Day (t)	21	22	23	24	25	26	27	28	29	30
Number of tweets	7	3	2	3	2	3	3	1	2	3

Day (t)	31	32	33	34	35	36	37	38	39	40
Number of tweets	5	7	2	0	1	3	1	1	0	0

Day (t)	41	42	43	44	45	46	47	48	49	50
Number of tweets	0	1	1	1	1	1	0	0	0	0

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УДК 51-77 10.23947/2587-8999-2019-1-1-17-28

Политический онлайн-флэшмоб 632305222316434

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Предмет исследования. В статье рассматривается случай онлайн-флешмоба 63230522231643, который должен был продемонстрировать негодование российской оппозиции по поводу оспариваемых парламентских выборов 2011 года. Организаторы призвали всех полагавших, что выборы были сфальсифицированы, разместить указанное число в любом месте в Интернете, чтобы оно могло быть проиндексировано поисковыми системами. Идея заключалась в том, что это число вряд ли могло появиться в каком-либо другом контексте. Таким образом, используя количество страниц с данным числом, найденных поисковой системой Google, каждый желающий смог бы оценить размах негодования, который представлялся членами политической оппозиции как очень широкая. Однако флэшмоб не получил поддержки ни от одного крупного оппозиционного веб-ресурса, газеты или известного политика. В результате он мобилизовал лишь небольшое количество участников и не смог достичь своих политических целей. В то же время, флэшмоб представляет собой редкий примером распространения информации в так называемом разреженном мире. Другими словами, пользователи, чьи политические установки и готовность к онлайн-активности делают их доступными для участия, составляют социальную сеть с относительно небольшим количеством ребер, которая является подсетью более плотной и крупной сети. Методы. В статье представлены эмпирические данные о ежедневном количестве твитов, участвующих во флешмобе. Также построена математическая модель для описания динамики флешмоба в Твиттере и проведено сравнение результатов моделирования с эмпирическими данными. Результаты. Модель правильно представляет и объясняет некоторые важные особенности динамики флэшмоба. Для объяснения других особенностей требуется больший объем эмпирических данных, позволяющий построить и квантифицировать более сложную модель.

Ключевые слова: онлайн флешмоб, разреженный мир, Твиттер, политический протест, математическое моделирование, модели слухов.

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UDC 519.6 10.23947/2587-8999-2019-1-1-29-34

Computer modelling of primers search in the DNA chain*

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Polymerase chain reaction (PCR) is one of the most common experimental methods for solving DNA analysis problems. The possibility of PCR experiment conduction and its success are vastly depend on oligonucleotide structures. Oligonucleotide primers are important component of any PCR, and therefore, there are a number of requirements for their design. In this regard, it is essential to provide computer analysis for the primer selection. In current paper a new approach is proposed for a specific primer design which is based on Boyer-Moore search algorithm. Computer software is developed for computer-aided primer design, which noticeably simplifies the pre-experiment phase and improves PCR results.

Keywords: polymerase chain reaction, primer design, Boyer-Moore algorithm, computer analysis.

Introduction. Oligonucleotide primers determine specificity, efficiency and possibility of PCR reaction in the presence of all other components. The specificity of PCR is based on the formation of complementary complexes between a matrix and primers – short synthetic oligonucleotides with length from 10 to 30 bases. Each primer is complementary to one of the two chains of the double-stranded matrix and limits the beginning and the end of the amplified region. Reaction temperature depends on a particular composition of primers. Therefore, there are a number of requirements for the selection of nucleotide sequences and their lengths in primers in a view of problem being solved and object of experiment.

There are several well-known software solutions for the computer-aided primer design [1-5]. However, it is not always possible to implement a specific search, adjust parameters and initial conditions in case of using the aforementioned computer programs. Therefore, a new software is developed that allows primer design with the ability of introducing more stringent conditions on the desired primers and their location in a particular genome. It allows repeatedly perform computer analysis in several variations in order to determine the most favorable PCR conditions.

The object of research. Polymerase chain reaction (PCR) is one of the most common experimental method for solving DNA analysis problems. This method of gene diagnostics is widely used in various fields of biology and medicine. The essence of this analysis consists in a

* The reported study was funded by RFBR according to the research projects № 17-44-020120.
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multiple increase the amount of specific fragments by using special enzymes that repeatedly copy them for particular genomes.

PCR is performed in three stages. The first stage is denaturation: the divergence of two DNA chains (temperature 94-96° C). The second stage is annealing. Reaction temperature is reduced after the chains divergence so that the primers can bind to the one-chained matrix. Then the replication occurs (the synthesis of affiliated molecule DNA) where the primer is used as a priming [6].

Oligonucleotide primers (artificially created oligonucleotides that search for the desired DNA fragment) are important component due to the specificity of the PCR reaction, as well as its possibility occurs in the presence of all other components [7]. Thus, it is important to conduct a preliminary computer analysis for a further direct experimental research. There is a number of software solutions implementing design of oligonucleotide primers [8]. However, such software does not allow more detailed design of primers (for example, a specific composition of a primer, narrow PCR temperature range). Hence, there is no opportunity to solve small routine subtasks.

One of the computer-aided tasks is searching and determination of short sequences localization (primers) up to nucleotide. It is necessary in order to determine the possible places for primers annealing and their number. In fact, the task is similar to the searching for a word (10-20 characters length) in some text (up to 1 billion characters). In this case, the alphabet has the following letters determine four nucleotides: A (adenine), G (guanine), C (cytosine), and T (thymine). In its turn the molecule consists of nucleotides mentioned above. It is important not only to locate the «words» but also the number of its occurrences.

Searching short sequences has two destinations. The first one is for random PCR. It is important to know how many times the primer occurs in entire DNA chain and at what position it is located. In this case, the considered length of short sequences, as a rule, is from 8 to 25 nucleotides. The more often the desired site occurs, the higher the likelihood of a successful experiment. Figure 1 shows the search pattern.

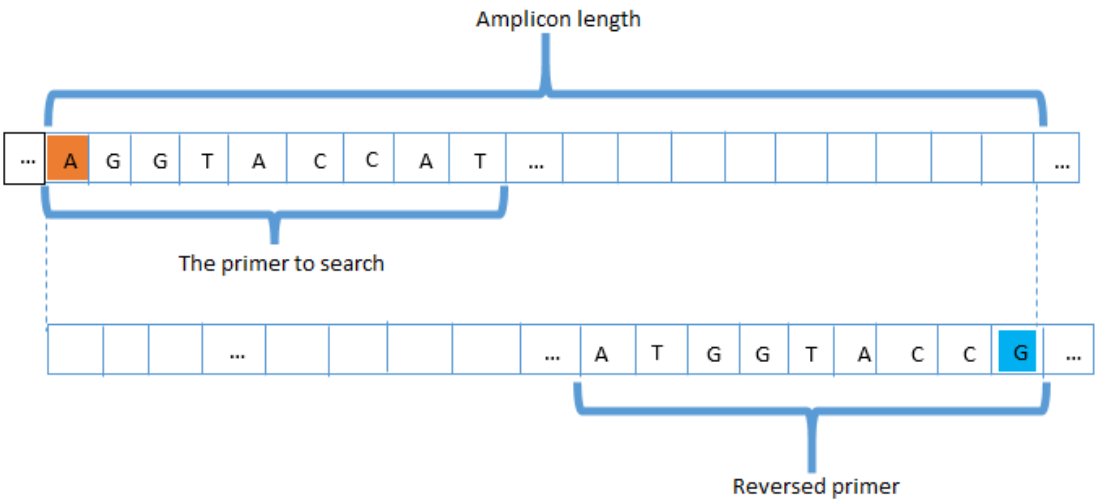

Fig. 1. Searching for primers (random PCR).

The second application is a searching for the annealing sites of slightly longer primers which should occur on the average of every 16 million nucleotides. A subsequent sequence of nucleotides after

each site is of interest assuming that three rather than four nucleotides are taken in the amplification reaction. The termination of chain (completion of the synthesis) occurs on the missing one. In this case, we are interested not only in position of the primer, but also in the adjacent DNA segments. It is worth noting, the forward and reverse primers are considered as equivalent in this case. That is why both primers are used to search for the annealing site. The scheme of this search is presented on Figure 2. Therefore, the proposed approach is take into account only such places of annealing where specific nucleotide is not met on the sufficiently long distance (for example, guanine G as shown on Figure 2). Moreover, it is important to know the length of sections, the total molecular mass of their constituent nucleotides.

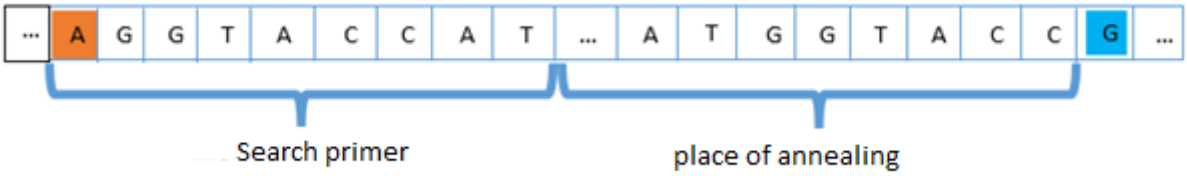

Fig. 2. Search for primers and annealing sites in the nucleotide sequence

Results of research. In order to solve the above problems, an algorithm was developed for searching short primers in the DNA chain. The proposed approach was based on the Boyer-Moore algorithm [9-10] with the additional conditions for the choice of primers. This algorithm allows to find the inclusion of specific fragments of sequences in the DNA chain up to nucleotide, as well as to determine the composition and size of the amplicons. During the search, a selection of primers was produced taking into account the stated requirements.

	A	B	C	D
1	# GGATCTTT	AAAGATCC	length of amplicon	
2	39883835	39884052	217	
3	55375264	55375548	284	
4	29569657	29569969	312	
5	38393029	38393375	346	
6	49519668	49520023	355	
7	41540764	41541163	399	
8	8231987	8232448	461	
9	37414390	37414862	472	
10	56234084	56234565	481	
11				

(a)

	A	B	C	D
1	# GGATCTTT	AAAGATCC	length of amplicon	
2	39883835	39884052	217	
3	55375264	55375548	284	
4	29569657	29569969	312	
5	38393029	38393375	346	
6	49519668	49520023	355	
7	41540764	41541163	399	
8	8231987	8232448	461	
9	37414390	37414862	472	
10	56234084	56234565	481	
11				

(b)

Fig. 3. The output of the program
(a) search sequence GGATCTTT (reverse primer AAAGATCC) for the analysis of random PCR
(b) search for GGATCTTTAC sequence (reverse primer GTAAAGATCC) to detect annealing sites

The software was developed using Python 3.5 language and BioPython library [11]. This library contains tools for calculations in the field of computational biology and bioinformatics. In addition, library tools allow to work with files in fasta-format (text format for nucleotide or polypeptide sequences, in which

nucleotides or amino acids are indicated using single-letter codes) [12]. All calculations were done for the model objects (chromosomes of Arabidopsis). The program output is presented on Figure 3.

Conclusion. The proposed software allows varying the size of a primer, the length of an amplicon. Moreover the developed computer-aided system could change the conditions for the annealing site (such as size and nucleotide composition).

The results obtained allow to predict the conditions for experimental PCR. On the base of the algorithm, a computer program was developed that allows computer-aided primer design. On the base of performed computer analysis, it was revealed that it is inexpedient to carry out experimental studies of PCR diagnostics since there are a small number of sites containing the required primers or they do not exist at all. The received results simplifies and optimizes the work of geneticists and experimenters are providing PCR experiments. If the size of the amplicons expected from computer analysis and their number are known, we can them on the gel electrophoresis in the form of bands during the PCR. In case of the absence of the desired sites in the genome under study the successful conduct of a full-scale experiment is unlikely.

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УДК 519.6 10.23947/2587-8999-2019-1-1-29-34

Компьютерное моделирование поиска праймеров в цепи ДНК*

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Полимеразная цепная реакция (ПЦР) является одним из самых распространенных экспериментальных методов при решении задач анализа ДНК. Олигонуклеотидные праймеры являются важной составляющей любой ПЦР, и поэтому существует ряд требований к их дизайну. От данных структур зависит успешность и возможность проведения эксперимента в целом. В связи с этим появилась необходимость проведения компьютерного анализа подбора праймеров. Разработан алгоритм на основе алгоритма поиска Бойера-Мура для специфичного дизайна праймеров. В настоящей работе представлены две вариации поиска праймеров. На основе алгоритма разработана программа, позволяющая проводить компьютерный дизайн праймеров перед непосредственным экспериментальным проведением ПЦР. Что значительно упрощает проведение натурного эксперимента. На данный момент расчеты проведены для модельных объектов (хромосом арабидопсиса).

Ключевые слова: полимеразная цепная реакция, дизайн праймеров, алгоритм Бойера-Мура, компьютерный анализ.

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* Работа выполнена при частичной поддержке гранта РФФИ № 17-44-020120.
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UDC 519.6 10.23947/2587-8999-2019-1-1-35-49

Mathematical modeling of the delay process in regulation of population dynamics based on the theory of cellular automation *

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The paper covers the research and parameterization of the delay effect in regulation of biological kinetics processes for interacting populations, including the modification of the mathematical model to describe the development of population fluctuations. Numerical implementation of the modified Conway algorithm for a cellular automaton with a ternary state of cells was developed for analysis the model scenarios of dynamics of nonlinear interacting biological populations, taking into account factors that have a significant influence on the nature of researched processes. The transformation conditions of the cells' state show that the formalized delay can refer to the dynamics of interaction of species and supporting the living conditions of the environment. A numerical implementation of a fundamentally different version of the cellular automaton was proposed. The cellular automaton allow modeling the processes of population dynamics regulation taking into account the delay effect on the basis of three dynamically interacting factors: ontogenetic delay, the necessary to restore resources, and diffusion component depending on the development rate of individuals in the population.

Keywords: cellular automaton, population dynamics, delay effect, mathematical model, algorithm, program.

Introduction. In the 70-s of XX century Kolmogorov A.N. assumed that with «the development of modern computing in many cases the examination of actual phenomena is reasonable conduct, avoiding the intermediate stage of it stylization in the spirit of the mathematics of the infinite and continuous, and passing directly to discrete models». Indeed, there is a large variety of mathematical systems based on the principle of fine-grained parallelism, and, most importantly, there were software and hardware systems that can simulate the operation of such systems today [1].

The main distinctive feature of systems with fine-grained parallelism is the possibility of simultaneous (parallel) changes in conditions of the entire system, while each section of it interacts only with its immediate neighbors. Due to this property, the events occurring at the micro level can associate with changes in the macro-level of the simulated object.

The classical system with fine-grained parallelism is a cellular automaton – a discrete model, which is a grid of arbitrary dimension. Each cell of grid at any given time can take one of a finite set of conditions with a given rule of cell transition from one condition to another.

