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NUMERICAL STUDY OF A MATHEMATICAL MODEL OF AN AUTOCATALYTIC REACTION WITH DIFFUSION IN A TUBULAR REACTOR

O. V. Gavrilova, South Ural State University, Chelyabisk, Russian Federation, gavrilovaov@susu.ru

The article analyzes analytically and numerically the model of the autocatalytic reaction with diffusion in the degenerate case on a finite connected directed graph **G** with the Showalter – Sidorov condition. The mathematical model of the autocatalytic reaction with diffusion is based on the system of distributed Brusselator equations. The system of degenerate equations of a distributed Brusselator whose functions satisfy the conditions of continuity and flow balance belongs to a wide class of semilinear Sobolev type equations. To investigate the existence of a solution of this system of equations, the phase space method which was developed by G. A. Sviridyuk and his students to study the solvability of Sobolev type equations will be used. We will show the simplicity of the phase space and the existence of a unique local solution of the given Showalter – Sidorov problem. The theoretical results of this article served as the basis for developing an algorithm for numerical study of the model in a Maple environment. The algorithm of numerical investigation is based on the Galerkin method, which allows us to take into account the phenomenon of degeneracy of the equation. The article gives several examples illustrating the results of the computational experiment obtained on the three-ribbed and five-ribbed graphs.

Keywords: Sobolev type equation; Brusselator; Showalter – Sidorov problem; reaction-diffusion models; local solution.

Introduction

In 1958, A. A. Belousov published a report on an unusual chemical reaction of citric acid oxidation with potassium bromate in the presence of a catalyst – three- and four-valence cerium vapor. The unusuality of that reaction was that the reagents, instead of reacting with the formation of a new substance, created a kind of chemical clock: namely, the solution with reagents periodically changed color from red to blue and vice versa. The work of Belousov was continued and developed by A. M. Zhabotinsky, who discovered the appearance of spiral waves in an initially homogeneous chemical mixture. To date, many Belousov – Zhabotinsky reactions are known, which usually occur at 25° C in a reaction mixture consisting of potassium bromate, malonic or bromo-malonic acid and cerium sulfate or an equivalent substance soluble in citric acid. The research works on the reactions mechanism resulted in arising of ordered temporal and (or) spatial structures arise, and after that some mathematical models were obtained in the form of reaction-diffusion equations

$$\begin{cases} \varepsilon_1 v_t = \alpha\Delta v + f(v,w), \\ \varepsilon_2 w_t = \beta\Delta w + g(v,w). \end{cases} \tag{1}$$

Here, $v = v(s,t)$ and $w = w(s,t)$ are the functions characterizing the reagent concentrations; the first summands on the right sides of the equations, according to Fick's law, characterize the diffusion of the reagents ($\alpha, \beta \in \mathbb{R}_+$ are the diffusion coefficients), the vector functions f and g are responsible for the interaction of the reagents.

At the present time, the studies of self-organization phenomena in various nonequilibrium systems, consisting in the occurrence and evolution of ordered space-time structures are carried out. An example of the latter can serve are autowaves, which are formed in excitable media in response to an external disturbance. There are many examples of excitable media: nerve and muscle tissues, colonies of microorganisms, a number of chemical solutions and gels, magnetic superconductors with current, and some solid-state systems [1–4].

System of equations (1) has been studied in various aspects, and in many studies the case $\varepsilon_1 > 0$, $\varepsilon_2 > 0$ is discussed along with the case $\varepsilon_1 = 0$ or $\varepsilon_2 = 0$ [5]. The necessity of studying the case $\varepsilon_1 = 0$ or $\varepsilon_2 = 0$ is related to the fact that the rate of change of one of the components significantly exceeds the other. This leads to systems of equations of the form

$$\left\{ \begin{array}{l} v_t = \alpha\Delta v + f(v,w), \\ 0 = \beta\Delta w + g(v,w). \end{array} \right. \tag{2}$$

Equations (2) in the case when

$$\begin{array}{c} f(v,w) = \gamma - (\delta+1)v + v^2 w, \\ g(v,w) = \delta v - v^2 w, \end{array} \tag{3}$$

describe the distributed Lefebvre – Prigogine Brusselator [6], proposed as a model of an autocatalytic reaction with diffusion [7]

$$\left\{ \begin{array}{r} v_t = \alpha\Delta v + \gamma - (\delta+1)v + v^2 w, \\ 0 = \beta\Delta w + \delta v - v^2 w. \end{array} \right. \tag{4}$$

The parameters $\gamma, \delta \in \mathbb{R}_+$ characterize the concentrations of the initial reagents, which are assumed to be constant.

We will consider the chemical reactions taking place in a system of narrow long tubes (multidimensional tubular reactor), along which substances can diffuse, the ends of the tubes, as well as their walls, are impermeable for reacting substances. The mathematical model of this tubular reactor, with the specified parameters, is the finite connected oriented graph $\mathbf{G}$. Each function in the system of equation considered on the graph satisfies the continuity condition and the flow balance condition [8]. It should be noted that the reaction-diffusion equations on graphs have been studied poorly, mainly for linear systems [7].

