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# NUMERICAL ANALYSIS SOLUTION OF THE PROBLEM BIMOLECULAR REACTION

*Abstract: In the work, the problem of a bimolecular reaction called the "Brusselator" is numerically solved. After some simplifications, a nonlinear system of ordinary differential equations with two or three unknowns is obtained, which depends on only one parameter (for example, α). The compiled Cauchy problem was solved by the fourth-order Runge-Kutta method of accuracy with a constant step. The problems of singular points, stability, and the limit cycle are analyzed, as well as the graphs of the trajectories in the phase space and their projections on the planes for various values of the parameter α. Also solved the "Brusselator" problem with DDE.*

*Key words: bimolecular reaction, brusselator, system of ordinary differential equations, singular point, limit cycle, stability.*

*Language: English*

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**Introduction**

As we know, the molecular behavior of a chemical reaction in the process of chemical technology is the number of molecules that participate in the reaction. Molecular reactions are divided into three types: multi-, two- and three-molecular. A multimolecular type reaction is $A \rightarrow B$ or $A \rightarrow B + C$, and a bimolecular type reaction is $A + B \rightarrow C$ or $2A \rightarrow B$. Three-particle reactions are rare, with the reaction of three particles colliding. Let us take a look at the model of Lefever and Nicolis (1971), which is called the problem «Brusselator». In this case, a bimolecular reaction is studied and the reaction of six substances is studied [5,7,8]. The following are numerical solutions to such a private issue with the help of MATLAB software.

**Example 1.** As a test, we first solve the Cauchy's problem with the 4-order Runge-Kutta method [5,7,8]:

$$y_1' = y_2, \quad y_2' = 2y_1^2(1 - 4x^2 y_1), \tag{1}$$
$$y_1(0) = 1, \quad y_2(0) = 0.$$

**Solution.** The exact solution to the problem (1) has the form:

$$y_1 = \frac{1}{1 + x^2}, \quad y_2 = -\frac{2x}{\left(1 + x^2\right)^2}.$$

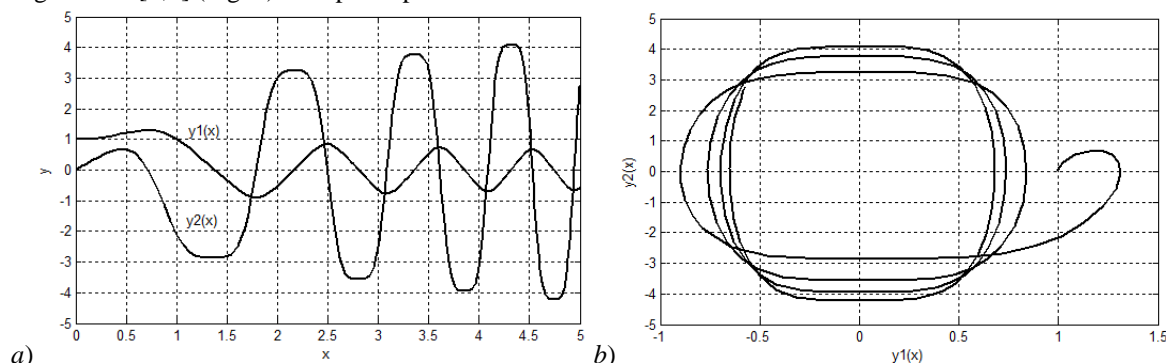Below are the results of a numerical solution this Cauchy's problem (1) with the MATLAB program in the segment $x \in [0;5]$ (Fig. 1). The phase portrait in the figure shows the existence and uniqueness of the limit cycle [1,6,10].



a)

b)

**Fig. 1. Graphs of the results approximate solution of the test system (1)**
**(*a* – graphs of functions *y₁*(*x*) and *y₂*(*x*); *b* – phase portrait).**

**Example 2.** Now let's look bimolecular reaction reducible to the two-dimensional «Brusselator» problem. for simplicity, assume that according to the law of mass interaction, excluding the effects of two substances on the reactions of other substances, amount of two substances constant, two substances have no effect on the reaction of the rest of the substance. In this case, the Cauchy problem will be represented by a system of two nonlinear ordinary first-order differential equations [5,7,8]:

$$y_1' = 1 + y_1^2 y_2 - (\alpha + 1) y_1, \quad y_2' = \alpha y_1 - y_1^2 y_2,$$
$$y_1(0) = 1, \quad y_2(0) = 3. \tag{2}$$