* The paper was supported with the financial support by the grant № 17-11-01286 of the Russian Science Foundation.
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The idea of cellular automation was appeared in the late 40-s of XX century. It was conceived and formulated by John von Neumann and Conrad Zuse independently as a universal computing environment for constructing, analyzing and comparing the characteristics of different algorithms.

The definition of cellular automata is given in the paper of Toffoli T., Margolus N. [2]: «Cellular automata are discrete dynamical systems whose behavior is fully defined in terms of local dependencies. To a large extent, this is also the case for a large class of continuous dynamical systems defined by partial differential equations. In this sense, cellular automata in computer science are analogous to the physical concept of «field», and cellular automata can be thought of as a stylized world. The space is represented by a uniform grid, each cell of which contains several bits of data; time goes forward in discrete steps, and the laws of the world are expressed by a single set of rules or a small reference table, by which any cell at each step calculates its new condition by the states of its close neighbors. Thus, the laws of the system are local and the same everywhere. «Local» means that in order to find out what will happen here a moment later, it is enough to look at the condition of immediate environment: no long-range action is allowed. «Sameness» means that the laws are the same everywhere: I can distinguish one place from another only by the shape of the landscape, not by any difference in the laws». Note that cellular automata are not just machines performing with a field divided into cells. The field of application of cellular automata is almost limitless: from the simplest «cross-zero» to artificial intelligence. The theme of cellular automata is very relevant, as it can lead to the solution of many issues in the world.

A two-dimensional cellular automation can be defined as a set of finite automata on a surface indicated with integer coordinates (i, j), each of which can be in one of conditions $\sigma_{i,j}$:

$$\sigma_{i,j} \in \sum \equiv \{0,1,2...k-1,k\}.$$

The change of automation conditions occurs according to the rule of transition

$$\sigma_{i,j}(t+1) = \phi(\sigma_{k,l}(t) \big| (k,l) \in N(i,j)),$$

where $N(i, j)$ is some neighborhood of a point (i, j).

For example, the von Neumann neighborhood:

$$N_N^1(i, j) = \left\{(k,l) \middle\| i-k\right| + \left|j-l\right| \le 1\right\},$$

and the Moore neighborhood:

$$N_M^1(i, j) = \left\{(k,l) \middle\| i-k\right| \le 1, \left|j-l\right| \le 1\right\}.$$

Four types of cellular automation were proposed by Stephen Wolfram in the book «A New Kind of Science». According to it, all cellular automation can be separate depending on the type of their evolution [3]. The Wolfram classification was the first attempt to classify the rules themselves rather than the types of behavior of the rules separately.

The cellular automaton, known as «Conway's Game of Life» [4], was popularized by John Conway to explain the processes of self-organization in various natural sciences and simply as a visual model in teaching programming. Popularity is explained by only two calculation rules of the next generation of group of cells which can be alive or dead: if there's a dead cell with three living, the dead becomes alive; a living cell remains in its state if there’re two or three living cells nearby.

The playing field may be limited, withdrawn – in the form of a computer simulation of the torus surface. Such technique in the simulation is called the setting of boundary conditions of cyclic type or periodic boundary conditions (the most common option) or infinite, as originally believed Conway. At the same time, the simplicity of the rules with binary cell division provides a huge variety of forms and interesting variants of the arrangement of living cells in the first generation, which lead to stable or periodic variants of the final arrangement, called figures. There is a game modification with the continuous space without cells with a very impressive visual implementation. The situations that arise in the course of the game invented by him are very similar to the real processes that occur at the birth, development and death of a colony of living organisms. They are born with a favorable combination of relevant factors and die if the conditions of their existence become unbearable. The conditions of birth and death are determined exclusively by the mutual arrangement of participants.

Although the game consists of simple rules, nevertheless, it attracts the attention of scientists for more than forty years. The game «Life» and its modifications influenced (in some cases mutually) many sections of such exact Sciences as mathematics, computer science, physics. In addition, many of the patterns found in the game have their analogies in other, sometimes completely «non-mathematical» disciplines. Perhaps, this game is connected with other scientific phenomena, including those about which modern science is still unknown. It is also possible that the laws of «Nature and Society» that are not open today will become more understandable thanks to «Life» and its modifications.

Thus, cellular automata have found and are widely used in many spheres of human activity, many of problems which became possible to solve only with the help of a computer.

The use of cellular automata to research the processes of biological kinetics is reflected in the historically first model of exponential population growth $N(t) = N(0)e^{rt}$. To describe changes in the state of small populations, no separate formalization of the existing mechanisms of regulation in the functional form was assumed, only at the level of correction of the basic value of the reproductive parameter r [5].

The parameter r is a – reproductive potential (also known as «malthusian parameter») and defined as the difference between instant birth and death $r = \alpha - \beta$. It was supposed a priori $r > 0$ irrespective from t. The exponential growth equation $N = rN_t$ has long been unused, referred to as an anomaly in the history of mathematical biology, although it is obvious from many examples of alien species infestations that the properties of reproductive activity simply cannot be preserved $\forall t$.

For example, a system of deterministic equations describing the petroleum hydrocarbons biodegradation processes by introducing the *Chlorella vulgaris Beijer* green algae into the water on the basis of combined methods of mathematical modeling using the stochastic approach, with its probabilistic submodels, takes into account the simultaneous influence of external factors, including the spatial distribution of salinity, temperature and illumination, on the rate of mass transfer:

$$\left(P_i\right)'_t + div\left(\mathbf{u}\, P_i\right) = \mu_i \Delta P_i + \varphi_i,\ i \in \overline{1,4},$$

where P_i is a concentration of *i-th* component: 1 is the petroleum, 2 is the biogenic matter, 3, 4 are the *Chlorella vulgaris Beijer* green algae and its metabolite; $\mathbf{u}$ is the velocity vector of water flow; μ_i are diffusion coefficients; φ_i is a chemical-biological source.

If the second equation of the considered system taking into account the fluctuations of the environment has the form:

$$\dot{P}_2 = (\alpha - \beta + y(t))P_2, \quad m(t) = P_2^0 e^{(\alpha-\beta)t}, \ \sigma^2(t) = P_2^0 e^{2(\alpha-\beta)t}(e^{\sigma^2 t} - 1),$$

where α, β are growth rate and mortality of phytoplankton; $r = \alpha - \beta$ P_2^0 is a concentration of P_2 at the initial time; $m(t)$, $\sigma^2(t)$ are the mathematical expectation and variance of fluctuations $y(t)$, that at $r < \sigma^2$ the probability of degeneration of the *Chlorella vulgaris Beijer* population over time increases, in an effort to limit the unit – the population is probability unstable, i.e. long enough effects of disturbances are most likely to lead to her death. At $r > \sigma^2$ the probability of degeneration decreases, and at $t \to \infty$ the population tends to zero – the population in this sense is stable.

The adequacy of probabilistic observational models can be checked using the randomness criterion, which takes into account the variance values of a number of actual parameters and its random component caused by the influence of randomness elements [6].

In the future, Multispecies interaction models were developed. One of the problems was the confirmation of the existence of closed cyclic trajectories for the number of opposing populations in practice of observations or in experiments, which predicts the well-known «predator-prey» model by Lotka-Volterra.

The oscillations of two species were obtained in experiments of Utid S. for another type of biological interaction «parasite-host». To explain the contradictions, the hypothesis arose that the effect of self-regulation does not act from the current state, but from the one, existed in the past and manifests itself after a while. This hypothesis was suitable for the existing mathematical means of modeling of elastic deformations – differential equations with a deviating argument.

As a result of the observations and laboratory experiments it was found that population fluctuations may also occur in isolated populations in the absence of interspecific trophic interactions [7]. The logistic equation with delay was proposed by Hutchinson G. for formation the appearance of population oscillations of a single-species self-regulating system [8]:

$$N_t' = rN(t)(1 - N(t-\tau)/K), \qquad (1)$$

where *t* is the time; *N* is the number of individuals in the population; *r* is a reproductive characteristic; *K* is a supporting habitat capacity; τ is the delay parameter.

The delay parameter τ in this equation is a characteristic of regulation, i.e. the regulating parameter of use and restoration of resources or accumulation/disintegration of toxic products of metabolism, not connected with the age of puberty. The Andronov-Hopf bifurcation is performed at increasing the value of delay τ (or the reproductive characteristic r) [9].

It is known that in most cases, the effect of delay was associated with the duration and stages of the formation of adult mature organisms. If the delay is some much then the critical value, the resulting cycle quickly acquires a relaxation form with very low and long minimums. A large number of equation modification (1) was proposed for improving the characteristics of the oscillation model cycle. The *«food-limited equation»* including periodically dynamic coefficients was the most famous among them [10]. This suggests that the method of harmonization of models and observational data has reached an impasse.

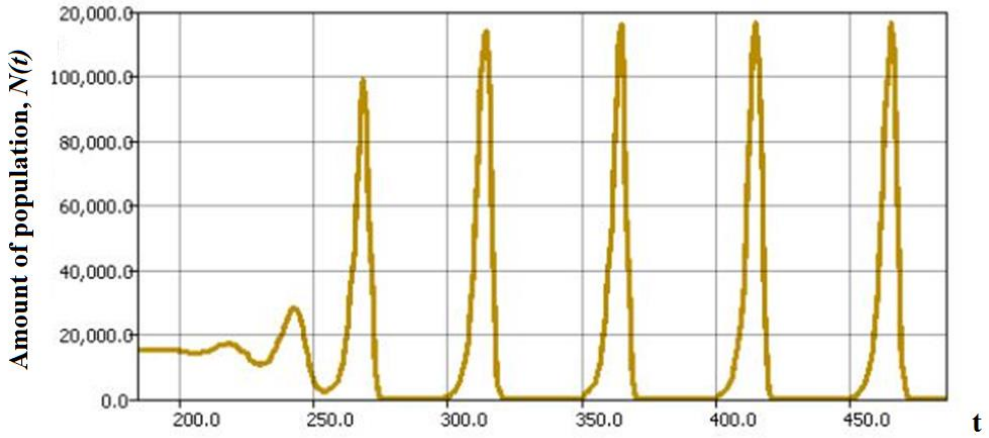

Fig. 1. Relaxation cycle in the Hutchinson equation, $K = 15000$.

According to experiments, conducted by the australian entomologist Nicholson with the laboratory population of flies, complex fluctuations of generational and regime change in behavior were occurred if the quantity and the regularity of receipt feed were changed; according to the modern analysis two frequency components were assigned in the oscillations [11].

However, in this case, the amount of feed is not a bifurcation parameter for the equation (1) considered above. A value K scales the amplitude of oscillations and represents the limit of the «ecological level». It's corresponded to the indicator of nutrient availability in (1). The fecundity and the time of passage of the stages of individual ontogenesis can be constant for the period of observation on average. It is obvious that in the experiment it was possible to simulate the change in the recovery rate of biological resources. According to the fact that the lack of food directly affects the mortality of larvae, it value is not isolated in the Hutchinson equation modifications. Therefore, it's necessary to take into account the instantaneous loss from the current population β (additional bifurcation parameter) was required for better agreement of experimental data simultaneously with the suppression of competition reproductive potential.

It was proposed a fundamentally different equation with delay, known as «Nicholson's blowflies equation» with the exponential nonlinearity, responsible for the self-regulation of reproduction efficiency [12]:

$$N_t' = \Upsilon N(t-\tau)e^{-\gamma N(t-\tau)} - \beta N(t), \quad (\Upsilon,\ \gamma,\ \beta = const\ > 0), \tag{2}$$

where γ is a characteristics of the population with the maximum effective reproduction.

The complex oscillations were occurred at the large values τ (τ = 15; β = 0.3); the damped oscillations were occurred with a smaller delay and smaller values β 1 (τ = 8, β = 0,015) – it's the scenario of soft completion of alien species invasive process with a single peak

The invasion of *Mnemiopsis leidyi* in the Black Sea refers to such scenario; but the dynamics of its number after entering the Caspian Sea does not fit into the known models. Mnemiopsis is a «short circuit breakers» in marine ecosystems, intercepting and mineralize flows of zooplankton organic matter, regenerate nutrients and thus stimulate the development of phytoplankton.

After the introduction of ctenophore in the Azov Sea the primary production was doubled with a concomitant increasing the organic matter in water and sediments and its turnover. One of the consequences of changes in the trophic chains in the Azov Sea ecosystem as a result of ctenophore introduction is an increase of detritus proportion [13]. *M. leidyi* can indirectly regulate the dynamics and distribution of summer phytoplankton through the consumption mechanism of zooplankters-phytophages, producing the «cascade» effect on the lowest trophic levels, through the zooplankton on phytoplankton and the chlorella «a». Eating of meroplankton by *Mnemiopsis* (larvae of benthic animals) and demersal plankton leads to decreasing of benthic biomass.

At modeling of hydrological processes (the interaction of plankton and ctenophores) in a shallow water – the Azov Sea – we take into account spatial distribution of salinity and temperature. The amount of *Mnemiopsis* depends on the range of its penetration and determined by the direction and velocity of wind currents that contribute to the drift of waters with high salinity. *Mnemiopsis* can live and reproduce only at salinity above 4.3‰ (for the Caspian Sea) [14]. The distribution of *Mnemiopsis* in the Azov Sea is limited by isogaline 3‰, due to its penetration from the Black Sea, where it's re-populated every year in spring or early summer, and lives until October, then dying out when temperature drops below 4°C.

Full-scale measurements obtained during the expedition in the Azov-Black Sea basin, and data of the «Analytical GIS» portal, developed by the Institute for information transmission problems of RAS (IITP RAS, Moscow) were used at modeling [15].

