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REGIMES OF A POPULATION DENSITY DESCRIBED BY A NONLINEAR REACTION-DIFFUSION MODEL

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Certain stationary and nonstationary solutions of a reaction-diffusion model are obtained. Results of a numerical simulation of problems involving boundary conditions of the first kind are presented. A classification of regimes of change in population density is determined.

Physicomathematical Statement of the Problem of Change in Population Density. Models described by a reaction-diffusion equation are widely used in physics, chemistry, biology, and ecology when the evolution of a population density is at issue [1-4]. In the present work we consider a model described by an equation of the form

$$\frac{\partial n}{\partial t} = \frac{\partial n}{\partial x}\left[D\frac{\partial n}{\partial x}\right] - an + bn^2 , \tag{1}$$

It is assumed that D has the following dependence on the concentration n [5]:

$$D = dn^{\delta} .$$

where for $\delta = 0$ we have the well-known linear case, i.e., the Kolmogorov–Petrovskii–Piskunov equation [6-12].

We will consider a boundary-value problem for a population density over the segment $0 \le x \le l$ with constant boundary conditions of the form

$$\begin{aligned} &n(0, t) = n_0 , \quad t \ge 0 ; \\ &n(l, t) = n_1 , \quad t \ge 0 . \end{aligned} \tag{2}$$

As the initial condition we take

$$n(x, 0) = n_1 , \quad 0 < x < l . \tag{3}$$

We introduce a dimensionless coordinate and time by making the replacement

$$x \Rightarrow lx , \quad t \Rightarrow \frac{l^2}{an_0^{\delta}} t ,$$

after which Eq. (1), boundary conditions (2), and initial conditions (3) take the form

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(u^{\delta}\frac{\partial u}{\partial x}\right) - \alpha u + \beta u^2 ; \tag{4}$$

$$\begin{aligned} &u(0, t) = 1 , \quad t \ge 0 ; \\ &u(1, t) = N , \quad t \ge 0 ; \end{aligned} \tag{5}$$

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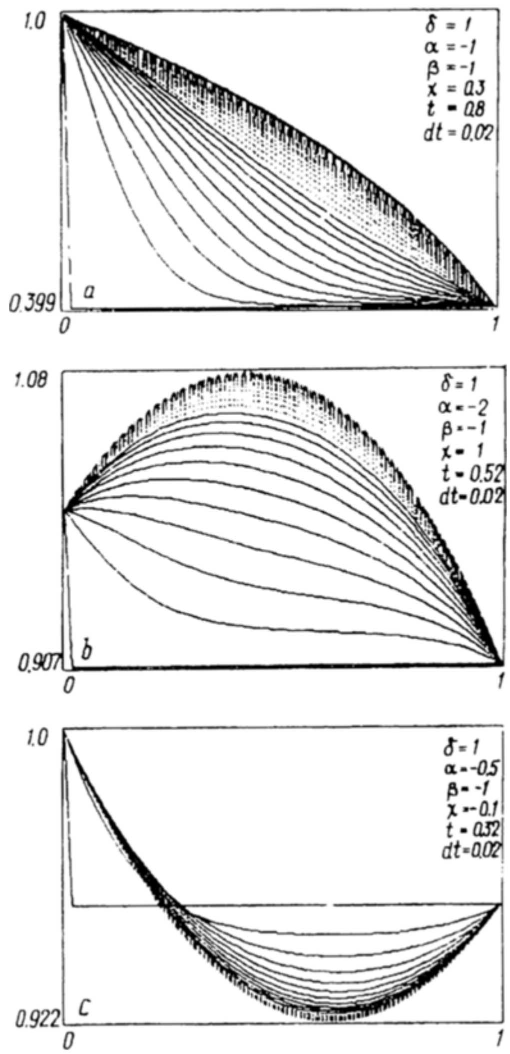

Fig. 1. Evolution of the dependence of the population density on the coordinate for the first (a), second (b), and the third (c) regimes of behavior; the population density and the coordinate are given in dimensionless variables.