**Solution.** The results of a corresponding study of system (2) of nonlinear ordinary first-order differential equations in the MATLAB program by the Runge-Kutta method at $\alpha = 0,1,2,3$ (the dependence of system components on time and phase portraits) are shown in Fig. 2-5 [1,3,9,10].
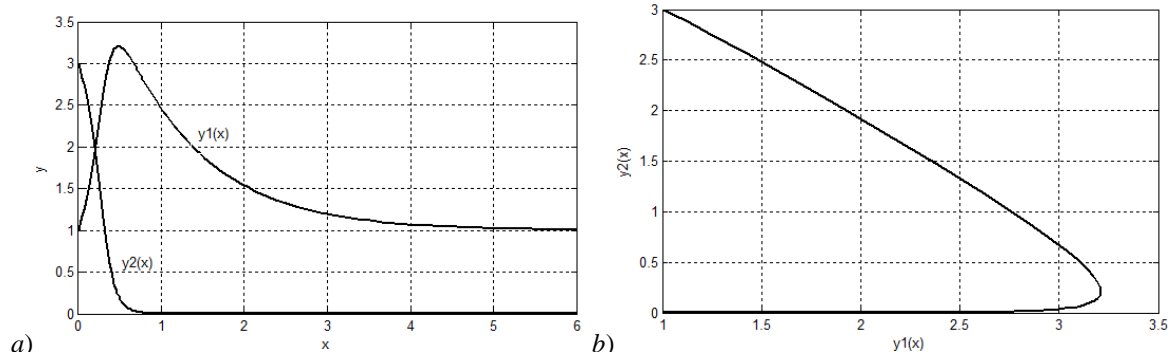


a)

b)

**Fig. 2. Graphs of the results approximate solution of the system (2) at $\alpha = 0$**
**(*a* – graphs of functions *y₁*(*x*) and *y₂*(*x*); *b* – phase portrait).**
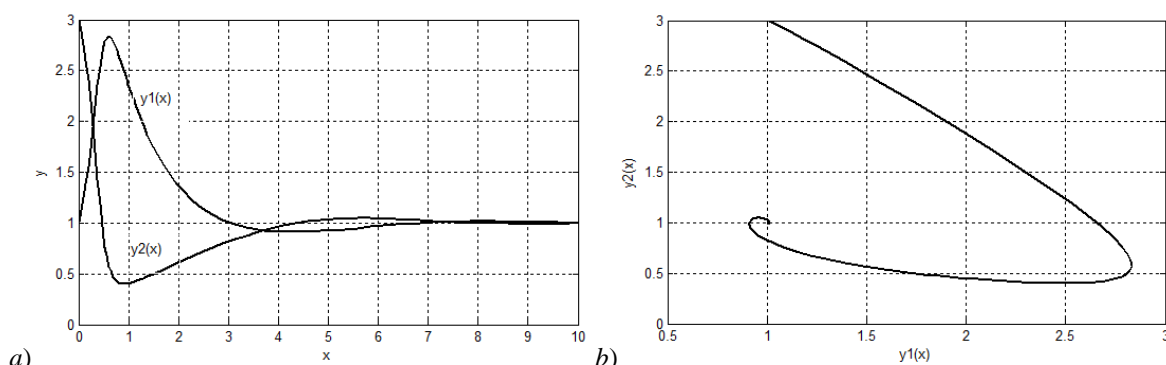


a)

b)

**Fig. 3. Graphs of the results approximate solution of the system (2) at $\alpha = 1$**
**(*a* – graphs of functions *y₁*(*x*) and *y₂*(*x*); *b* – phase portrait).**