In suitable constructed function spaces, the system of equations (4), where the functions satisfy the condition of continuity and balance of flows, is reduced to a semilinear Sobolev type equation

$$L\dot{u} = Mu + N(u), \ \ker L \neq \{0\}. \tag{5}$$

The classical initial condition for Sobolev type equations is the Cauchy condition

$$u(0) = u_0. \tag{6}$$

However, the consideration of condition (6) in the case of the degenerate equation (2) leads to the nonexistence of the solution for the derived initial values u_0. In [9] this phenomenon is studied in detail and it was shown that it is more natural to consider the initial Showalter – Sidorov condition for the degenerate equation (5)

$$L(u(0) - u_0) = 0, \tag{7}$$

than condition (6), and if the operator L is continuously invertible, then problem (7) is equivalent to problem (6) for equation (5). Thus, relying on the theory of relatively bounded operators or relative to sectorial operators, G. A. Sviridyuk, and later his successors [10, 11], found the conditions for the unique solvability of the problem (5), (7). In the case when the operator M is (L, p) sectorial and the phase space of the equation (5) is a simple Banach C^∞-manifold problem (5), (7) is uniquely solvable. A Banach C^∞-manifold is called simple if any of its atlas is equivalent to an atlas containing a single map. Also, it is worth mentioning about another important concept such as quasistationary (semi)trajectories passing through the point u_0, which pointwise lie in the phase space $\mathfrak{M}$ [12]. Any stationary trajectory of the equation (5) is quasistationary, but the converse is not true. In particular, if the operator M is $(L, 0)$ sectorial, then any solution (5), (7) is a quasistationary (semi)trajectory. However, the phase space of equation (5) may be not simple, then the solution of Showalter–Sidorov problem (7) for semilinear Sobolev type equations (5) is non-unique. It was shown in the papers [13, 14] that the Showalter – Sidorov problem for the Korpusov – Pletner – Sveshnikov equation can have two different solutions, and for the Plotnikov equation system – three. In addition, it should be noted that in the degenerate case (i.e. $\varepsilon_1 = 0$ or $\varepsilon_2 = 0$) the phase space of the system of equations (1) contains features such as the assemblies and folds of Whitney [15], therefore, can have one or more solutions or a solution may not exist.

Since the article besides theoretical studies also contains the results of numerical experiments, here it is necessary to mention the Galerkin method, which is the basis of computational experiments. Obtaining an analytical solution for Sobolev type equations (5) is not always possible, so the construction of algorithms for numerical methods of the problems being studied is in demand. In the case of degenerate semilinear equations, the Galerkin method is the most suitable, as it allows us to take into account the degeneracy of the equations for certain parameters. Using the Galerkin method, approximate solutions of models are constructed which coefficients satisfy a system of algebra-differential equations with the corresponding initial conditions [16, 17].

We will research the system of equations (4) on a finite connected oriented graph $\mathbf{G}$ with the Showalter – Sidorov condition (7). The simplicity of the phase space and the existence of a unique local solution of this problem will be shown. To illustrate the results obtained, examples will be given on the three-ribbed and five-ribbed graphs.

1. Formulation of the Problem

Let $\mathbf{G} = \mathbf{G}(\mathfrak{V}; \mathfrak{E})$ be a finite connected oriented graph, where $\mathfrak{V} = \{V_i\}$ is set of vertices, and $\mathfrak{E} = \{E_j\}$ is the set of arcs. Each arc E_j has the length $l_j > 0$ and the area cross section $d_j > 0$. On the graph $\mathbf{G}$ we consider the system of equations distributed of Brusselator:

$$\begin{cases} v_{jt} = \alpha v_{jss} + \gamma - (\delta + 1)v_j + v_j^2 w_j, \\ 0 = \beta w_{jss} + \delta v_j + v_j^2 w_j, \end{cases} \tag{8}$$

where each function $v_j = v_j(s,t)$ and $w_j = w_j(s,t), s \in (0, l_j)$ and $t \in \mathbb{R}_+$, satisfies the continuity condition

$$\begin{gathered} v_j(0,t) = v_k(0,t) = v_m(l_m,t) = v_n(l_n,t), \\ w_j(0,t) = w_k(0,t) = w_m(l_m,t) = w_n(l_n,t), \\ E_j, E_k \in E^\alpha(V_i), \\ E_m, E_n \in E^\omega(V_i), \end{gathered} \tag{9}$$

and flow balance condition

$$\begin{gathered}\sum_{E_j\in E^{\alpha}(V_i)} d_j v_{js}(0,t) - \sum_{E_j\in E^{\omega}(V_i)} d_j v_{js}(l_j,t) = 0,\\ \sum_{E_j\in E^{\alpha}(V_i)} d_j w_{js}(0,t) - \sum_{E_j\in E^{\omega}(V_i)} d_j w_{js}(l_j,t) = 0,\end{gathered} \tag{10}$$