$$u(x, 0) = N, \quad 0 < x < l, \tag{6}$$

where

$$N = \frac{n_1}{n_0}, \quad \alpha = \left(\frac{l^2}{n_0^{\delta} d}\right) a, \quad \beta = \left(\frac{l^2}{n_0^{\delta - 1} d}\right) b, \quad n = n_0 u.$$

Analysis of the Stationary Problem. Let us consider the stationary equation

$$\frac{d}{dx}\left(u^{\delta}\frac{du}{dx}\right) + \alpha u - \beta u^2 = 0, \tag{7}$$

which corresponds to the nonstationary equation (4) with boundary conditions (5). It is evident that this equation has the trivial solution $u = 0$ under the corresponding boundary conditions. We will seek solutions of Eq. (7) differing from the trivial one.

Equation (7) can be integrated once using the replacement

$$\frac{du}{dx} = y(u) . \tag{8}$$

After integration, taking account of Eq. (8), we obtain

$$\left(\frac{du}{dx}\right)^2 = y^2(u) = \frac{2\alpha}{\delta + 2} u^{2-\delta} - \frac{2\beta}{\delta + 3} u^{3-\delta} + \frac{\chi}{u^{2\delta}} . \tag{9}$$

In the general case integration of relation (9) proves to be difficult. However, it is to be noticed that this relation coincides with the equation of one-dimensional motion of a mass point with zero energy in the potential [13]

$$V(u) = -\left(\frac{2\alpha}{\delta + 2} u^{2-\delta} - \frac{2\beta}{\delta + 3} u^{3-\delta} + \frac{\chi}{u^{2\delta}}\right) .$$

Now we will introduce the new variables z and ξ, connected with the variables u and x by the relations

$$u = \left|\frac{\alpha}{\beta}\right| \frac{\delta + 3}{\delta + 2} z , \quad x = \sqrt{\left(\frac{1}{2} \left(\frac{\delta + 3}{|\beta|}\right)^{\delta} \left(\frac{|\alpha|}{\delta + 2}\right)^{\delta - 1}\right)} \, \xi ,$$

and the constant c, connected with the constant χ by the relation

$$\chi = 2 \left(\frac{\delta + 3}{|\beta|}\right)^{\delta + 2} \left(\frac{|\alpha|}{\delta + 2}\right)^{\delta + 3} c .$$

Here it was assumed that the values of α and β were taken from the range of values for which the replacement is valid. When $\alpha > 0$ and $\beta > 0$, Eq. (9) is written in the form

$$\left(\frac{dz}{d\xi}\right)^2 = z^{2-\delta} - z^{3-\delta} + \frac{c}{z^{2\delta}} . \tag{10}$$

When

$$z = z_0 = \frac{\delta + 2}{\delta + 3} , \quad c = c_0 = \frac{(\delta + 2)^{\delta + 2}}{(\delta + 3)^{\delta + 3}} , \quad u = u_0 = \frac{\alpha}{\beta} \tag{11}$$

the potential

$$V(z) = z^{3-\delta} - z^{2-\delta} - \frac{c}{z^{2\delta}}$$

and its first derivative vanish.

For further analysis, it is convenient to replace one of the boundary conditions (at the right end) by the condition for the constant $\chi(c)$, taking into account the corresponding sign of the derivative at the left end. In such a statement the problem corresponds to the Cauchy problem and is completely analogous to that of the motion of a point of mass 0.5 with zero energy in potential (11) with initial conditions of the form

$$z(0) = z_0 = \frac{\delta + 2}{\delta + 3} \left|\frac{\alpha}{\beta}\right| , \quad \frac{dz}{d\xi}(0) = \sqrt{\left(z_0^{2-\delta} - z_0^{3-\delta} - \frac{c}{z_0^{2\delta}}\right)} ,$$

and, moreover, the value of z_0 must lie in the "classically accessible region" of the potential $V(z)$, which is achieved by the corresponding choice of the constant c.