The model for describing the ecological and biological process of interaction between ctenophores and plankton has the form [16, 17]:

$$\left(P_i\right)_t' + \frac{1}{2}\sum_{\alpha=1}^{3}\left\{U_\alpha \left(P_i\right)_{x_\alpha}' + \left(U_\alpha P_i\right)_{x_\alpha}'\right\} = \mu_i \Delta P_i + \frac{\partial}{\partial x_3}\left(\nu_i \frac{\partial P_i}{\partial z}\right) + \psi_i,\ i \in \overline{1,9}.$$

$$\psi_1\left(P_1,P_2,P_3\right) = \left\{\alpha_1 P_3 - \delta_1 P_2 - \varepsilon_1\right\}P_1,\ \psi_2\left(P_1,P_2\right) = \left\{\alpha_2 P_1 - \varepsilon_2\right\}P_2, \qquad (3)$$

$$\psi_3\left(P_1,P_3,P_4\right) = \left\{\alpha_3 P_4 - \delta_3 P_1 - \varepsilon_3\right\}P_3,\ \psi_4\left(P_3,P_4,P_5\right) = \left\{\alpha_4 P_5 - \delta_4 P_3 - \varepsilon_4\right\}P_4,\ \alpha_4 = \left(\alpha_{04} + \gamma_4 P_6\right)$$

$$\psi_5\left(P_1,P_2,...,P_9\right) = \sum_{i=1,i\neq 5}^{9} \varepsilon_i P_i - \delta_5 P_4 P_5 + B\left(\overline{P}_5 - P_5\right) + f,$$

$$\psi_m\left(P_1,P_2,P_3,P_4,P_6,...,P_9\right) = \sum_{l=1}^{4} k_l P_l - \varepsilon_m P_m;\ m \in \overline{6,9},$$

where P_i are concentrations, $i \in \overline{1,9}$: 1, 2 are *Mnemiopsis leidyi* and *Beroe ovata* ctenophores; 3 is the zooplankton; 4 is the phytoplankton; 5 is the biogenic matter; 6, 7, 8, 9 are metabolites of ctenophores (6, 7) and plankton (zoo- (8) and phyto- (9)); ψ_i are functions of trophic interactions; α_l is the growth function of ctenophores and plankton, $l = \overline{1,4}$; α_{04}, γ_4 are the phytoplankton growth rate in the absence of metabolite and the impact parameter; B is the entering velocity of nutrients P_5; $\overline{P}_5$ is the maximum possible concentration of nutrients; ε_l is a mortality factor of l-th specie; ε_m are coefficients of metabolite decomposition, $m = \overline{6,9}$; k_l is an excretion rate of l-th specie (ctenophores ($l = \overline{1,2}$), zooplankton ($l = 3$), phytoplankton ($l = 4$)); $\delta_1, \delta_3, \delta_4$ are coefficients of loss due to eating;

$f = f(x_1, x_2, x_3, t)$ is the source function P_5 (pollution); $\mathbf{u}$ is the velocity field of water flow; $\mathbf{U} = \mathbf{u} + \mathbf{u}_{0i}$, $\mathbf{U} = (U_1, U_2, U_3)$ is the rate of convective transport of matter; $\mathbf{u}_{0i}$ is the sedimentation rate of i-th substance; μ_i ν_i are diffusion coefficients in horizontal and vertical directions of i-th substance.

The computational domain G is a closed basin limited by the undisturbed water surface Σ_0, the bottom $\Sigma_H = \Sigma_H(x, y)$ and the cylindrical surface σ for $0 < t \le T_0$. $\sum = \sum_0 \cup \sum_H \cup \sigma$ is the piecewise smooth boundary of the domain G.

We add boundary conditions to the system (3):

$$P_i = 0 \text{ на } \sigma, \mathbf{U}_\mathbf{n} < 0; (P_i)_\mathbf{n}' = \varphi_i \text{ на } \sigma, \mathbf{U}_\mathbf{n} \ge 0; (P_i)_z' = 0 \text{ на } \Sigma_0; (P_i)_z' = -\beta_i P_i \text{ на } \Sigma_H, \quad (4)$$

where β_i is an absorption coefficient of i-th component by bottom sediments; $\mathbf{n}$ is the vector of the external normal to the surface $\sum$.

Also, we add initial conditions:

$$P_i\big|_{t=0} = P_{i0}(x, y, z), i = \overline{1,9}. \quad (5)$$

Thus, there is a problem of ecological interpretation of delay τ, i.e., the determination of its magnitude with any direct population characteristics or properties of the environment. The analysis showed that taking into account the effect of delay in biological kinetics models can improve the accuracy of predictive modeling of population dynamics.

Continuity of measurement units is not necessary for population dynamics, because there are alternative methods for describing the processes of biological population dynamics, such as the cognitive graphs and cellular automata.

Results of numerical experiments. Rules of operation of new cellular automaton were defined in the paper [18]. Due to it, we can research the influence of the delay effect on the evolution of interacting biological populations. A mathematical game with more complex rules were introduced for illustration the problem of parametric expression of delay action in dynamic models and as a new object for determining the self-organization forms. According to it, the automaton cell has not two, but three acceptable conditions. The cellular automaton in which the parameter, relating to the nature of the occurrence of delayed regulation, will change during the game, simulating the evolutionary adaptation of the community to the emergence of new species, can be designed in the future.

Let's describe the rules of the «oaks-rodents» cellular automaton.

1. A cell field is defined as the same «Life» game (in the closed version). Each cell has 8 adjacent cells. Initially, the oak grows in each cell (N_1). The rodent (N_2) can settle in the cell, containing the oak.

2. Adult rodent can produce $r = 2$ offspring every season if also the rodent lives at least one of the adjacent to his cell.

3. If more than 5 cells are occupied around the rodent, the rodent dies from overpopulation, and the oak becomes free.

4. Rodents undermine the roots of the tree. The oak falls, and the rodent dies. Before the fall of the oak, a rodent may breed no more than $k = 5$ times.

5. The offspring of the rodent will become pubescent and will be able to give offspring through the season, if they will take a suitable oak at this moment, otherwise they die. The new rodent occupies the nearest free oak with the least number of occupied adjacent cells, examining the adjacent ones clockwise.

6. The rodent may have migrated for the season to a distance of not more than $l = 2$ of the neighboring cells to occupy the oak (similar to the speed of light in the Conway's game).

7. A new oak grows up for $\tau = 10$ seasons on place the fallen oak.

Several aspects, related to the phenomenon of delayed regulation, are determined in the transformation rule of cell conditions. Moreover, these factors are warring in the game. We propose to make the parameter τ as a «manager» to assess the impact in scenarios with slower recovery of resources, which was not in «Life», but is consistent with environmental reality.

The software that implements the operation of the cellular automaton was developed in the C# object-oriented programming language. Transition rules for cellular automation of the delay regulation are the basis of algorithm of software implementation. For a better research of the model of biological population interacting, all parameters of the cellular automation can dynamically change during the application.

The main window of the developed application with the original interface that allows to dynamically changing the parameters of the cellular automation is given in Fig. 4.

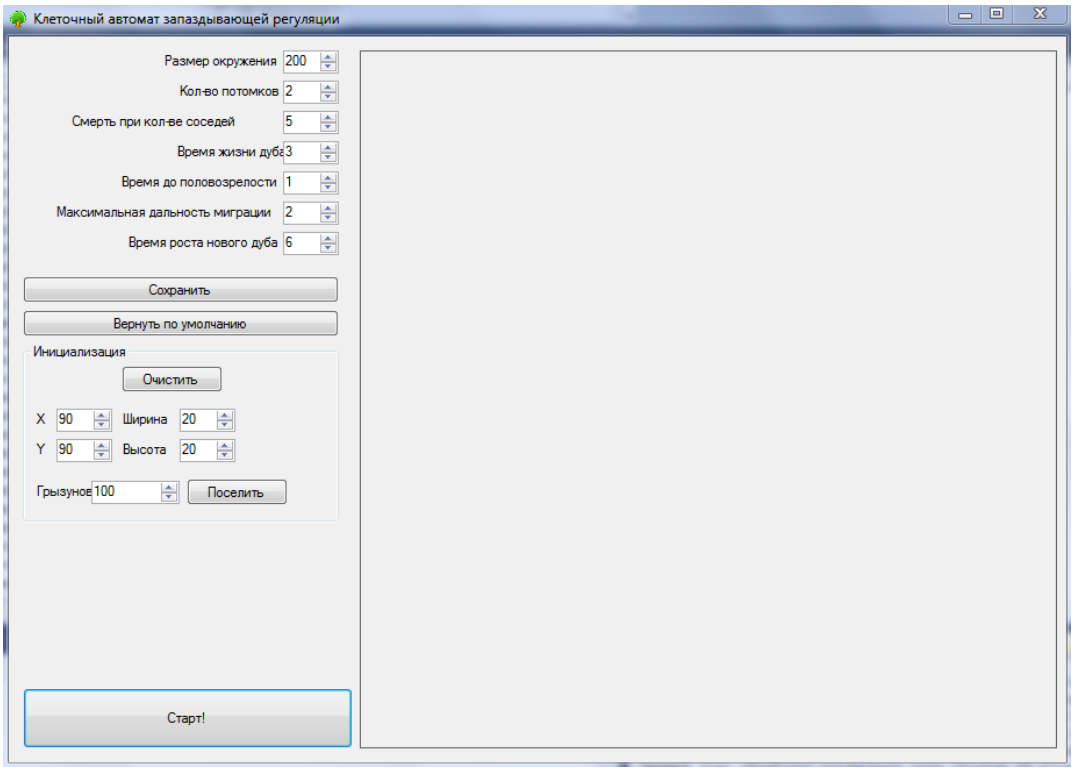

Fig.4. The interface of application.

We conducted a number of experiments with the developed application. Figures 5-8 shows the results of mathematical modeling the evolution process of two interacting species of biological

populations (the concentration N_1 denotes by the green color, N_2 – by the red color) taking into account the delay effect based on the previously introduced transition rules (algorithm) of the cellular automation.

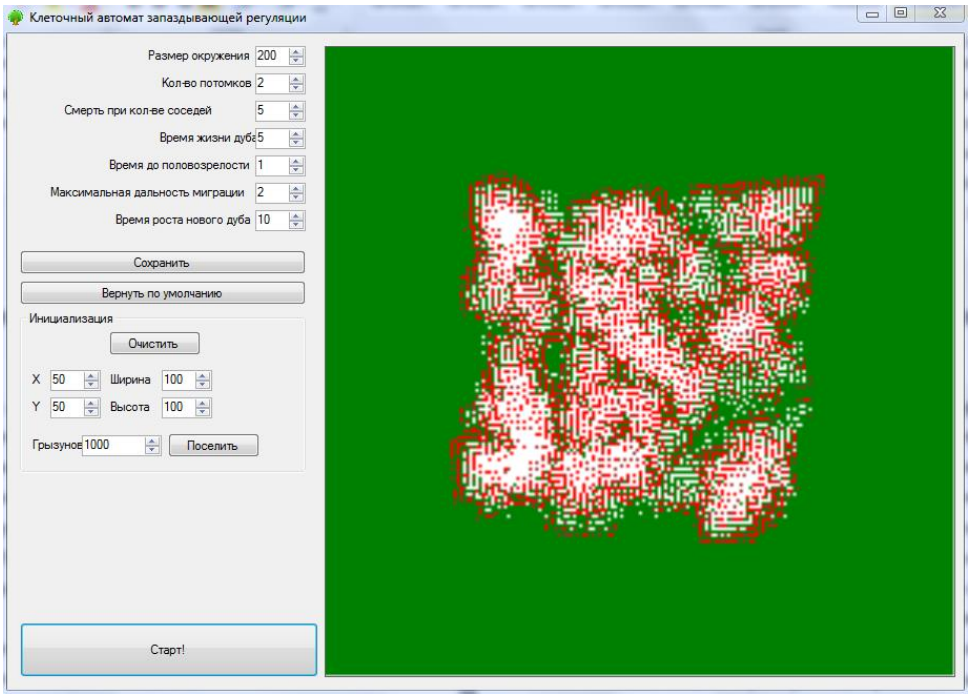

Fig. 5. The process of modeling the interaction of biological populations.

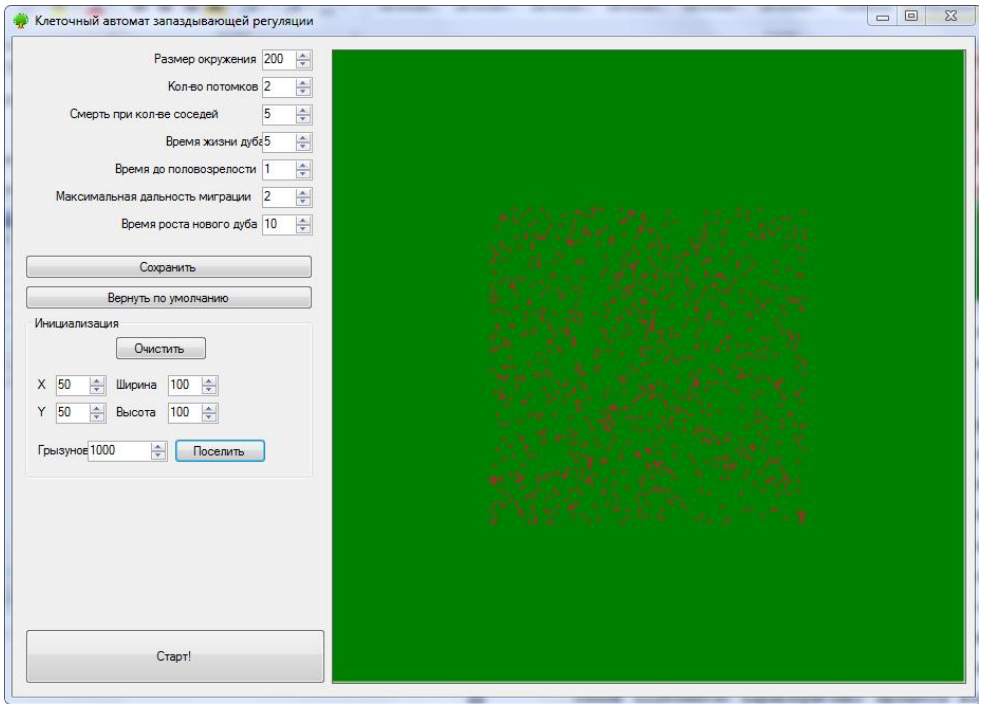

Fig. 6. Changes in the number of interacting populations at the initial time $(t = 0)$.

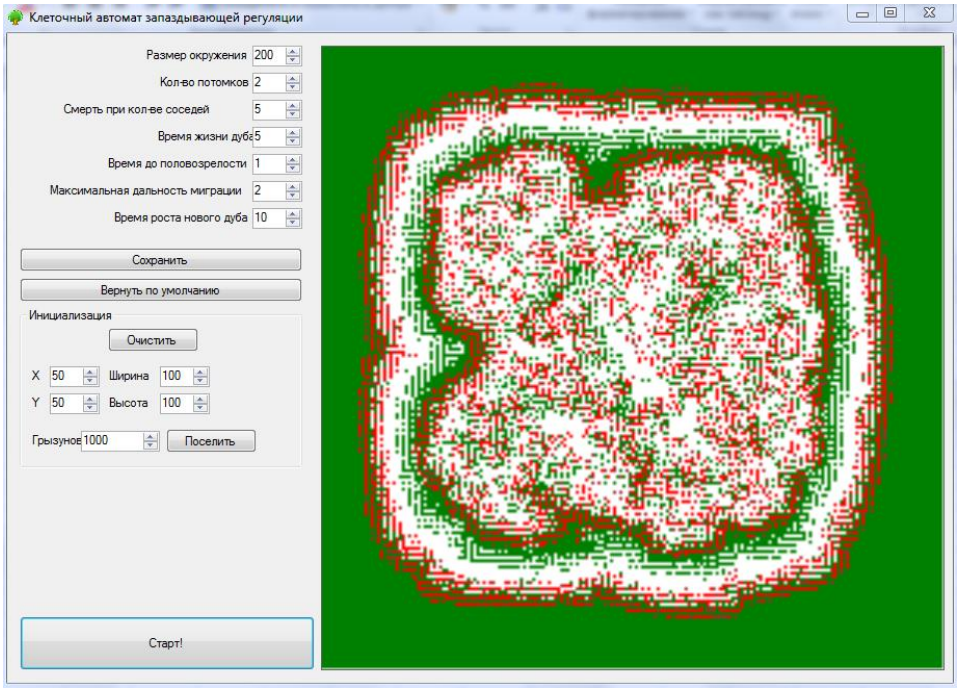

Fig. 7. The intermediate stage of the simulation $(t = 50)$.