where $E^{\alpha(\omega)}(V_i)$ denotes the set of edges with the beginning (end) at the vertex V_i. Based on the results obtained in [8], we introduce the set $L_2(\mathbf{G}) = \{g = (g_1, g_2, \ldots, g_j, \ldots) : g_j \in L_2(0,l_j)\}$. The set $L_2(\mathbf{G})$ is a Hilbert space with a scalar product $\langle g, h\rangle = \sum\limits_{E_j\in\mathfrak{E}} d_j \int\limits_0^{l_j} g_j h_j ds$.
We denote by $\mathfrak{R}$ the set $\mathfrak{R} = \{r = (r_1, r_2, \ldots, r_j, \ldots) : r_j \in W_2^1(0,l_j)$ and (9) $\}$ is satisfied. The set $\mathfrak{R}$ is a Banach space with norm $\|r\|^2_{\mathfrak{R}} = \sum\limits_{E_j\in\mathfrak{E}} d_j \int\limits_0^{l_j} (r^2_{js} + r^2_j) ds.$

We identify $L_2(\mathbf{G})$ with its conjugate, and denote by $\mathfrak{K}$ the dual space $\langle\cdot,\cdot\rangle$ to $\mathfrak{R}$. We fix $\lambda \in \mathbb{R}_+$ and with the formula $\langle A\varphi, \psi\rangle = \sum\limits_{E_j\in\mathfrak{E}} d_j \int\limits_0^{l_j} (\varphi_{js}\psi_{js} + \lambda\varphi\psi) ds$ define the operator $A : \mathfrak{R} \to \mathfrak{K}$.

In the paper [18] it was shown that the spectrum of the operator A is real, discrete, finite-fold and condensed only to $+\infty$. We construct the operator $B = A - \lambda\mathbb{I}$, then the operator $B \in \mathcal{L}(\mathfrak{R}; \mathfrak{K})$, and the spectrum $\sigma(B)$ of the operator B is discrete, finite and is condensed only to $+\infty$.

For reduction (8) – (10) to equation (5), we construct a Banach space

$$\mathfrak{H} = \{h = (h_1, h_2, \ldots, h_j, \ldots) :\ h_j \in W_2^2(0,l_j) \text{ and satisfies (9), (10)}\}$$

with the norm $\|h\|^2_{\mathfrak{H}} = \sum\limits_{E_j\in\mathfrak{E}} \int\limits_0^{l_j} (h^2_{jss} + h_{js} + h^2_j) ds.$

Denote by $\nu_k = -\lambda_k$, where $\lambda_k, k \in \{0\} \cup \mathbb{N}$ are the eigenvalues of the operator B. We construct the spaces $\mathfrak{U} = \mathfrak{F} = L_2(\mathbf{G}) \times L_2(\mathbf{G})$ with scalar product

$$[u, \zeta] = \langle v, \xi\rangle + \langle w, \eta\rangle,$$

where $u = col(v, w), \zeta = col(\xi, \eta)$ and define the operators

$$\begin{gathered}[Lu, \zeta] = \langle v, \xi\rangle,\ u, \zeta \in \mathfrak{U},\\ [Mu, \zeta] = \alpha\langle v_{ss}, \xi\rangle - \beta\langle w_{ss}, \eta\rangle,\ u, \zeta \in \mathfrak{H}.\end{gathered}$$

Lemma 1. [7] (i) *For any* $\alpha, \beta \in \mathbb{R}\backslash\{0\}$*, the operator* $L \in \mathcal{L}(\mathfrak{U}, \mathfrak{F})$, $\ker L = L_2(\mathbf{G}) \times \{0\}$*, and the operator* $M \in \mathcal{C}l(\mathfrak{U}; \mathfrak{F})$, dom $M = \mathfrak{H} \times \mathfrak{H}$.
(ii) *For any* $\alpha, \beta \in \mathbb{R}_+$*, the operator* M *is* $(L, 0)$*-sectorial.*

Remark 1. It should be noted that in the case of $(L, 0)$-sectoriality of the operator M, each solution of the problem (8) – (10) is a quasistationary trajectory [12].

We construct the operator

$$[N(u),\zeta] = \langle \gamma - (\delta+1)v + v^2 w, \xi\rangle + \langle \delta v - v^2 w), \eta\rangle$$

and let dom $N = L_4(\mathbf{G}) \times L_4(\mathbf{G}) = \mathfrak{U}_N$. Denote by $\mathfrak{U}_N^*$ the dual space to $\mathfrak{U}_N$ with respect to the duality $[\cdot,\cdot]$. By the Sobolev embedding theorem, there are dense and continuous embeddings

$$\mathfrak{H} \hookrightarrow \mathfrak{U}_N \hookrightarrow \mathfrak{U} \hookrightarrow \mathfrak{U}_N^*. \tag{11}$$

Lemma 2. *For any $\gamma, \delta \in \mathbb{R}$, the operator $N \in C^\infty(\mathfrak{U}_N; \mathfrak{U}_N^*)$.*