Now we consider cases where $\chi(c)$ takes certain values. Let $\delta = 1$, since the solution of Eq. (10) for $\delta \neq 1$ is the same. Then Eq. (10) for $\delta = 1$ will be written in the form

$$\left(\frac{dz}{d\xi}\right)^2 = z - z^2 + \frac{c}{z^2},$$

while the constants z_0, u_0, c_0, and χ_0 take the following values:

$$z_0 = \frac{3}{4}, \quad c_0 = \frac{27}{256}, \quad u_0 = \left|\frac{\alpha}{\beta}\right|, \quad \chi_0 = \frac{1}{6}\frac{|\alpha|^4}{|\beta|^3}.$$

Several cases are possible in the analysis. We consider each of them separately.

First we assume that the constants α and β are positive.

1) When $c < -c_0$ there is no solution.

2) At $c = -c_0$ there is a single solution coinciding with the trivial one $u = |\alpha|/|\beta|$.

3) When $-c_0 < c < 0$ a periodic solution can exist in the region $z_1 \leq z \leq z_2$, where z_1 and z_2 are the roots of the equation

$$z - z^2 + \frac{c}{z^2} = 0, \quad 0 < z_1 < z_2. \tag{12}$$

The period of the solution along the x axis is determined from the formula

$$T_x = \sqrt{\left(\frac{2}{|\beta|}\right)}\, 2 \int_{z_1}^{z_2} \frac{dz}{\sqrt{\left(z^2 - z - \frac{c}{z^2}\right)}}.$$

Here the boundary conditions at the left end should be chosen from the region $(z_1; z_2)$.

4) At $c = 0$ Eq. (9) can be integrated, and the solution obtained has the form

$$u(x) = \frac{4\alpha}{3\beta} \cos^2\left(\sqrt{\left(\frac{|\beta|}{2}\right)}\, \frac{x - x_0}{2}\right), \tag{13}$$

where x_0 is a constant determined from the boundary condition at the left end.

We will consider the stability of solution (13). Let us take a small perturbation and expand it in a Fourier series in time and space:

$$\delta u(x, t) = \sum_{k,\omega} \delta u_{k,\omega} e^{ikx - i\omega t},$$

Substituting the perturbed solution into Eq. (4) and making use of the fact that a nonperturbed function is a solution of (7), we obtain that harmonics for which $|\beta| < k$ will be damped.

5) When $c > 0$, a solution of the problem exists if $z < z_3$, where z_3 is the positive root of Eq. (12). At $z = z_3$, the solution can have a turning point. The boundary condition at the left end is chosen from the region $z \leq z_3$.

Now we consider cases where the constants α and β are negative. Equation (10) will be written in the form

$$\left(\frac{dz}{d\xi}\right)^2 = z^2 - z + \frac{c}{z^2}. \tag{14}$$

1) When $c > c_0$, a solution exists if the boundary condition at the left end is arbitrarily prescribed and $z > 0$.

2) At $c = c_0$ a solution exists if the boundary condition at the left end is arbitrarily prescribed and $z > 0$. The potential

$$V(z) = z^2 - z - \frac{c}{z^2}$$

has a second-order zero at the point $z = z_0$, and Eq. (14) will be written as

$$\left(\frac{dz}{d\xi}\right)^2 = (z - z_0)^2 p(z),$$

where $p(z)$ has no singularities at $z = z_0$. There is the unstable solution $u = |\alpha| / |\beta|$.

3) When $0 < c < c_0$, no solution exists if $z_1 < z < z_2$, where z_1 and z_2 are the roots of the equation

$$z - z^2 - \frac{c}{z^2} = 0, \quad 0 < z_1 < z_2. \tag{15}$$

At the points z_1 and z_2 the solution can have turning points. The boundary condition at the left end is chosen outside the region $(z_1; z_2)$.

4) At $c = 0$ Eq. (9) can be integrated, and the solution takes the form

$$u(x) = \frac{4|\alpha|}{3|\beta|} \operatorname{ch}^2 \left(\sqrt{\left(\frac{|\beta|}{2}\right)} \frac{x - x_0}{2}\right), \tag{16}$$

where the constant x_0 is determined from the boundary condition at the left end.