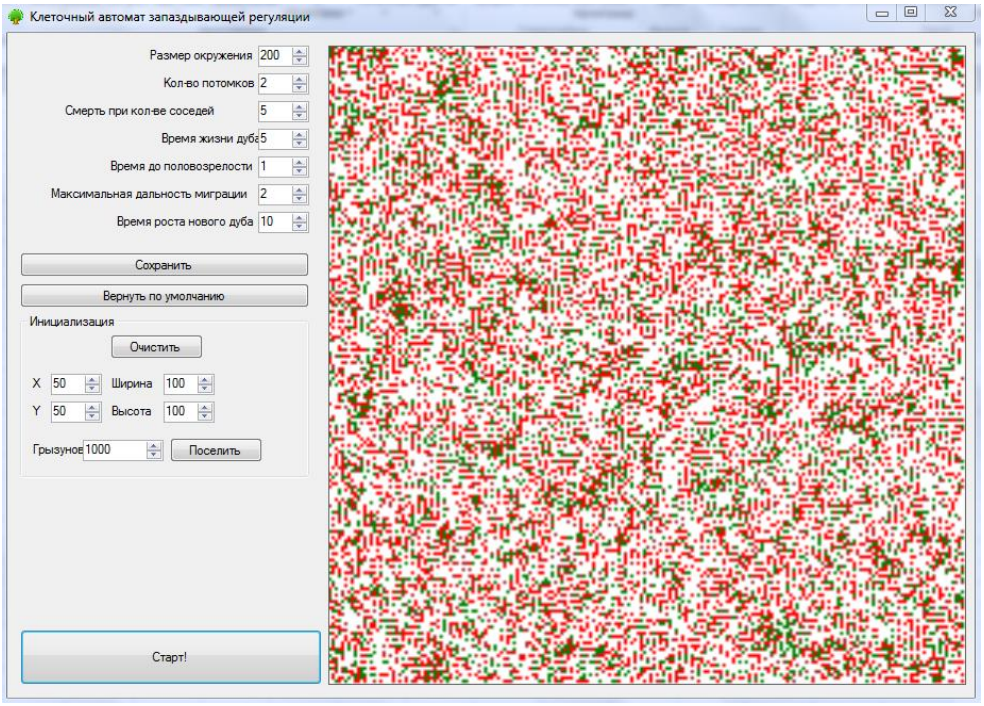

Fig. 8. Changes of the amount of interacting populations $(t = 500)$.

Graphs of population amount changes for different values (the time delay parameter) are given in Fig. 9-12.

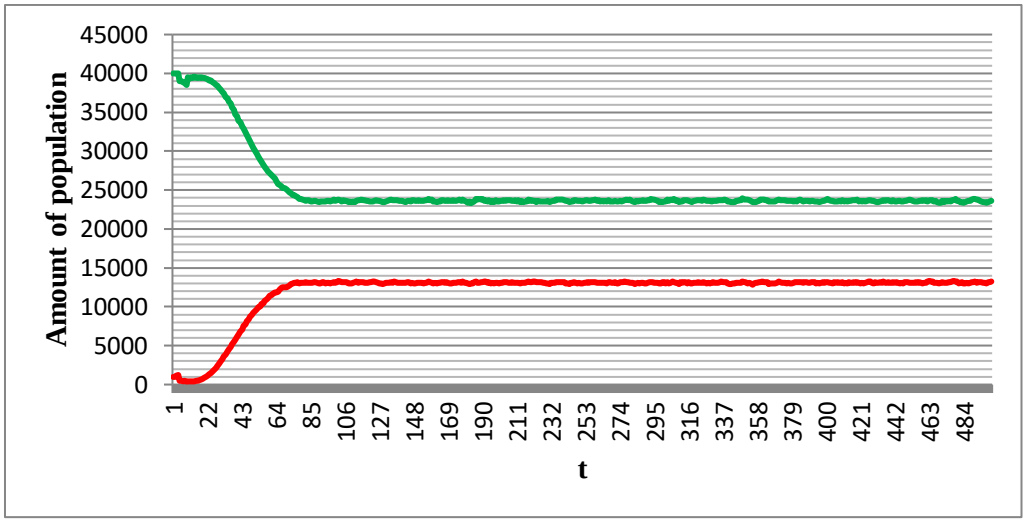

Fig. 9. Changes of population at $\tau = 5$.

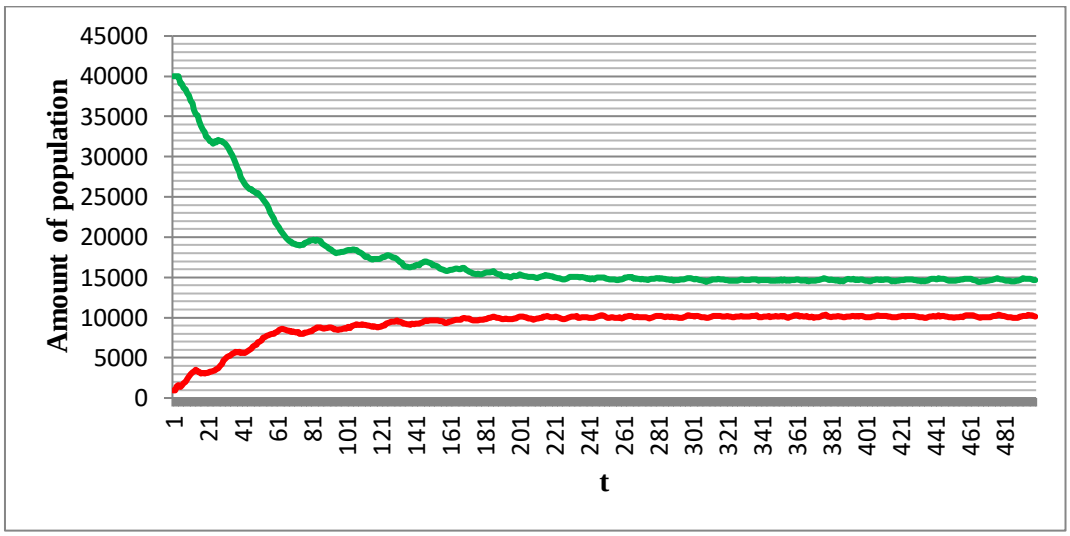

Fig. 10. Changes of population at $\tau = 10$.

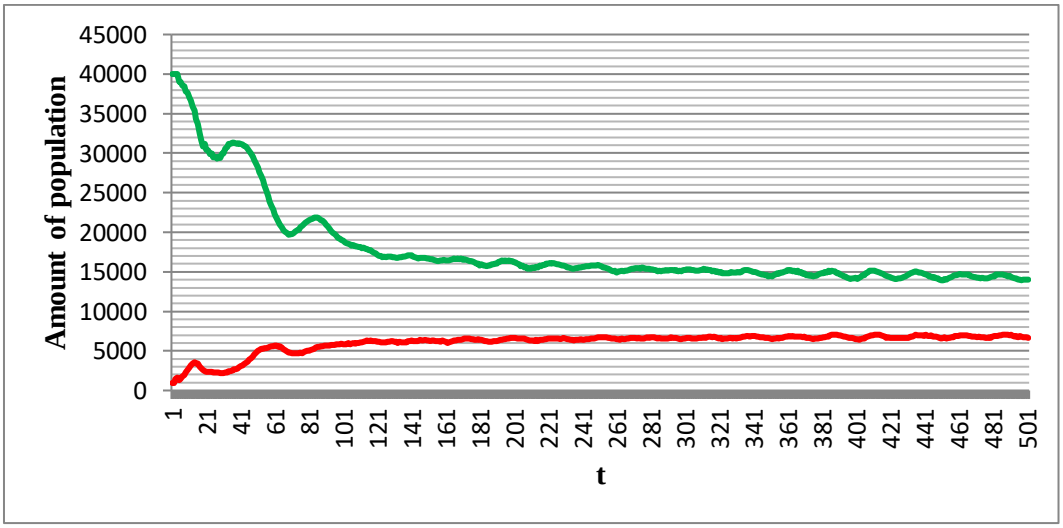

Fig. 11. Changes of population at $\tau = 15$.

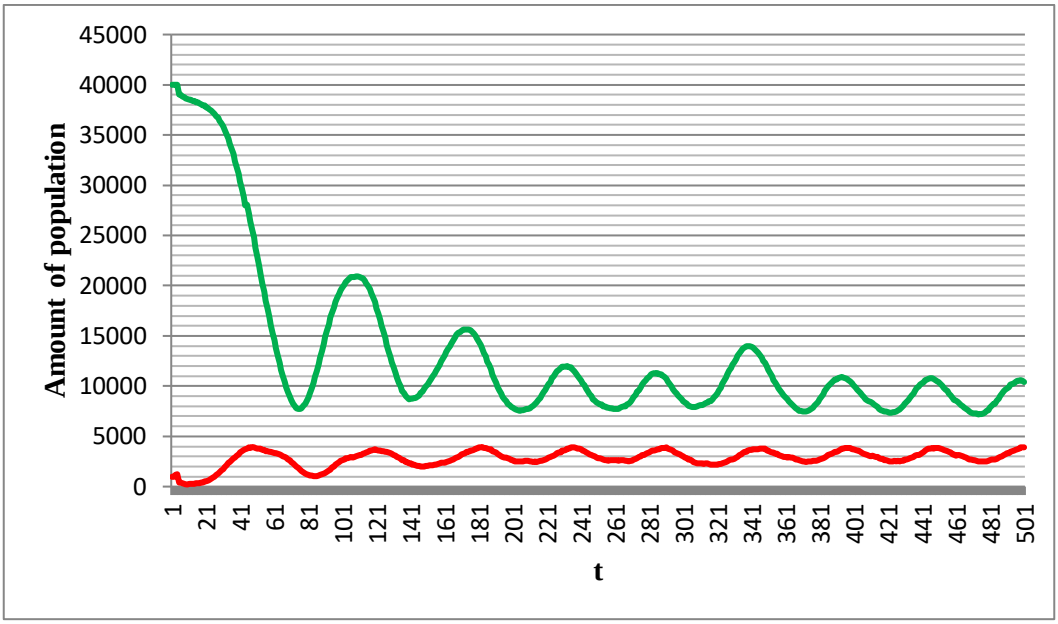

Fig. 12. Changes of population at $\tau = 30$.

According to the Fig. 9-12, it can be concluded that taking into account the delay effect can improve the accuracy of predictive modeling the interacting biological population evolution. As we can see that, the change of population is approaching the field data at increasing the τ parameter. Numerical experiments have shown that the results of population dynamics modeling coincide with the solution of equation (2) at the qualitative level (Fig. 2). The solution of the model problem at high values τ has the complex oscillations. The solution of the model problem gives a fast output to the stationary regime with a single significant deviation with the less delay.

The numerical implementation of the modified Conway algorithm made it possible to determine nontrivial input data that affect on the dynamics of environmental processes, tend to some established stationary or oscillatory regime. Although it is known that the initial conditions are not so significant characteristics in population dynamics.

Conclusion. A variant of the cellular automation, modeling the regulation processes of interacting biological population dynamics taking into account the delay effect, was considered. The application was developed for a computer in C# for modeling the nonlinear interaction of the cellular automation. Experiments were performed on the basis of developed application for researching various effects, including the delay, occurring at different input parameters of the cellular automation (the rules of transition). The algorithm of cell transformation includes three dynamically interacting factors: the ontogenetic delay, the need to restore resources for the further development of the population, and the diffusion component. The developed numerical implementation of the cellular automaton was based on the hypothesis that the delayed regulation does not belong to the properties of species or only the environment, but it is an additive characteristic of nonlinear interaction process of the researched biological populations.

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УДК 519.6 10.23947/2587-8999-2019-1-1-35-49

Математическое моделирование процесса запаздывания в регуляции популяционной динамики на основе теории клеточных автоматов*

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Работа посвящена изучению и параметризации эффекта запаздывания при регуляции процессов биологической кинетики для взаимодействующих популяций, в том числе модификация математической модели для описания развития популяционных флуктуаций. Для анализа модельных сценариев динамики нелинейно взаимодействующих биологических популяций с учетом факторов, оказывающих существенное влияние на характер протекания изучаемых процессов, разработана численная реализация модифицированного алгоритма Конвея для клеточного автомата с троичным состоянием клеток. Условия трансформации состояния клеток показывают, что формализуемое запаздывание может относиться к динамике взаимодействия видов и поддерживающей условия жизни среды. Предложена численная реализация принципиально отличного варианта клеточного автомата, моделирующего процессы регуляции популяционной динамики с учетом эффекта запаздывания на основе трех динамически взаимодействующих факторов: онтогенетической задержки, необходимости восстановления ресурсов и диффузионной составляющей, зависящей от темпа развития особей популяции.

Ключевые слова: клеточный автомат, популяционная динамика, эффект запаздывания, математическая модель, алгоритм, программа.

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* Работа выполнена при поддержке РНФ, проект № 17-11-01286.

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UDC 519.17+51-74 10.23947/2587-8999-2019-1-1-50-59

Application of graph theory to describe the process of oxidative regeneration of catalysts in oil refining processes*

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The application of graph theory to describe the various processes of oil refining is an urgent problem. This facilitates the development, analysis and design of production data. In the future, it is possible to obtain qualitative and quantitative characteristics of these processes. This article presents a description using the theory of graph processes for the oxidative regeneration of catalysts of dehydrogenation of butane and catalytic cracking. The obtained regularities using graphs can be used to optimize these processes.

Keywords: catalyst, catalytic cracking, dehydrogenation of butane, graph, graph theory, kinetic model, mathematical modeling, operator scheme, oxidative regeneration.