Proof. We show first that $N \in C(\mathfrak{U}_N; \mathfrak{U}_N^*)$. Indeed, by the Hölder's inequality and the continuity of the embedding $\mathfrak{U}_N \hookrightarrow \mathfrak{U}$, we have

$$|[N(u),\zeta]| \le (C_1 + C_2||u||_{\mathfrak{U}_N} + C_3||u||^3_{\mathfrak{U}_N})||\zeta||_{\mathfrak{U}_N},\ \zeta \in \mathfrak{U}_N$$

$$|[N'_u\zeta_1,\zeta_2]| \le (C_4 + C_5||u||^2_{\mathfrak{U}_N})||\zeta_1||_{\mathfrak{U}_N}||\zeta_2||_{\mathfrak{U}_N},\ \zeta_1,\zeta_2 \in \mathfrak{U}_N$$

where the constants $C_1, C_2, C_3, C_4, C_5 \in \mathbb{R}_+$ do not depend on u, nor on ζ, ζ_1, ζ_2, a N'_u is the Frechet derivative of the operator N at the point u. Similarly, the continuity of the second derivative is proved, the remaining ones are equal to zero. Thus, the inclusion $N \in C^\infty(\mathfrak{U}_N; \mathfrak{U}_N^*)$ is proved.

□

We construct an auxiliary interpolation space [19] $\mathfrak{U}_\alpha = \mathfrak{R} \times \mathfrak{H}$, by (11) we have dense and continuous embeddings

$$\mathfrak{H} \hookrightarrow \mathfrak{U}_\alpha \hookrightarrow \mathfrak{U}_N \hookrightarrow \mathfrak{U}, \tag{12}$$

then the operator $N \in C^\infty(\mathfrak{U}_\alpha; \mathfrak{U}_N^*)$. So, we reduced problem (8) – (10) to a semilinear Sobolev type equation (5).

2. Showalter – Sidorov Problem

We now turn to the problem (8) – (10) with Showalter – Sidorov condition (7). Condition (7) in this particular case will have the following form:

$$v(0) = v_0. \tag{13}$$

Thus, we are interested in the solvability of the problem (8) – (10), (13) for any $u_0 = col(v_0, w_0) \in \mathfrak{U}_\alpha$. The operator M is $(L,0)$-sectorial; hence, in our case all the solutions of the problem (8) – (10) are quasistationary trajectories passing through the point u_0, i.e. lie pointwise in the phase space

$$\mathfrak{M} = \{u \in \mathfrak{H} : \langle \beta w_{ss} + \delta v - v^2 w), \eta\rangle = 0\}.$$

Lemma 3. *For $\gamma, \delta \in \mathbb{R}$ and $\langle(\beta w_{ss} - v_0^2 w), \eta\rangle \ne 0$, then for any vector $v \in \mathfrak{U}_\alpha$ there exists a unique vector $w \in W_2^2(\mathbf{G})$ such that $u = col(v,w) \in \mathfrak{M}$.*

Proof. We construct an auxiliary operator $\langle D(w), \eta\rangle = \langle \beta w_{ss} - v^2 w), \eta\rangle$, $w, \eta \in W_2^2(\mathbf{G})$, dom $D = W_2^2(\mathbf{G})$, a $\langle\cdot,\cdot\rangle$ is the scalar product in $L_2(\mathbf{G})$.

Because the $|\langle D(w), \eta\rangle| \leq (C_1 + C_2||w||_{W_2^2(\mathbf{G})})||\eta||_{L_2(\mathbf{G})}$, where the constants $C_1, C_2 \in \mathbb{R}_+$ depends on β, δ, λ and does not depend on w, η.

Note that the operator $D : W_2^2(\mathbf{G}) \to L_2(\mathbf{G})$ is linear and by the hypothesis of the lemma $\ker D = \{0\}$, hence, the inverse operator D^{-1}: $L_2(\mathbf{G}) \to W_2^2(\mathbf{G})$ exists. Therefore, for any $v \in \mathfrak{U}_\alpha$ there exists a unique vector $w \in W_2^2(\mathbf{G})$ such that $u = col(v, w) \in \mathfrak{M}$.

□

Theorem 1. *Let $\gamma, \delta \in \mathbb{R}_+$ and $\langle(\beta w_{ss} - v_0^2 w), \eta\rangle \neq 0$. Then the phase the space of the equation* (8) *is a simple Banach C^∞-manifold $\mathfrak{M}$.*

Hence, by Theorem 1, Cauchy Theorem [20], and the classical result obtained in the paper [21], it follows that

Theorem 2. *Let the point $u_0 = (v_0, w_0) \in \mathfrak{M}$, where $\langle(\beta w_{ss} - v_0^2 w), \eta\rangle \neq 0$ for all $w, h \in \mathfrak{H} \setminus \{0\}$. Then there exists a unique local solution of the problem* (8) – (10), (13).

3. Numerical Experiment

Algorithm to found the approximate solution of the Showalter – Sidorov problem (8) – (10), (13) based on the modified Galerkin method was developed for illustrate the results of theoretical research.