5) When $c < 0$, the region $z_3 \le z$ is accessible for the solution, where z_3 is the positive root of Eq. (15). At the point $z = z_3$ the solution can have a turning point. The boundary condition at the left end should not be situated in the region $z \ge z_3$.

Solution of the Stationary Equation in the Case $\delta = -1$. This solution is of purely theoretical interest.

For $\delta = -1$, under the square root sign of Eq. (9) we can factor a perfect square, and this equation takes the form

$$\frac{du}{dx} = \pm (au^2 - bu),$$

where

$$a = \sqrt{|\beta|}, \quad b = \frac{|\alpha|}{\sqrt{|\beta|}}, \quad \chi = \frac{\alpha^2}{|\beta|}.$$

Here we assume that $\alpha < 0$ and $\beta < 0$. Integrating this equation, we obtain the solution

$$u(x) = \frac{|\alpha|}{\sqrt{|\beta|}\left(|\beta| + \exp\left(\pm \frac{|\alpha|(x - x_0)}{\sqrt{|\beta|}}\right)\right)},$$

where x_0 is the integration constant. This solution corresponds to a stationary shock wave.

Certain Analytical Solutions of the Nonstationary Problem. We will consider the problem of the eigenfunctions and eigenvalues for the operator

$$L(u) = \frac{d}{dx}\left(u^{\delta}\frac{du}{dx}\right) - \beta u^2,$$

that corresponds to the boundary-value problem (7). Here the constant α plays the part of the eigenvalue and the boundary conditions are taken in accordance with the initial problem (5). The solution u depends parametrically on α.

Let the solution of Eq. (7) be represented in the form

$$u(x, g(t)) = g(t) f(x),$$

where $f(x)$ is a function independent of α (as the function $f(x)$ we can take functions corresponding to the solutions (13) and (16)) and $g(t)$ depends on time. Then Eq. (4) will be written as

$$\frac{dg(t)}{dt} = (g(t) - \alpha) g(t).$$

The solution of this equation has the form

$$g(t) = \frac{\alpha}{1 + \exp(\alpha(t - t_0))},$$

where t_0 is the integration constant. The solution of the nonstationary equation is obtained in the form

$$u(x, t) = \frac{\alpha f(x)}{1 + \exp(\alpha(t - t_0))}.$$

Taking into account stationary solutions of the type of (13) and (16), we have

$$u(x, t) = \frac{\alpha}{1 + \exp(\alpha(t - t_0))}\frac{4}{3\beta}\operatorname{ch}^2\left(\sqrt{\left(\frac{|\beta|}{2}\right)}\frac{x - x_0}{2}\right),$$

$$u(x, t) = \frac{\alpha}{1 + \exp(\alpha(t - t_0))}\frac{4}{3\beta}\cos^2\left(\sqrt{\left(\frac{|\beta|}{2}\right)}\frac{x - x_0}{2}\right).$$

It should be noted that these solutions exist only for the corresponding assignment of the initial condition.

Method of Mathematical Simulation. Numerical solution of the stationary problem (7) was performed under an initial condition of the form $u(0) = 1$ with a prescribed value for the constant χ that replaced the second boundary condition. The equation was solved by the Runge–Kutta method of the fourth order of accuracy.

Nonstationary problem (4)-(6) was solved numerically with the use of the following implicit difference scheme [14]:

$$\frac{u_j^{n+1} - u_j^n}{\tau} = \frac{1}{h^2}\left(\left(\frac{u_{j+1}^{n+1} + u_j^{n+1}}{2}\right)^{\delta}(u_{j+1}^{n+1} + u_j^{n+1}) - \left(\frac{u_j^{n+1} + u_{j-1}^{n+1}}{2}\right)^{\delta}(u_j^{n+1} - u_{j-1}^{n+1})\right) -$$

$$- \alpha u_j^{n+1} + \beta(u_j^{n+1})^2, \quad 0 < j < J, \quad 0 \le n,$$

where u_j^n is the population density at the j-th point on the n-th temporal layer. The scheme is absolutely stable, and therefore the values of the time τ and space h intervals were selected on the basis of the best approximation.