Introduction. Chemical industry production includes complexes of various processes. Before building a chemical plant, it is necessary to develop a production process plan, which involves developing the individual process technologies, considering their interconnections. «Any complex technology is not a mechanical sum of separate processes. The optimal modes for carrying out particular processes independently do not ensure the best work of the whole plant» [1]. Each process shall be harmonious not only from a technical point of view; it shall also fulfill the economic requirements [2]. The objective of achieving the minimum prime cost is very complicated. The issue of reducing the production costs is solved by analyzing the structure of processes, the nature of production costs, etc. [3–8]. A prerequisite for the successful solution of these tasks is the analysis of chemical and technological processes in general.

The study of complex chemical industries is called the study of processes (the study of flow structure). The word «process» here is understood in the widest sense, since it can apply to anything from a single device to an entire plant [9]. The object of study is the production facilities of modern chemical industry analyzed based on technological schemes or using graphs that are more illustrative.

Analysis of chemical production facilities using the theory of graphs. Such a study started with the comparison of technological schemes, but it was found out that they could not be used for the comparison. Within the framework of the study of processes, they can be compared by substitution of technological schemes for the graphs and the subsequent analysis based on the theory of graphs. It emerged that any chemical production facilities, even the most complex ones, can be represented as consisting of objects and each of such objects can be classified within one of the four classes.

1. Reactors – devices in which chemical transformations take place.
2. Allactors – devices in which only physical processes occur.
3. Tanks – construction for the storage of intermediate products.

* The study was partially supported by the Russian Foundation for Basic Research, research project No. 18-07-00341.
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4. Lines – devices for managing the flows.

Objects 1, 2 and 3 are hereinafter referred to as the operational units.

Such classification allows both to describe the chemical production facilities and study them quantitatively using the theory of graphs, while technological schemes provide only qualitative information. A quantitative analysis of chemical production facilities using the theory of graphs becomes possible due to the fact that the set of processes described by graphs is modeled by matrices [9, 10]. Since the method of analysis is graphical, the word «graph», first suggested by Koenig [11, 12], appeared.

The graph theory is a mathematical tool for analyzing the schemes, in which the objects are represented by points in two-dimensional space, and the relationship between the objects is shown by lines [10]. The points of the set in the graph theory are called the points of the graph, and the lines connecting them are called edges. In the graphs of chemical production facilities, the points are operational units, and the edges are the lines.

A characteristic feature of graphs describing the processes of industrial chemistry is that they are the directed graphs, that is, the directions can be assigned to all their edges. This is due to the fact that the movement of flows along the lines in the processes of industrial chemistry usually occurs only in one direction. When the process is represented by graphs, the points of graph do not differ qualitatively, that is, they can denote any object. In the processes of industrial chemistry, the points (operational units) can be of three types, and they are not exchangeable.

Initially, all the points of graphs were designated by the same points, and the lines along which the material or energy is transferred were indicated by arrows pointing in the direction of motion [11].

Then it emerged that the graphs of industrial chemistry become more illustrative if their points contain the information on the purpose of a particular operational unit. Also, two extreme types of graphs are used to illustrate the processes: principal and technological graphs. Principal graphs provide only a scheme of the model of the chemical process of processing raw materials into the final product. They illustrate only the most important reactors, and, if necessary, some allactors. All reactors, allactors, tanks, all equipment for the transfer and all routes of materials are illustrated on technological graphs.

Legend.

Operational units corresponding to the points of the graph are designated with the symbols shown below:

Reactor: black circle (●).

Allactor: white circle (O).

Reservoir: square (□).

Tanks for storing raw materials and finished products are not shown on the graphs at all, as they do not characterize the process.

Devices for transferring materials (which correspond to the edges on the graph) are shown depending on the aggregate state of the substance being transferred.

Designation of edges of the graphs of the processes of industrial chemistry:

Solid matter: ------ →

Liquid matter: →→

Gaseous matter: ·····→·····

Suspension: -·-·-·→·-·

Arrows indicate the direction of movement.

The graphs of industrial chemistry can be classified into four types:

1. Direct-flow open graph, i.e. a graph in which the mass flows have the same direction.
2. Counter-flow open graph, i.e., a graph in which the major mass flows have opposite directions.

3. Direct-flow closed-loop graph represents the process in which the circulation of one of the substances takes place. The number of subgraphs can be open or closed.

4. Counter-flow closed-loop graph represents the process in which the counter-flow circulation of two substances takes place.

Based on the analysis of properties of the industrial chemistry processes, it can be mathematically demonstrated that only the above four types of graphs can exist [11].

The difference between the graphs of industrial chemistry and other graphs is that the conditions for the movement of mass flows in the processes are determined.

Each process in industrial chemistry is characterized by three factors:

1. Directional movement of incoming and outgoing mass flows, due to which each graph of industrial chemistry is directed as noted above.

2. The sum of the masses at the input ($\sum_{i=1}^{n} Ai$) is equal to the sum of the masses at the output ($\sum_{j=1}^{m} Aj$), since it is impossible to accumulate matter inside the process scheme $\sum_{i=1}^{n} Ai = \sum_{j=1}^{m} Aj$

3. The number of incoming (n) and outgoing (m) flows can be correlated by three types of dependences: $n < m$, $n = m$, $n > m$.

Graphs of processes of industrial chemistry can be of different complexity. The simplest model representing only the chemical scheme of the technological process without the auxiliary equipment is called the principal graph. The technological graph is obtained by representing a complex chemical production (chemical plant). Between these two cases there is a range of transition graphs, the shape of which varies depending on the number of operations under consideration.

Complex technological graphs can be made more illustrative by splitting them into subgraphs. This option is expedient when representing complex technological processes, especially in case of complex processes of combined production. As a result, complex graphs and combined graphs are obtained [9]. Let us consider the application of the theory of graphs for particular industrial processes important for today's industrial chemistry.

Application of the theory of graphs to simulate the process of oxidative regeneration of butane dehydrogenation catalyst. The process of deactivation takes place in any petrochemical industry, accompanied by the deposition of carbon on the surface of the catalysts thus reducing their activity. This problem can be solved by oxidative regeneration.

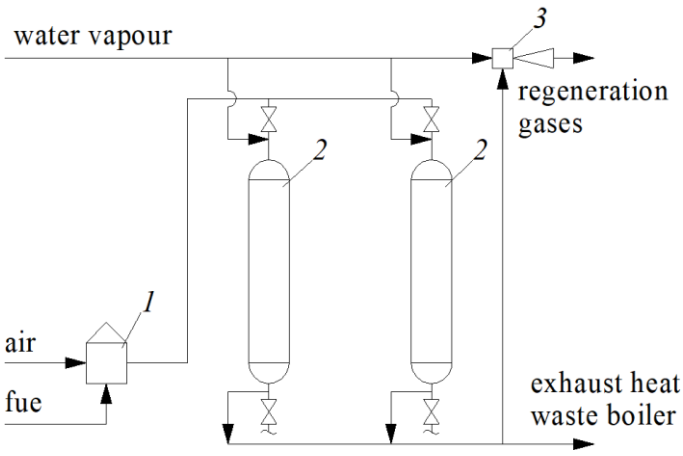

Fig. 1. Scheme of oxidative regeneration of catalyst of one-stage butane dehydrogenation. 1 – furnace, 2 – reactors, 3 – ejector.

The oxidative regeneration of cocked catalysts is a combination of chemical reactions proceeding when oxygen interacts with coke, as a result of which coke is removed in the form of gaseous oxidation products: carbon oxides, water vapor, and sulfur oxides in some cases [12].

Let us consider the chemical-technological graph of the process of oxidative regeneration of catalysts.

The catalyst of vacuum dehydrogenation of butane is regenerated in a contact apparatus, the reactive unit is composed of eight apparatuses that ensure the continuity of the process. After completion of the dehydrogenation cycle, the apparatus is blown and air is fed into it. Coke burn off is performed at a temperature of 600-650℃. The regeneration cycle lasts for 8 minutes, the gases are removed by a 3-ejector, the catalyst is restored when the hydrocarbon gas is fed from the reactor.

Dehydrogenation of butanes to butadiene takes place in a system of two reactors with a fixed-bed catalyst. One apparatus operates in catalyst regeneration mode, and the other - in dehydrogenation mode. The regeneration is performed by a steam-air mixture at a temperature of 620-650 ℃, oxygen concentration is within 1-2%, the duration of two cycles is 30 minutes. Dehydrogenation takes place first, followed by regeneration. The switching of the operation from the dehydrogenation phase to the regeneration phase consists in replacing the butane in the vapor mixture with a certain amount of air [13].

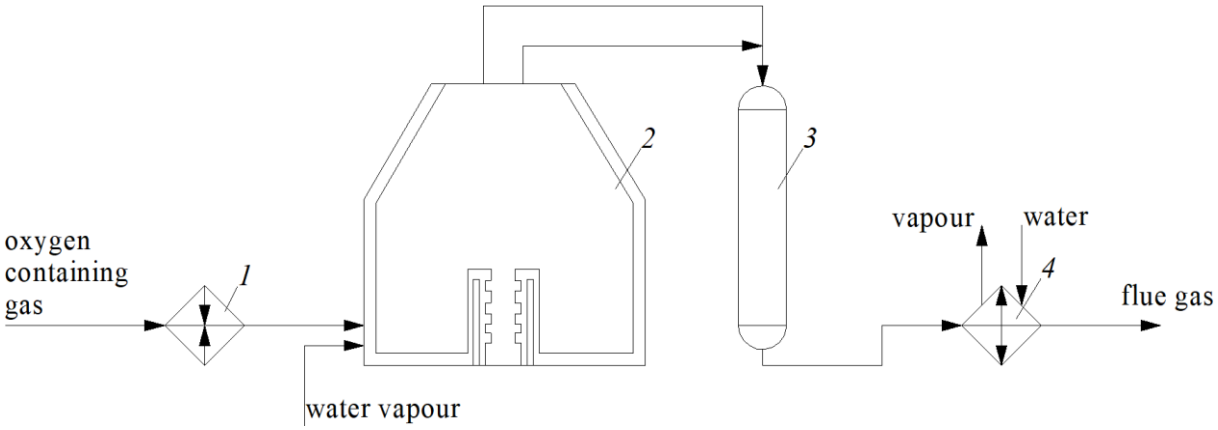

Fig. 2. Technological scheme of regenerations of catalyst for dehydrogenation of butenes:
1 – heat exchanger; 2 – furnace; 3 – reactor; 4 – wasteheat exchanger.

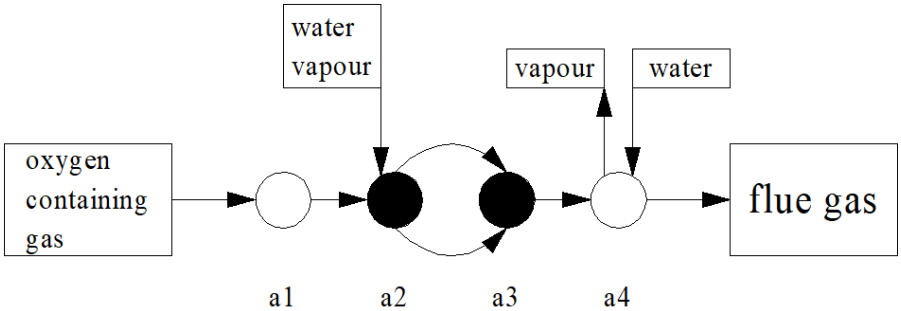

Fig. 3. Graph of regenerations of catalyst for dehydrogenation of butanes:
allactor a^1 – heat exchanger; a^2 – furnace; a^3 – reactor; a^4 – wasteheat exchanger.

The comparison of Figures 2 and 3 shows that the graphs are perceived much more easily than the traditional technical schemes. This is due to the fact that the range of operational units is shown using one point of the graph (in this case – a).

Application of the theory of graphs to simulate the process of oxidative regeneration of cracking catalyst. Let us consider more complicated refining processes, which, for example, include catalytic cracking to produce high-octane gasoline components. The quality of the process products is influenced by the composition of the raw materials, the technological parameters of the process, such as temperature and pressure, as well as the properties of the catalyst. During the process of cracking, coke deposits are formed on the catalyst, such deposits can be removed by catalyst regeneration. Fig. 4 shows the example of a reactor unit [14].

Therefore, the process of catalyst regeneration occurs in one apparatus. However, several processes take place in the regenerator. The air is heated up to the regeneration temperature in the preheater, then the air is mixed with the coked catalyst. A chemical reaction of oxidation (combustion) of coke from the catalyst surface occurs, after which the combustion gases are removed from the regenerator and the catalyst returns to the reactor after cooling. Thus, an operational technological scheme of the process of regeneration of catalytic cracking catalyst can be developed on the basis of the above. The scheme is shown in Figure 5.

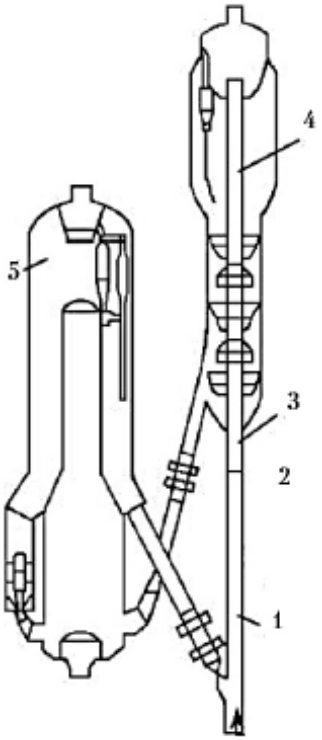

Fig. 4. Technological scheme of a reactor unit of a modern catalytic cracking unit:
1 – catalyst uplift zone; 2 – raw material sprayer; 3 – overflow device with ideal upward plug-flow; 4 – riser; 5 – regenerator [14].

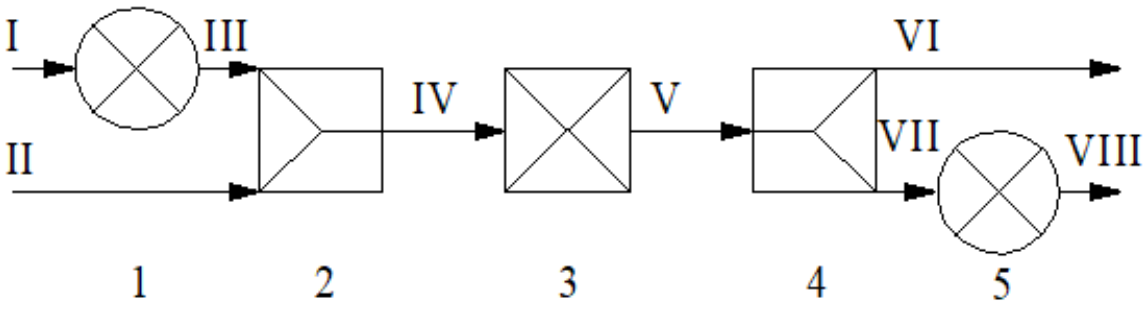

Fig. 5. Operational scheme of catalytic cracking catalyst regeneration process.