We denote by $\sigma(A)$ the spectrum of the operator A, constructed in Section 1. We recall that the spectrum $\sigma(A)$ is nonnegative, discrete, finite-fold, and condensed only to ∞. Following the Galerkin method, we seek an approximate solution $\tilde{u} = (\tilde{v}, \tilde{w})$ of the problem (8) – (10) in the form of sums

$$\tilde{v}_i(s,t) = \sum_{l=1}^{n} v_i^l(t)\varphi_l(s), \quad \tilde{w}_i(s,t) = \sum_{l=1}^{n} w_i^l(t)\varphi_l(s),\ i = 1, ..., m,$$

where $\varphi_l(s)$ are the eigenfunctions of the operator A on the l-th edge of the graph.

To find the unknowns $v_i^l(t)$, substitute the Galerkin sums in the equation (5), and then multiply the resulting equation scalarly in $L_2(\mathbf{G})$ by the eigenfunctions $\varphi_l(s)$, we obtain a system of algebra-differential equations

$$\langle L\tilde{u}_t, \varphi_l\rangle + \langle M\tilde{u}, \varphi_l\rangle = \langle N(\tilde{u}), \varphi_l\rangle,\ l = 1, \dots n \tag{14}$$

with the conditions of Showalter – Sidorov

$$\langle v(0) - v_0, \varphi_l\rangle = 0. \tag{15}$$

Based on this algorithm, a program for the numerical solution of the (8) – (10), (13) problem in the Maple programming language was developed and implemented in the Maple 17.0 for Windows environment. The developed program functions as follows:

1. The numerical solution of the Showalter – Sidorov problem for the distributed brusselator (by default the Runge – Kutta method of 4 or 5 order is used) is found from the given coefficients on the basis of Galerkin's method.

2. A graphic representation of this approximate solution at the initial and final point in time is obtained.

The result of the program is shown in the examples.

Example 1. It is required to find a numerical solution of the problem (8) – (10), (13) for given coefficients $\gamma = 1$, $\alpha = 1$, $\beta = 1$, $\delta = \frac{1}{4}$ and $m = 3$ on the graph **G** (Fig. 1) consisting of three edges and four vertices $d_i = 1, l_i = \pi, i = 1, \ldots, 3$, $T = 1$, and initial functions

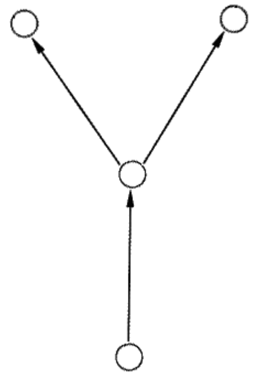

Fig. 1. Graph **G**

$$v_{01}(s) = \sqrt{\frac{2}{3\pi}}\left(\cos\left(\frac{7s}{2}\right) + \cos\left(\frac{5s}{2}\right) + \cos\left(\frac{3s}{2}\right)\right),$$
$$v_{02}(s) = -\left(\sqrt{\frac{2}{3\pi}} + 1\right)\left(\sin\left(\frac{7s}{2}\right) + \sin\left(\frac{5s}{2}\right) + \sin\left(\frac{3s}{2}\right)\right),$$
$$v_{03}(s) = \sin\left(\frac{7s}{2}\right) + \sin\left(\frac{5s}{2}\right) + \sin\left(\frac{3s}{2}\right).$$

The results of a numerical solution of a system of algebraic differential equations with initial conditions taken into account are presented in Table 1 (with an accuracy of 10^{-7}).

Table 1

The numerical solution of the problem

t	$v_1(t)$	$v_2(t)$	$v_3(t)$	$w_1(t)$	$w_2(t)$	$w_3(t)$
0	5,2554618	10,5109236	15,7663854	−0,0008576	0,0001728	0,0084892
0,1	3,0166314	2,7163826	1,2252387	0,0232671	0,0063418	0,0001835
0,2	1,7103189	0,6975324	0,0937483	0,0320726	0,0038489	0,0000780
0,3	0,9584756	0,1776861	0,0054537	0,0234993	0,0014607	0,0000127
0,4	0,5314025	0,0450486	−0,0013787	0,0141977	0,0004237	−0,0000070
0,5	0,2903006	0,0114000	−0,0019023	0,0079701	0,0001119	−0,0000095
0,6	0,1544920	0,0028831	−0,0019420	0,0042772	0,0000286	−0,0000098
0,7	0,0780490	0,0007290	−0,0019449	0,0021661	0,0000072	−0,0000099
0,8	0,0350308	0,0001843	−0,0019451	0,0009729	0,0000018	−0,0000099
0,9	0,0108238	0,0000466	−0,0019451	0,0003006	0,0000004	−0,0000099
1,0	−0,0027975	0,0000117	−0,0019451	−0,0000777	0,0000001	−0,0000099

Figs. 2, 3 illustrate the behavior of the model functions $v(s,t)$ and $w(s,t)$ on the first and the second edges of the graph at the initial and at the final time.