At each time step we solved the system by the iterative process

$$\frac{u_j^s - u_j^{\text{old}}}{\tau} = \frac{1}{h^2}\left(\left(\frac{u_{j+1}^{s-1} + u_j^{s-1}}{2}\right)^{\delta}(u_{j+1}^s - u_j^s) - \left(\frac{u_j^{s-1} + u_{j-1}^{s-1}}{2}\right)^{\delta}(u_j^s - u_{j-1}^s)\right) - \alpha u_j^s + \beta u_j^s u_j^{s-1},$$

where u_j^s is the value of the desired function on the next temporal layer at the s-th iteration; as a zero iteration we took the value of the function on the previous temporal layer u_j^{old}. The iterations were calculated by the pivot method [15, 16]. The initial and boundary conditions were prescribed in the form

$$u_0^n = 0, \quad 0 \le n;$$

$$u_J^n = N, \quad 0 \le n;$$

$$u_j^0 = N, \quad 0 \le j \le J.$$

The calculation was carried out in the following order. First we prescribed the boundary condition at the left end ($u(0) = 1$), the value of the constant χ, and the sign of the derivative at the point $x = 0$, and then we solved Eq. (9) by the Runge–Kutta method. The value of the function at the right end u determined in this way was taken as the second boundary condition and initial data for the evolution problem (4)-(6), which then was solved. In all the cases for simplicity of calculations we took $\delta = 1$. The calculations were performed for different regimes specified by the values of α and β and the value of the constant χ. In all calculations with stationary boundary conditions the solution of the evolution problem approached the solution of the stationary problem (9) obtained by the Runge–Kutta method.

Results of Numerical Simulation. Results obtained by numerical simulation of the processes of evolution of the population density are given in Fig. 1. Each graph displays several distributions of the population density over the coordinate at equal time intervals. It is evident how the initial distribution of the population density goes over into a stationary distribution. On each graph the value of α, β, and χ are indicated for which the calculation was performed as well as the time t up to which the evolution problem (4)-(6) was calculated and the time intervals dt at which the given graphs were obtained.

It is established that a solution has one of four characteristic regimes of behavior.

The first regime (Fig. 1a). The solution attains a stationary distribution; the value at each point does not exceed the maximum value at the ends and is not smaller than the minimum one. In this case the spatial derivative has the same sign everywhere. This regime can be realized in any of the cases in which a solution exists.

The second regime (Fig. 1b). The solution attains a stationary distribution that exceeds the maximum one from the boundary conditions, i.e., protrusion of the density above the boundary values is observed. This regime can be realized when $\alpha > 0$ and $\beta > 0$, if $\chi > -\chi_0$, and when $\alpha < 0$ and $\beta < 0$, if $0 < \chi < \chi_0$.

The third regime (Fig. 1c). The solution attains a stationary distribution that at certain points is smaller than the minimum value at the boundary, i.e., a "dip" in the density below the boundary values occurs. This regime can be realized when $\alpha > 0$, $\beta > 0$, and $-\chi_0 < \chi < 0$ and when $\alpha < 0$, $\beta < 0$, and $\chi_0 < \chi$.

The fourth regime. The solution attains a constant. This regime is realized when $\alpha > 0$, $\beta > 0$, and $\chi = -\chi_0$ and when $\alpha < 0$, $\beta < 0$, and $\chi = \chi_0$ under the corresponding boundary conditions.

NOTATION

n, population density; a, b, d, α, β, and N, constant coefficients; D, diffusion coefficient; t, time; x, coordinate; δ, positive quantity characterizing the dependence of the diffusion coefficient on the population density; χ and c, integration constants; u and z, dimensionless population densities; ξ, dimensionless coordinate; u_j^n, value of the population density at the j-th point on the n-th temporal layer; τ, time step of the grid; h, spatial step of the grid; u_j^s, value of the population density on the next temporal layer at the s-th iteration.

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