Let us demonstrate the process of oxidative regeneration of catalytic cracking catalyst using the theory of graphs. To optimize the chemical and technological process, the following classification of graphs is used [15]:

1) Flowgraphs;
2) Informational flowgraphs;
3) Signal flow graphs;
4) Reliability graphs.

The main properties of the graphs in relation to the description of chemical and technological processes are as follows:

1) Orientation, since the movement of matter and energy in the system has a certain direction;
2) Asymmetry, since not all neighboring elements of the system are interconnected by reverse process flows;
3) Connectedness, since all the elements of the system are interconnected by a single chain of flows of matters or energy.

Flowgraphs include [15]:

1) Parametric graphs;
2) Material graphs compiled according to the flowrates of physical flows;
3) Thermal graphs.

Let us compile a flowgraph for the process of oxidative regeneration of catalytic cracking catalyst based on the operational scheme (Fig. 5).

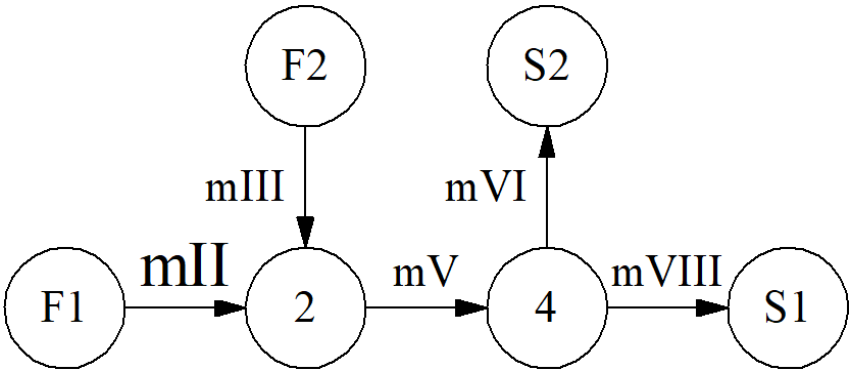

Fig. 6. Flowgraph for the process of oxidative regeneration of catalytic cracking catalyst: the physical flow of the system is characterized by the following parameters: m_i – total flowrate of a physical flow.

Only the system elements with the changing flowrate are used to compile a material graph of the flowrates of physical flows. The operators in which the flowrate changed are the points of the graph; the flows themselves are the edges of the graph. Flowrates do not change in operators 1, 3, 5. In operator 1 the airflow is heated, i.e. the temperature rises, but the air flowrate does not change. In operator 3 chemical transformation (burning) takes place, but the flowrate remains the same. In operator 5 cooling takes place, i.e. temperature drops, but the catalyst flowrate does not change. Flowrate changes only in operators 2, 4, consequently, these operators are the points of the graph. In addition to the operators, raw material and product flows shall be included in the material graph of flowrates. Therefore, the graph includes F1 and F2 – the flows of catalyst and air, respectively. S1 and S2 are the output of products, regenerated catalyst and combustion gases, respectively.

Fig. 7 shows the thermal flow graph.

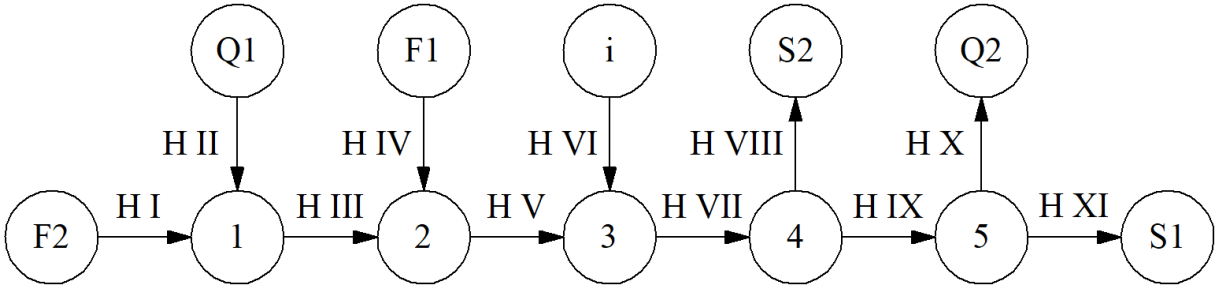

Fig. 7. Thermal graph for the process of oxidative regeneration of a catalytic cracking catalyst**:** 1-5 are the numbers of the points corresponding to operators;
F_1 is the flow of coked catalyst; F_2 is the flow of fresh air;
S_1 is the flow of regenerated catalyst; S_2 is the flow of combustion gases;
Q_1 is the flow of heat supplied to the system for air heating;
Q_2 is the flow of heat carried away when cooling the regenerated catalyst; $i_Г$ is the heat of coke combustion;
$H_1 – H_{11}$ are the heat flows inside the system.

Chemical graphs can be used to describe the chemical mechanism of processes, including the catalytic ones. Chemical graphs are classified as follows [15]:

1) Molecular;
2) Bipartite;
3) Signal.

Molecular graphs characterize the structure of a chemical bond. Molecular graphs allow to solve problems with coding, structural peculiarity, branching, etc. Atoms are the points of the graphs, and chemical bonds are the edges. The structure of catalysts can also be illustrated by molecular graphs.

Bipartite graphs are used to optimize paths; they require the smallest number of intermediate reactions, the minimum number of reagents. Molecules are the points of such graphs, and interactions between molecules, i.e. chemical bonds are the edges.

Signal graphs characterize the kinetics of chemical processes. Information variables are the points of the graphs, signal interconnections are the edges.

An adjacency matrix, an incidence matrix, is compiled based on the theory of graphs. Mathematical models can be developed on the basis of these matrices.

For the catalytic cracking process let us consider one of the known variants of the mechanisms of the kinetics of this process [16].

$$K + O_2 \leftrightarrow [K\text{-}O_2] \rightarrow [K\text{-}O]$$
$$[K\text{-}O_2] \rightarrow CO_{2адс} \rightarrow CO_2\uparrow$$
$$[K\text{-}O] \rightarrow CO_{адс} \rightarrow CO\uparrow$$
$$[K\text{-}O] \rightarrow H_2O_{адс} \rightarrow H_2O$$
$$CO + 1/2O_2 \rightarrow CO_2$$

Bipartite graph for this reaction is shown below in Fig. 8.

Using this graph, adjacency and incidence matrices can be compiled and the order of analysis of the target system of chemical reactions can be defined.

The advantages of graph models include their flexibility, wide possibilities and variety of applications. Theoretical graph algorithms and the search for control procedures based on them are much more efficient than others in many cases. The advantage of this method is that the method allows to determine the fastest way to solve a problem in case of a significant number of possible solutions. The graphs can also be used to determine the method of analyzing a complex system, the solution of which is not obvious at first glance.

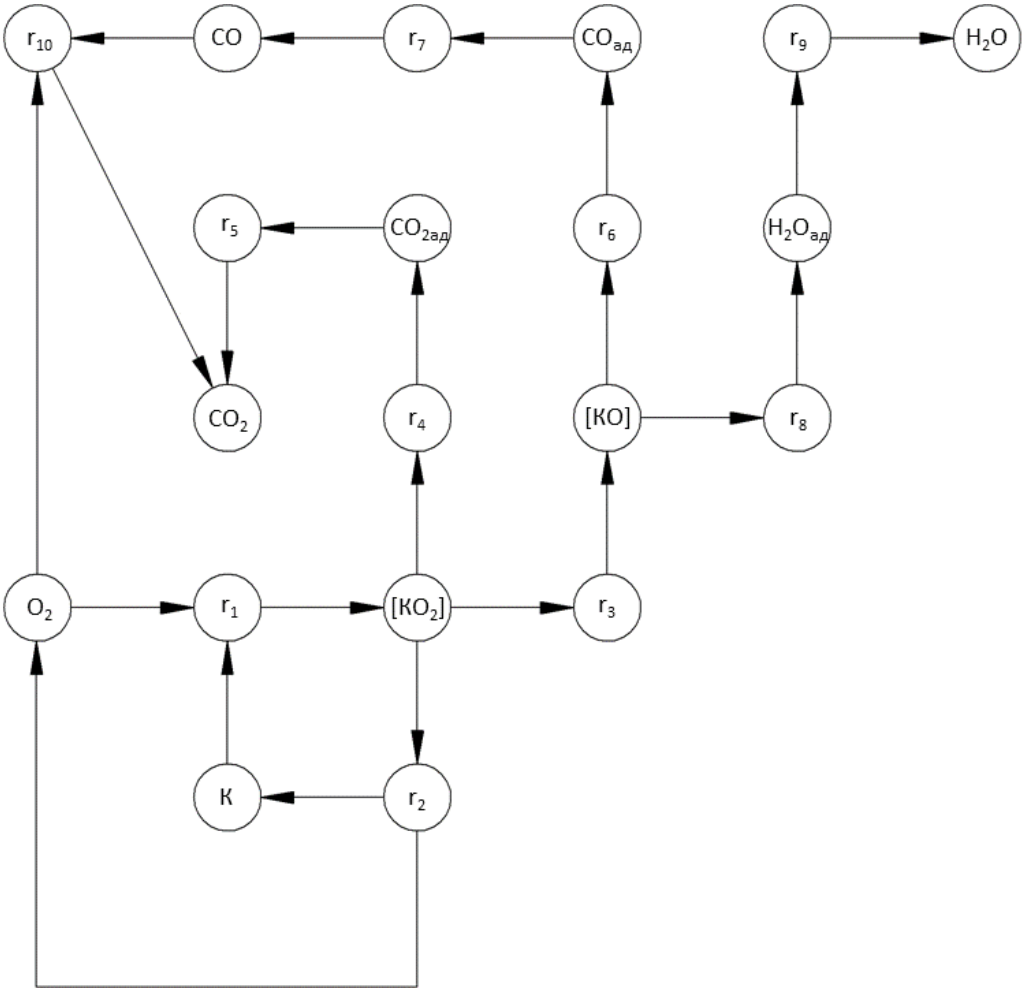

Fig. 8. Bipartite graph for the process of oxidative regeneration of hydrocarbon cracking catalyst.

Conclusion. Thus, the presentation of a process with the graphs is more illustrative as compared with the technical scheme. The presentation of process of industrial chemistry on the basis of the theory of graphs described above has a purely qualitative nature at the initial stage. But such a presentation allows to determine the procedure for analyzing the equipment for the compilation of a mathematical model, which will allow to optimize the oxidative regeneration processes of the butane dehydrogenation catalyst and the oxidative regeneration of the cracking catalyst to reduce the prime cost of products.

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УДК 519.17+51-74 10.23947/2587-8999-2019-1-1-50-59

Применение теории графов для описания процесса окислительной регенерации катализаторов в процессах нефтепереработки *

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Применение теории графов для описания различных процессов нефтепереработки является актуальной проблемой. Это облегчает разработку, анализ и проектирование данных производств. В дальнейшем можно получить качественные и количественные характеристики данных процессов. В данной статье представлено описание с применением теории графов процессов окислительной регенерации катализаторов дегидрирования бутана и каталитического крекинга. Полученные закономерности с помощью графов могут быть использованы при оптимизации данных процессов.

Ключевые слова: граф, дегидрирование бутана, катализатор, каталитический крекинг, кинетическая модель, математическое моделирование, окислительная регенерация, операторная схема, теория графов.

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* Работа выполнена при частичной поддержке гранта РФФИ № 18-07-00341.

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UDC 004.94 10.23947/2587-8999-2019-1-1-50-63

Probabilistic modeling of overhead irrigation processes*

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The article is devoted to the development of a sprinkling process model that is in relation to the probabilistic similarity to the simulated process, the numerical implementation of which allows to calculate the matrix of irrigation doses in the sprinkling area, or at the test site. The study was performed using system analysis and probabilistic modeling. The uniform distribution of fluid over the area until 2004 was estimated by the RD 10.11.1–9-89 by the effective irrigation coefficient, insufficient irrigation coefficient, and excessive irrigation coefficient. After the introduction of the interstate standard ISO 7749-2-2004 it is estimated by the Christiansen coefficient. New mathematical models and software were designed for probabilistic modeling of the sprinkling process. In constructing the model, the event combining theorem and the Lyapunov theorem were used. As the example, analysis of the operation of twelve sprinklers was carried out. The presented computational experiment was performed to optimize the positioning of the apparatuses according to the criteria of irrigation uniformity and the coefficient of ac-counting completeness of water, which falls on the test site. The obtained results can be used in the process of optimizing the placement of vehicles on «Volzhanka» and «Dnepr» machines. Probabilistic mathematical models of the sprinkling process make it possible to optimize the positioning of apparatuses according to the criteria of uniform irrigation. The programs for modeling water distribution by devices from four positions are applicable only when the distance between the positions is greater than the radius of the sprinkling zone. Irrigation uniformity indicators do not meet agrotechnical requirements. Optimization of the positioning of the apparatus in twelve positions provides excellent indicators for irrigation uniformity. The optimization programs and techniques that were used in the study are applicable to optimize the distribution of other liquids in agricultural technologies, for example, for the distribution of pesticides.

* The reported study was funded by RFBR according to the research project № 19-07-00623.
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Keywords: calculation of uniformity indicators, sprinkling uniformity, irrigation uniformity, Christiansen uniformity coefficient, effective irrigation coefficient, insufficient irrigation coefficient, excess irrigation coefficient.

Introduction. The purpose of the research is to design probabilistic model of the sprinkling process. That model is in relation to the probabilistic similarity to the simulated process, the numerical implementation of which is presented in the form of software that calculates matrix of irrigation doses in the irrigation zone, or at test site according to the water flow through the apparatus and statistical characteristics of the jet, performing imitation of the movement of the machine and the overlapping of zones from several vehicles, calculating indicators of irrigation uniformity at different steps of apparatus installation, issuing the result in the form of matrices or graphs.

The objective function of the sprinkling system is to reduce the unproductive water consumption while maintaining the irrigation rate by optimizing the sprinkling process using probabilistic modeling. Sprinklers do not require field layout. Some of them work with slopes of 0.05 and more. Exceeding the sprinkling intensity as compared with the soil absorbency in such field leads to flooding of some sites, to surface runoff, that is, to the increase of unproductive consumption of the most important natural resource and soil erosion, causing environmental damage to reservoirs that receive waste water, and reduction of crop yields and others.

Materials and methods. The study was performed using system analysis and probabilistic modeling. The uniform distribution of fluid over the area until 2004 was estimated by the RD 10.11.1–9-89 by the effective irrigation coefficient, insufficient irrigation coefficient, and excessive irrigation coefficient. After the introduction of the interstate standard ISO 7749-2-2004 it is estimated by the Christiansen coefficient.