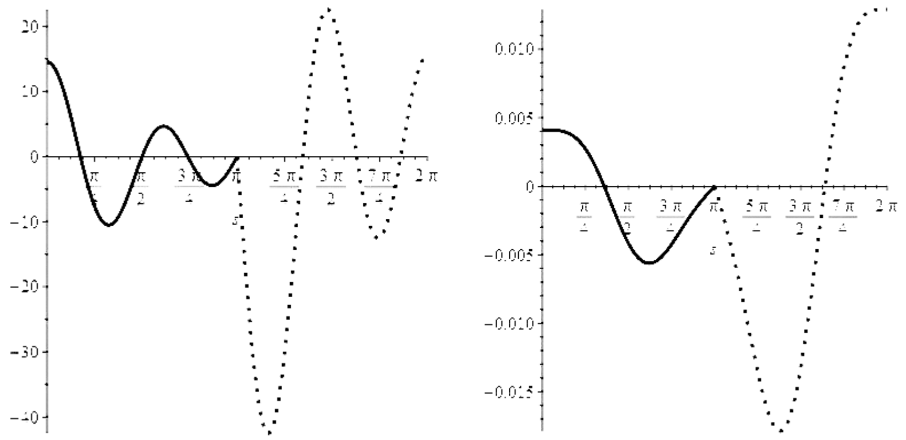

Fig. 2. $v(s,0)$ and $v(s,1)$ of the first and the second edges of the graph **G**

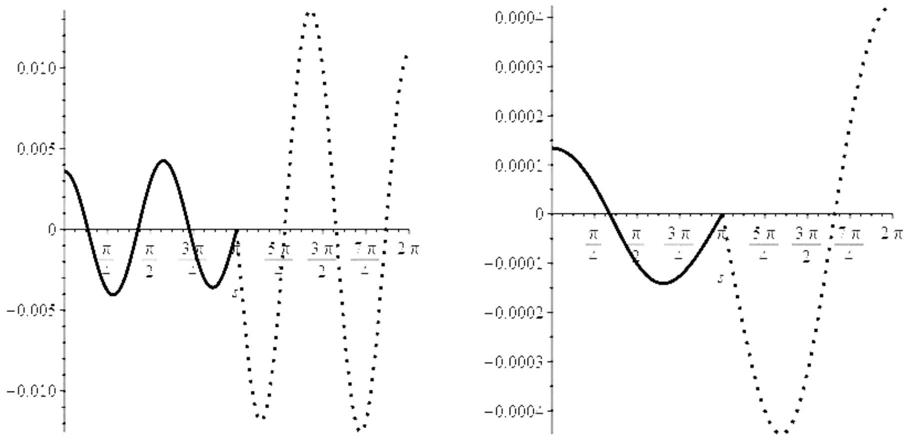

Fig. 3. $w(s,0)$ and $w(s,1)$ of the first and the second edges of the graph $\mathbf{G}$

Figs. 4, 5 illustrate of the behavior of the model functions $v(s,t)$ and $w(s,t)$ on the first and the third edges of the graph at the initial and at the final point in time.

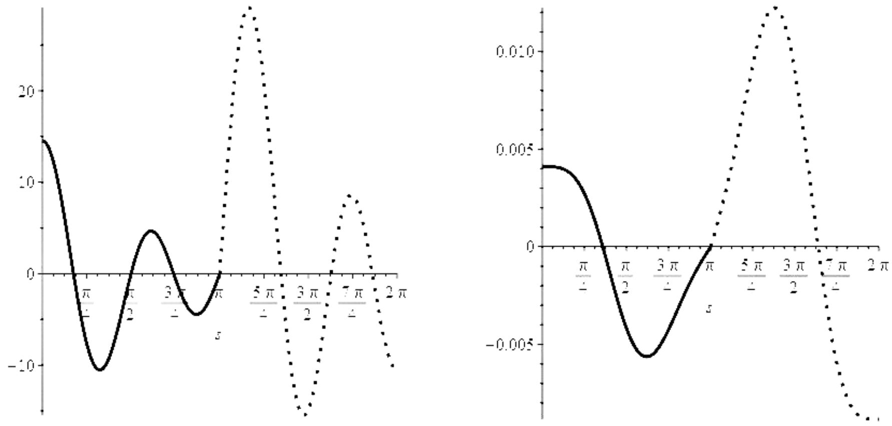

Fig. 4. $v(s,0)$ and $v(s,1)$ of the first and the third edges of the graph $\mathbf{G}$