Research results. The intensity of sprinkling should not exceed the absorbency of the soil. The effectiveness of the system is assessed by the compliance of the average dose, uniformity and intensity of sprinkling to the established standards. To assess the effectiveness of the system in the field the reporting area is to be indicated.

The size of the site is set by integers. The platform is divided into meter squares. There is set the cycles and calculated the coordinates of the middle of each meter square. According to the coordinates there is defined the distance of the squares to each of the devices involved in the irrigation of the test site. The distance matrix is used when calculating the sprinkling intensities from each apparatus. Intensities are summed to obtain an intensity matrix. By the intensity matrix, the uniformity index, the dose matrix, the average dose are calculated. The dosage matrix checks the fulfillment of the water intake condition and the absence of surface water flow. Calculation of the system performance indicators is conducted using software probabilistic process models that are designed further.

Defining the cycles of changing the distances between the devices, there is calculated the performance indicators for all values of the parameters A and B, optimal positioning of the devices is determined.

The most important step in system analysis is the design of adequate probabilistic models of the process. Improvement of the adequacy of the models is achieved using the statistical results of testing devices by the radial method.

Design, testing and adjustment of sprinkling machines are associated with significant labor and material resources, and take a lot of time. The use of computer-aided design systems for these purposes allows to accelerate the designing of machines, reduce costs [2].

The rotation of the apparatus is considered to be uniform, if in one cycle of pulsed movement the displacement is significantly less than the size of the sprinkling zone. The device operates in a circle or sector.

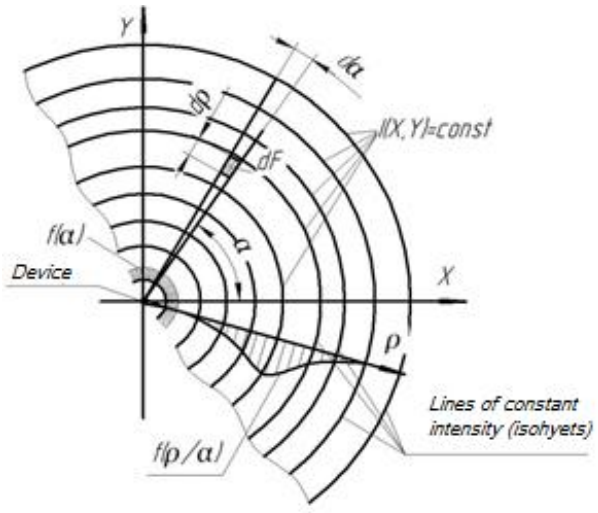


Fig. 1. Diagram of water distribution simulation with the sprinkling mashine

Sprinkler machines DShK-64A «Volzhanka» and DF-120 «Dnepr» work positionally. The Sprinkler machine DF-120 works from the hydrants located at distance of 54 meters. The pipeline is equipped with the flaps of 27 meters in length, at the ends of which medium jet sprinklers are installed. The layout of the apparatus during sprinkling can be represented as the rectangle with dimensions $A \times B$, where A is the distance between the apparatus on the pipeline; B is the distance between positions or flaps.

Stationary sprinkler systems have the same layout of the apparatus, therefore, the modeling of water distribution by such systems can be performed according to programs designed for positional action machines. For the programs to work, it is enough to obtain experimental data on the water distribution along the radii of the irrigation zone, the other characteristics are calculated by the simulation method.

Simulation is performed under the assumption of uniform rotation of the apparatus. In one cycle of impulse movement, the displacement is significantly smaller than the size of the sprinkling zone, therefore, after the overlapping of the sprinkling zones, the distribution of water is obtained in the same way as with uniform continuous rotation of the apparatus. The apparatus of such machines usually work in a circle.

Sprinklers create rain fan that irrigates circle on the field. The area that is irrigated by one apparatus is called the sprinkling zone.

Mathematical models of the process are presented under the following assumptions (Fig. 1) rain distribution by fan angle or circle is known and defined by empirical density of angle probability $f(\alpha)$ and flow Q; density of the water flow per angle unit equals to $q_\alpha = Q \cdot f(\alpha)$; the distribution of the flight distance of the droplets by radius is known and given by the empirical probability density of the distances $f(\rho)$; wind speed is zero; consumption Q and installation height of the devices are constant; the surface of the field is horizontal.

Let the device be in the center of the *XOY* coordinate system and work in a circle (Fig. 1). The position of the site dF is set in rectangular and polar coordinates. The need to have two coordinate systems is explained by the fact that the apparatus moves along angle and emits jet along radius, and the uniformity of rain must be determined by the area in rectangular coordinates.

Вероятность попадания жидкости на элементарную площадку dF, выделенную в зоне дождевания двумя радиусами с углом между ними $d\alpha$ и двумя окружностями с приращением радиуса $d\rho$, определится как произведение вероятностей попадания в диапазон угла $d\alpha$ и радиуса $d\rho$, т.е.

The probability of fluid entering elementary platform dF, that is marked in the sprinkling zone by two radii with the angle between them $d\alpha$ and two circles with increment of radius $d\rho$, is defined as the multiplication of the probabilities of falling into range of angle $d\alpha$ and radius $d\rho$, i.e.

$$P\{dF\} = f(\alpha) \cdot d\alpha \cdot f(\rho) d\rho .$$

The intensity of rain on the site is equal to the amount of water falling on it per unit of time divided by its area. With independent units ρ and α it is

$$I = \frac{Q \cdot f(\alpha) \cdot d\alpha \cdot f(\rho) \cdot d\rho}{\rho \cdot d\alpha \cdot d\rho} = \frac{Q \cdot f(\alpha) \cdot f(\rho)}{\rho} . \quad (1)$$

In the SI system, the sprinkling intensity is measured in kg/m^2·s, which is equivalent to such usual units for land reclamation as mm of layer per second.

Initially, in formula (1), on the basis of the Lyapunov limit theorem, the normal laws of the distribution of the angle and distance of the jet's flight were applied. Subsequently, any empirical distribution was approximated by the method of cubic spline interpolation and the resulting function was used to calculate the intensities by the formula (1)

The dose of irrigation of any site by the stationary device is determined by the multiplication of the intensity and the operating time *T*, i.e.

$$q_F = I \cdot T, кг / м^2 . \quad (2)$$

The rectangular coordinates of the site *dF* are related to the polar relations:

$$\begin{cases} X = \rho \cdot \cos\alpha \\ Y = \rho \cdot \sin\alpha . \end{cases} \quad (3)$$

Inkjet apparatus when working in a circle rotates uniformly, therefore, all values of the angle are equally probable and the probability density of the angle is determined by the formula

$$f(\alpha) = \frac{1}{2 \cdot \pi} . \quad (4)$$

The probability density of drops' flight distance of a single-nozzle apparatus, such as the «Rosa-1», is approximated by normal distribution law

$$f(\rho) = \frac{1}{\sigma_\rho \sqrt{2 \cdot \pi}} \exp(-\frac{(\rho - M_\rho)^2}{2 \cdot \sigma_\rho^2}), \quad (5)$$

where ρ is drops' flight distance; M_ρ, σ_ρ are mathematical expectation and standard deviation of drops' flight distance.

The probability density of drops' flight distance of apparatus with two nozzles is determined by the formula of the composition of the distribution laws

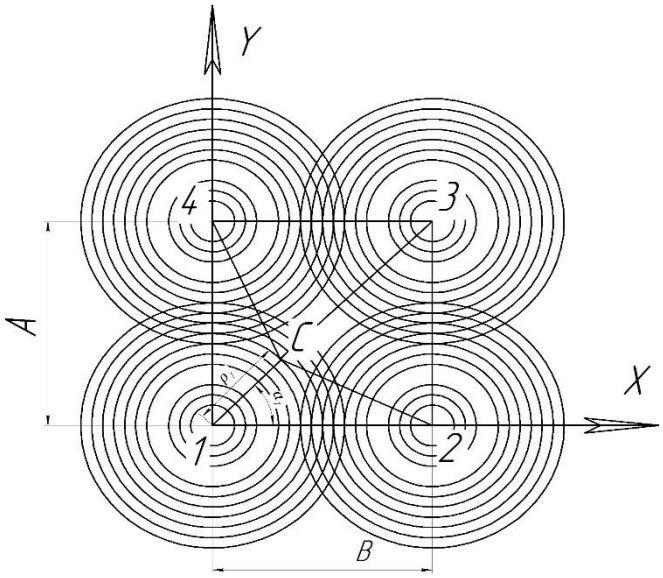


Fig. 2. Simulation scheme of water distribution by four sprinklers.

$$f(\rho) = \frac{C_1}{\sigma_{\rho 1} \sqrt{2 \cdot \pi}} \exp(-\frac{(\rho - M_{\rho 1})^2}{2 \cdot \sigma_{\rho 1}^2}) + \frac{C_2}{\sigma_{\rho 2} \sqrt{2 \cdot \pi}} \exp(-\frac{(\rho - M_{\rho 2})^2}{2 \cdot \sigma_{\rho 2}^2}, \quad (6)$$

where C_1, C_2 are weight coefficients; $M_{\rho 1}, \sigma_{\rho 1}$ are mathematical expectation and standard deviation of drops' flight distance from the first nozzle; $M_{\rho 1}, \sigma_{\rho 1}$ are mathematical expectation and standard deviation of drops' flight distance from the second nozzle.

The weight coefficients and numerical characteristics of the drops' flight distance are selected at modeling by the condition of the most uniform distribution of water by radius or by sprinkling area.

Further, there are proposed algorithms and programs for mathematical modeling and optimization of water distribution processes by stationary sprinklers or ones that are installed at positional action machine taking into account random and deterministic factors.

There is presented the modeling of water distribution using example of "Rosa-1" type irrigation system.

According to the technical characteristics of the device there is accepted $M_\rho = 11m$; $\sigma_\rho = 3,2m$; Q = 1,2 l/s.

The first device is located at the beginning of coordinates XOY, the second one is shifted along the X axis by distance B, the third one has coordinates of (B, A), the fourth one has coordinates of $(0, A)$.

For clarity of modeling, there were set the dimensions of the general sprinkling area and calculated the irrigation dose by all four devices using the designed algorithm (Fig. 3).

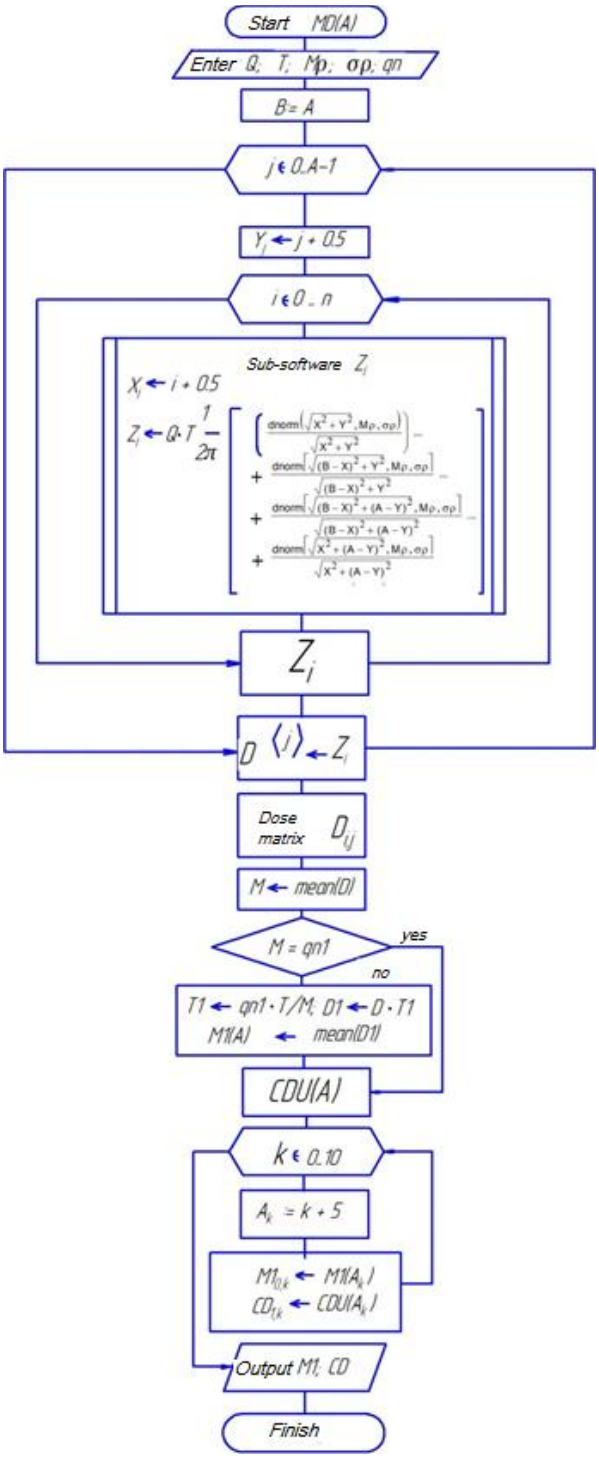


Fig. 3. Block diagram of calculation of doses and indicators of irrigation uniformity for four devices.

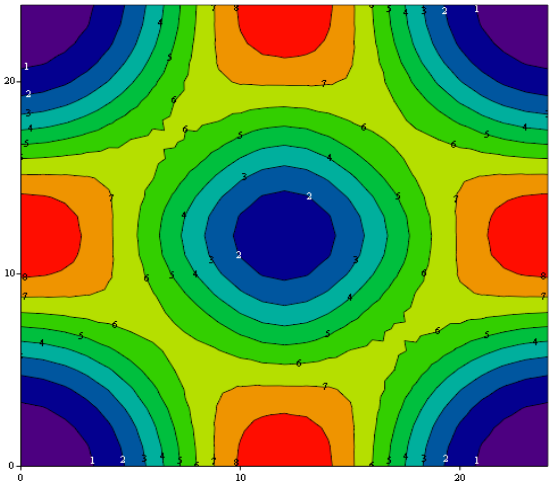


Fig. 4. The result of calculating the irrigation uniformity on the area irrigated by four devices at $A = B = 25$ m

To do this, the coordinates of the point *C(X, Y)* are set in the form of matrix with the step of one meter. Changing the distances between the devices, they were chosen under condition of more uniform water distribution. However, this task was quite difficult.

Quantitative assessment of uniformity on the rectangle area with dimensions *A* and *B* was performed using irrigation dose matrix. The limits of the *X*, *Y* coordinates are set so that the square area bounded by the lines connecting the points of location of the apparatuses is divided into meter sections. Doses of sprinkling are calculated in the center of each site.

Based on the calculation results, there were obtain a matrix of doses *MD* with the number of elements *A·B*. According to the dose matrix, there were calculated the variation coefficients, the minimum, average and maximum doses for different values of *A* and *B*. For calmness, it is logical to set $A = B$.

Variational series were compiled using dose matrices and the coefficients of effective, excessive and insufficient irrigation were calculated. The average dose was calculated by the matrix and compared with the value of

$$q_{Fsr} = \frac{Q \cdot T}{A \cdot B}. \qquad (7)$$

Studies have revealed the difficulty of obtaining uniform distribution of water with single-jet stationary devices. The coefficient of effective irrigation was much less agronomic standards. Over- and under-irrigation ratios were twice the agronomic standard.

To perform the optimization, dose calculation softwares were designed for squares bounded by lines connecting the points of location of the apparatuses [3].

The algorithm has two cycles of calculating the coordinates of meter squares. In the center of each square, irrigation dose of is calculated, matrix $M_{i,j}$ is created. Next, there are calculated the average value of the elements of the dose. Check is performed for the absence of wastewater, if necessary, the sprinkling time is recalculated or the water flow through the apparatus is adjusted.

If the distance between positions *A* is greater or equals to (Fig. 5, a) the maximum radius of sprinkling, then water from the four devices gets to the site *F*, bounded by lines connecting points 1,

2, 3, 4 of the devices' location. Its quantity is equal to the multiplication of flow through one apparatus at the sprinkling time.

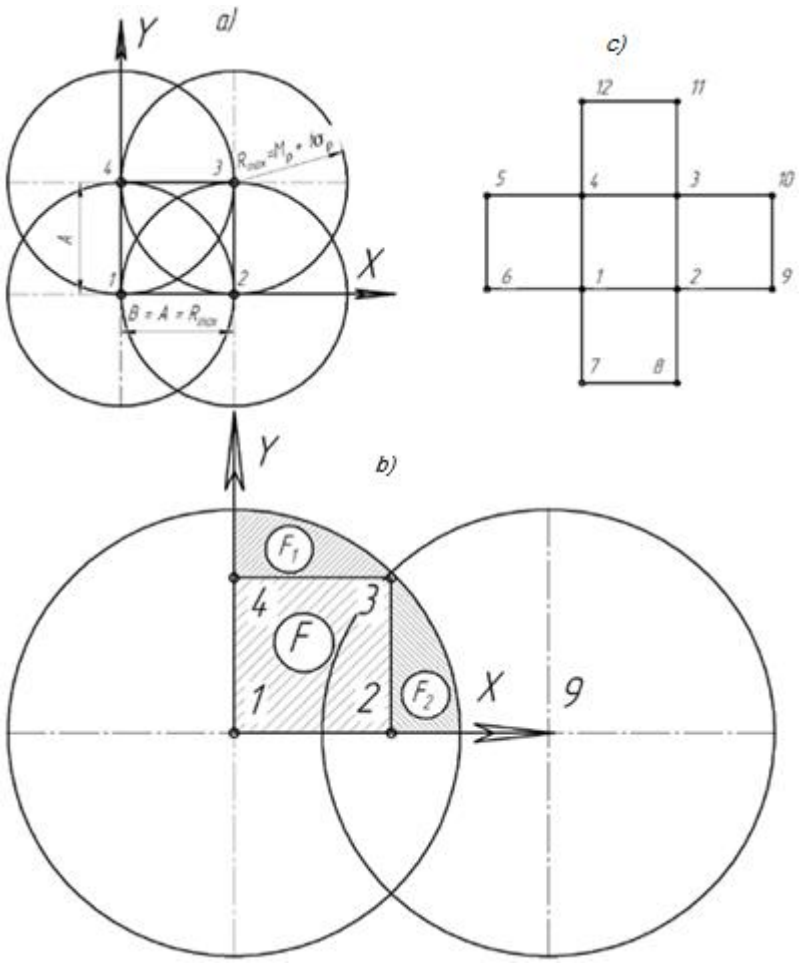


Fig. 5. Schemes of sprinkling model design

At site *F*, each device produces a fourth part of the flow, other devices do not participate in sprinkling the site. The models for calculating the sprinkling dose are relatively simple, the assessment of the irrigation uniformity of the entire field is the same as the test area *F*. However, as calculations presented, it is not possible to obtain distribution with a single-jet apparatus within limits. When the distance between the positions decreases (Fig. 5, b), the sprinkling area of the apparatus goes beyond the test site. The first apparatus has areas the water on which supplements the irrigation of adjacent areas irrigated with fourth and ninth positions (Fig. 6, c). In this case, accurate assessment of the sprinkling uniformity of the test site should be carried out taking into account the work of twelve vehicles according to Fig. 6, c.

The preliminary assessment can be performed on four devices, but to calculate the coefficient of completeness of accounting, that is equal to the ratio of the sum of doses on the test site to the product of the flow through one device for the watering time. The smaller this coefficient is than 1, the less reliable is the uniformity estimation. The data of the matrix shows that with A = 10 m the distribution is very uniform, although the overlap is large.

However, the coefficient of accounting completeness is less than 0.7, therefore it is necessary to develop modeling software from twelve positions. Previously it can be noted the possibility of uniform watering with single-jet sprinklers.

Software *MD12 (A)* is designed to calculate the dose of watering by twelve single-jet devices installed in the corners of the squares on the Fig. 5, c.

The test site is located between the devices 1, 2, 3, 4.

Software *Ke12 (A*) [4] includes software *MD12(A)* and according to the dose matrix there is performed calculations of the Christiansen, insufficient, effective and excessive irrigation coefficients and the coefficient of accounting completeness. The program is supplemented with cycle of changing the distance between the positions.

The output of the calculation results in the form of matrix (Fig. 6) allows to select the optimal distance between the positions of the devices.

$i := 0..4 \quad j := 0..8 \quad A_j := j + 9 \quad M_{i,j} := Ke12(A_j)_i \quad M_{5,j} := A_j$

$$M = \begin{pmatrix} 96.448 & 96.738 & 98.251 & 91.012 & 83.152 & 76.818 & 72.146 & 67.974 & 64.464 \\ 0 & 0 & 0 & 0 & 0.071 & 0.204 & 0.231 & 0.297 & 0.304 \\ 1 & 1 & 1 & 0.972 & 0.781 & 0.571 & 0.516 & 0.469 & 0.346 \\ 0 & 0 & 0 & 0.028 & 0.148 & 0.224 & 0.253 & 0.234 & 0.349 \\ 0.976 & 0.991 & 0.997 & 0.999 & 0.999 & 0.999 & 0.999 & 0.999 & 0.999 \\ 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 & 17 \end{pmatrix} \begin{pmatrix} CDU \\ Knd \\ Kef \\ Kiz \\ Ky \\ A \end{pmatrix}$$

Fig. 6. Matrix of calculation results of uniformity indicators of water distribution by single-jet apparatus

Matrix in Fig. 6 shows that a single-jet apparatus distributes irrigation water in accordance with agrotechnical requirements only when the distance between positions is less than 13.5 m. In this case, the Christiansen coefficient is about 80%. The calculations were performed with the expectation of the drops' flight distance of 10 m and the standard deviation of the distances of 3 m. Insufficient watering under the vehicles was eliminated by the fact that the maximum intensity of the adjacent apparatus almost coincides with the point of the neighboring one. When the distance between the apparatuses is less than 13.5 m, the irrigation dose on all meter sites in the overlap zone equals to the agrotechnical limits $M(1 \pm 0,25)$. The coefficient of accounting completeness is equal to 0.997, which testifies to the full account of the water flow to the teating site from twelve devices. The possibility of uniform irrigation using single-jet sprinklers is proven, but the distance between the positions is close to the mathematical expectation of the drops' flight distance.

The designations in Fig. 6 are written at the right of the counting matrix: $M_{0,j}$ is the Christiansen ratio; $M_{1,j}$ is the underflow coefficient; $M_{2,j}$ is the coefficient of effective watering; $M_{3,j}$ is the coefficient of over-irrigation; $M_{4,j}$ is the coefficient of accounting completeness; A is the distance between the positions of the apparatus.

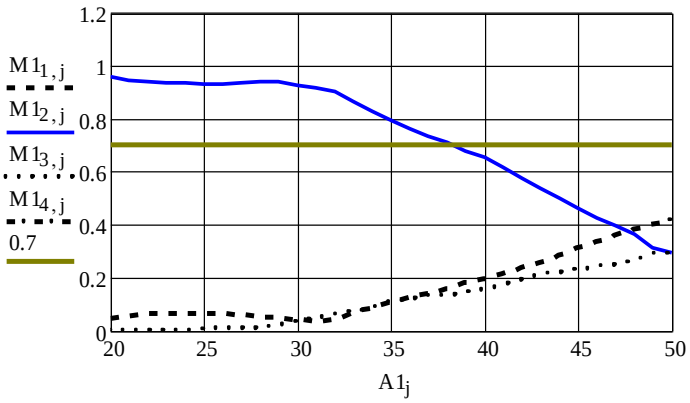
Fig. 6 shows that the coefficient of accounting completeness is very close to 1. The coefficient of effective irrigation is 0.7 and the coefficient of uniformity according to Christiansen is obtained of

0.8 when the apparatus is installed at step of 13.4 m, which is one meter more than at the evaluation of four positions.

M1 =

	18	19	20	21	
0	81.812	80.406	78.792	76.959	CDU
1	0.158	0.179	0.194	0.215	Knd
2	0.711	0.679	0.654	0.616	Kef
3	0.131	0.143	0.151	0.169	Kiz
4	1.777	1.797	1.818	1.838	Ky
5	38	39	40	41	A

$i := 0..3 \quad j := 0..30 \quad A1_j := j + 20 \quad M1_{i,j} := Ke2S12(A1_j)_i \quad M1_{5,j} := A1_j$



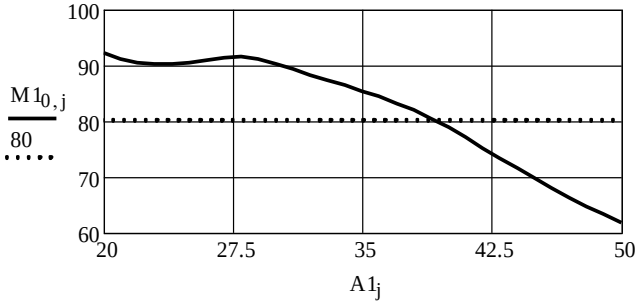


Fig. 7. Matrix of doses and graphs of indicators of uniform water distribution by a double-jet apparatus when working at twelve positions $M_{\rho 1} = 15m; \sigma_{\rho 1} = 5m; M_{\rho 2} = 7m, \quad \sigma_{\rho 2} = 2m; C_1 = 0,7; C_2 = 0,3.$

Next, simulation of the operation of the «Rosa-3» type apparatus was performed.

There was considered the work of the two main nozzles.

The following input data is accepted: $Q = 8l/s; \quad M_{\rho 1} = 15m; \quad \sigma_{\rho 1} = 5m; \quad M_{\rho 2} = 7m,$ $\sigma_{\rho 2} = 2m; \quad C_1 = 0,7; \quad C_2 = 0,3.$

Software $D1(A)$ calculates the matrix of doses of the two-jet apparatus.

Selection of weight coefficients, is conducted by mixing the two laws of normal distribution.

Along the lines of equal irrigation doses increase in the irrigation uniformity can be noted. Excess irrigation is observed on the horizontal and vertical lines connecting the centers of rotation

centers of the apparatuses, and there is insufficient irrigation at the intersection of the diagonals. The uniformity estimation showed that the effective irrigation coefficient is 0.893.

The use of additional nozzle to equalize the water distribution along the radii proved to be effective, the best simulation result was obtained.

The coefficient of effective watering is more than 0.7 with installation step of devices of less than 37 *m*. Uniformity according to Christiansen is more than 80% in the same range of distances between the apparatuses.

Discussion and conclusion. The method of modeling the water distribution by sprinklers can be used in the design of new and modernization of existing machines.

The considered examples can be used to optimize the placement of apparatus on «Volzhanka» and «Dnepr» machines.

According to the results of the work, number of conclusions can be formulated:

1. Probabilistic mathematical models of the sprinkling process make it possible to optimize the positioning of the apparatuses according to the criteria of irrigation uniformity.

2. Programs for modeling water distribution by devices from four positions are applicable only when the distance between the positions is greater than the radius of the sprinkling zone. In this case irrigation uniformity indicators do not meet agrotechnical requirements.

3. Optimization of the positioning of the apparatus in twelve positions provides excellent indicators of irrigation uniformity.

4. Optimization programs and techniques used in the research are applicable to optimize the distribution of other liquids in agricultural technologies, for example, for the distribution of pesticides.

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УДК 004.94 10.23947/2587-8999-2019-1-1-50-63

Вероятностное моделирование процессов дождевания*

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Статья посвящена разработке модели процесса дождевания, находящейся в отношении вероятностного подобия к моделируемому процессу, численная реализация которой позволяет выполнить расчет матрицы доз полива в зоне дождевания, или на зачётной площадке. Исследование выполнено с применением системного анализа и вероятностного моделирования. Равномерность распределения жидкости по площади до 2004 года на основании РД 10.11.1–9-89 оценивали коэффициентом эффективного полива, коэффициентом недостаточного полива, коэффициентом избыточного полива. После введения межгосударственного стандарта ИСО 7749-2-2004 – коэффициентом Христиансена. Разработаны новые математические модели и программное обеспечение для вероятностного моделирования процесса дождевания. При построении модели использовались теорема о совмещении событий и теорема А.М. Ляпунова. Для примера был проведен анализ работы двенадцати дождевальных аппаратов. Представленный вычислительный эксперимент выполнен для оптимизации позиционирования аппаратов по критериям равномерности орошения и по коэффициенту полноты учета воды, попадающей на зачетную площадку. Обсуждение и заключения. Полученные результаты могут быть использованы в процессе оптимизации размещения аппаратов на машинах «Волжанка» и «Днепр». Вероятностные математические модели процесса дождевания позволяют оптимизировать позиционирование аппаратов по критериям равномерности орошения. Программы моделирования распределения воды аппаратами с четырех позиций применимы только при расстоянии между позициями большем радиуса зоны дождевания. Показатели равномерности орошения при этом не соответствуют агротехническим требованиям. Оптимизация позиционирования аппаратов по

* Работа выполнена при частичной поддержке гранта РФФИ № 19-07-00623.
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двенадцати позициям дает отличные показатели по равномерности орошения. Программы и методики оптимизации, использованные при исследовании, применимы для оптимизации процессов распределения других жидкостей в агротехнологиях, например для распределения пестицидов.

Ключевые слова: расчет показателей равномерности, равномерность дождевания, равномерность полива, коэффициент равномерности Христиансена, коэффициент эффективного полива, коэффициент недостаточного полива, коэффициент избыточного полива.

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