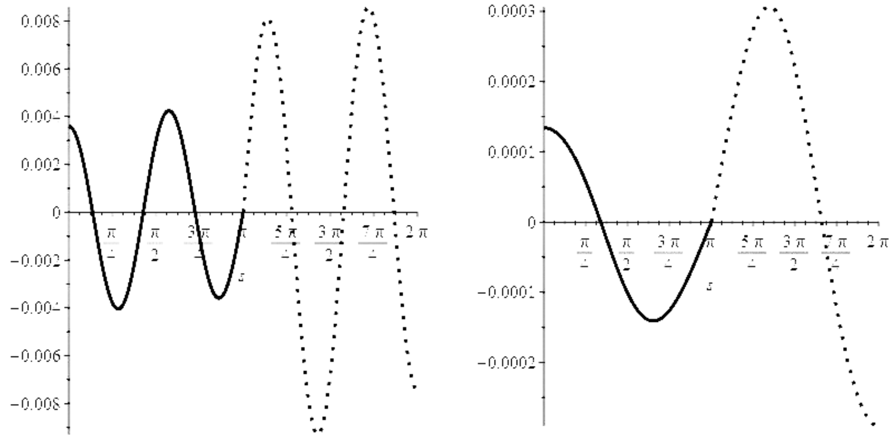

Fig. 5. $w(s,0)$ and $w(s,1)$ of the first and the third edges of the graph $\mathbf{G}$

Example 2. It is required to find a numerical solution of the problem (8) – (10), (13) for set coefficients $\gamma = 1$, $\alpha = 2$, $\beta = 4$, $\delta = \frac{1}{4}$ and $m = 3$ on the graph **G** (Fig. 6) consisting of five consecutively connected edges and six vertices $d_i = 1, l_i = \pi, i = 1, \ldots, 5$, $T = 1$, and initial functions

$$v_{01}(s) = \sqrt{\tfrac{2}{5\pi}}\left(\cos\left(\tfrac{2s}{5}\right) + \cos\left(\tfrac{s}{5}\right) + 1)\right),$$
$$v_{02}(s) = \sqrt{\tfrac{2}{5\pi}}\left(\cos\left(\tfrac{2s}{5} + \tfrac{2\pi}{5}\right) + \cos\left(\tfrac{s}{5} + \tfrac{\pi}{5}\right) + 1\right),$$
$$v_{03}(s) = \sqrt{\tfrac{2}{5\pi}}\left(-\sin\left(\tfrac{2s}{5} + \tfrac{3\pi}{10}\right) + \cos\left(\tfrac{s}{5} + \tfrac{2\pi}{5}\right) + 1\right),$$
$$v_{04}(s) = \sqrt{\tfrac{2}{5\pi}}\left(-\cos\left(\tfrac{2s}{5} + \tfrac{\pi}{5}\right) - \sin\left(\tfrac{s}{5} + \tfrac{\pi}{10}\right) + 1\right),$$
$$v_{05}(s) = \sqrt{\tfrac{2}{5\pi}}\left(\cos\left(\tfrac{2s}{5} + \tfrac{\pi}{10}\right) + \cos\left(\tfrac{s}{5} + \tfrac{3\pi}{10}\right) + 1\right).$$

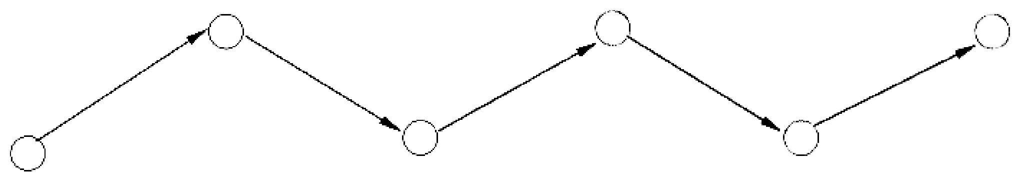

Fig. 6. Graph **G**

The result of the numerical solution of the system of algebraic differential equations with allowance for the initial conditions is presented in Table 2 (with an accuracy of 10^{-7}); in Fig. 7 we illustrate the behavior of the model function $v(s,t)$ on each edge of the graph at the beginning and at the end of time, Fig. 8 shows an illustration of the behavior of the model function $w(s,t)$ on each edge of the graph at the initial and at the final instant of time.

Table 2

The numerical solution of the problem

t	$v_1(t)$	$v_2(t)$	$v_3(t)$	$w_1(t)$	$w_2(t)$	$w_3(t)$
0	2	3	4	0,1253301	−0,0551093	0,2458884
0,1	2,0763675	2,6940882	3,4927618	0,2581374	−0,1060352	0,1703706
0,2	2,1454677	2,4203842	3,0536960	0,4250503	−0,1703084	0,0677417
0,3	2,2079922	2,1756744	2,6752924	0,5899671	−0,2314321	−0,0371085
0,4	2,2645667	1,9568104	2,3493521	0,7174804	−0,2735610	−0,1187750
0,5	2,3157574	1,7608072	2,0676155	0,7958981	−0,2921211	−0,1677739
0,6	2,3620766	1,5849967	1,8227596	0,8337800	−0,2918655	−0,1889439
0,7	2,4039880	1,4270819	1,6088404	0,8454240	−0,2799346	−0,1916727
0,8	2,4419110	1,2851002	1,4211853	0,8425436	−0,2620205	−0,1839739
0,9	2,4762252	1,1573600	1,2560966	0,8326644	−0,2417243	−0,1711564
1,0	2,5072739	1,0423845	1,1105816	0,8200689	−0,2210712	−0,1563395

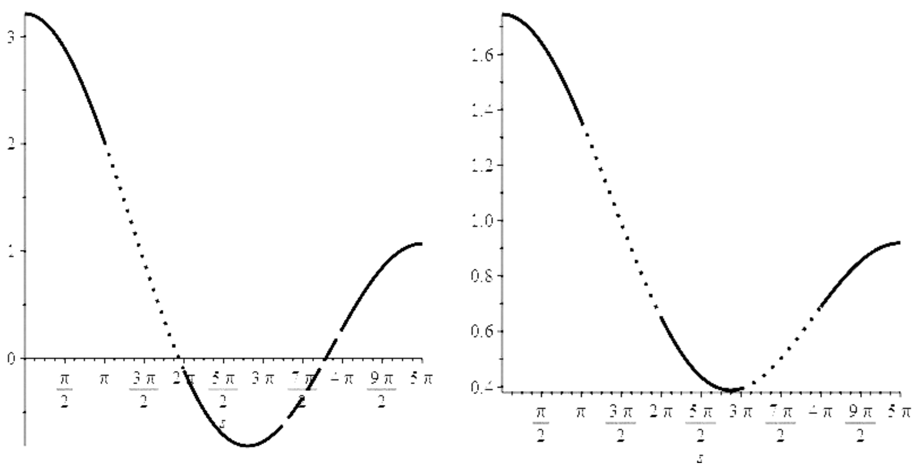

Fig. 7. $v(s,0)$ and $v(s,1)$ sequentially on each edge of the graph $\mathbf{G}$

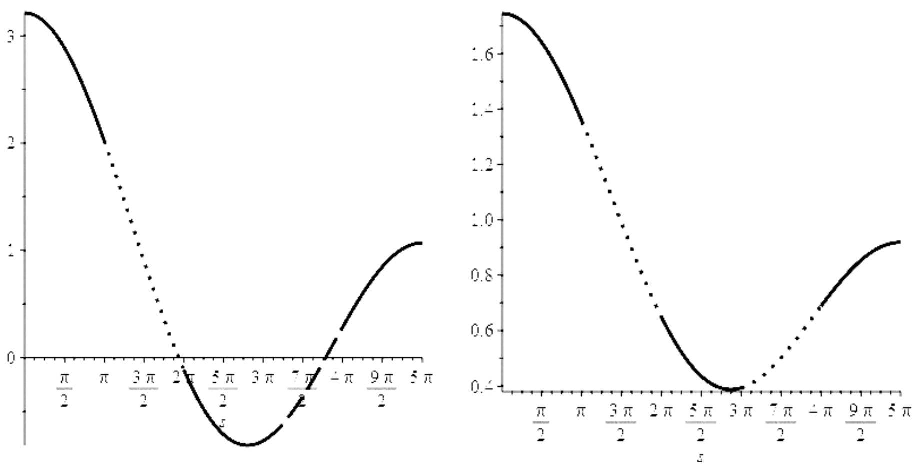

Fig. 8. $w(s,0)$ and $w(s,1)$ sequentially on each edge of the graph $\mathbf{G}$

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Olga V. Gavrilova, PhD Student, Department of Mathematical Physics Equations, South Ural State University, Chelyabinsk, Russian Federation, gavrilovaov@susu.ru.

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ЧИСЛЕННОЕ ИССЛЕДОВАНИЕ ОДНОЙ МАТЕМАТИЧЕСКОЙ МОДЕЛИ АВТОКАТАЛИЧЕСКОЙ РЕАКЦИИ С ДИФФУЗИЕЙ В ТРУБЧАТОМ РЕАКТОРЕ

О. В. Гаврилова

В статье проводится аналитическое и численное исследование модели автокаталической реакции с диффузией в вырожденном случае на конечном связном ориентированном графе **G** с условием Шоуолтера – Сидорова. В основе математической модели автокаталической реакции с диффузией лежит система уравнений распределенного брюсселятора. Система вырожденных уравнений распределенного брюсселятора, функции которой удовлетворяют условиям непрерывности и баланса потока, относится к широкому классу полулинейных уравнений соболевского типа. Для исследования существования решения данной системы уравнений будет использован метод фазового пространства, который был разработан Г. А. Свиридюком и его учениками для исследования разрешимости уравнений соболевского типа. Нами будет показана простота фазового пространства и существование единственного локального решения данной задачи Шоуолтера – Сидорова. Теоретические результаты данной статьи проиллюстрированы с помощью численного исследования модели, проведенного в среде Maple. В основе алгоритма численного исследования лежит метод Галеркина, который позволяет учесть феномен вырожденности уравнения. В статье приводятся несколько примеров иллюстрирующих результаты вычислительного эксперимента, полученные на трехреберном и пятиреберном графах.

Ключевые слова: уравнения соболевского типа; брюсселятор; условием Шоуолтера – Сидорова; уравнения реакции-диффузии; локальное решение.

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Гаврилова Ольга Витальевна, аспирант, кафедра уравнений математической физики, Южно-Уральский государственный университет (г. Челябинск, Российская Федерация), gavrilovaov@susu.ru.

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