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This system has a unique singular point $y_1' = y_2' = 0$ at $y_1 = 1$, $y_2 = \alpha$. The linearized equation around this point is nonlinear only for $\alpha > 2$. Continuing to study the field of research, we conclude that $y_1'$, $y_2'$ or $(y_1 + y_2)'$ are positive or negative, which means that all solutions to this system are limited. Thus, at $\alpha > 2$ has a limit cycle, and numerical calculations show that it is unique.
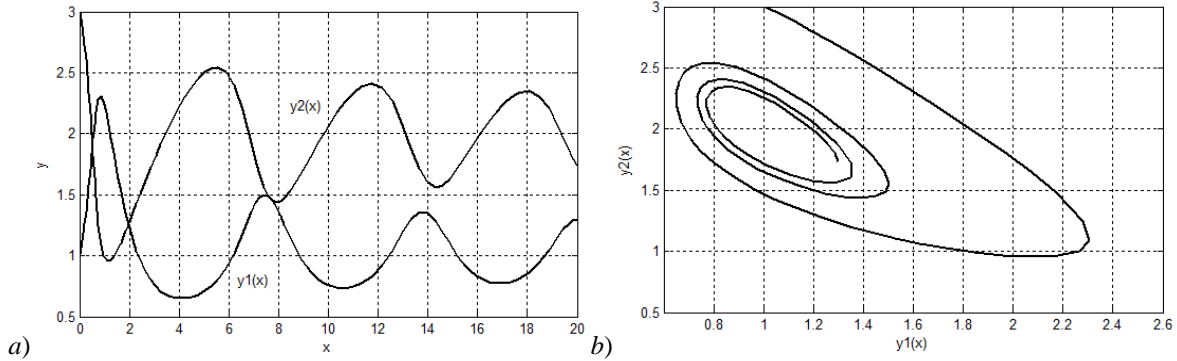


*a)*        *b)*

**Fig. 4. Graphs of the results approximate solution of the system (2) at $\alpha = 2$**
**(*a* – graphs of functions $y_1(x)$ and $y_2(x)$; *b* – phase portrait).**
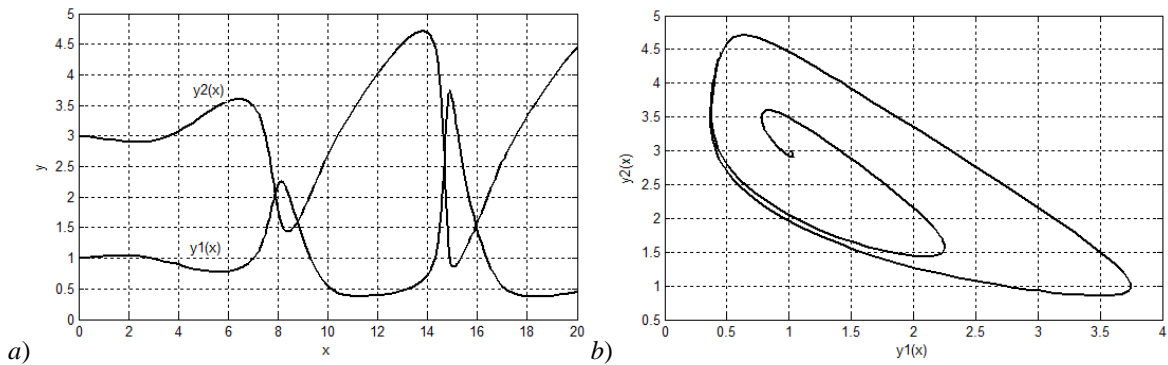


*a)*        *b)*

**Fig. 5. Graphs of the results approximate solution of the system (2) at $\alpha = 3$**
**(*a* – graphs of functions $y_1(x)$ and $y_2(x)$; *b* – phase portrait).**

To confirm the above, we refer to the Zonneveld method. The calculations of the Sonneveld method for two systems of first-order differential equations given above have the form [6]:

$$\vec{y}_{i+1} = \vec{y}_i + \left( -\frac{1}{2}\vec{k_1} + \frac{7}{3}\vec{k_2} + \frac{7}{3}\vec{k_3} + \frac{13}{6}\vec{k_4} - \frac{16}{3}\vec{k_5} \right),$$

$$\vec{k_1} = h\vec{f}(x_i, y_i), \quad \vec{k_4} = h\vec{f}\left( x_i + h, y_i + \vec{k_3} \right),$$

$$\vec{k_2} = h\vec{f}\left( x_i + \frac{1}{2}h, y_i + \frac{1}{2}\vec{k_1} \right),$$

$$\vec{k_3} = h\vec{f}\left( x_i + \frac{1}{2}h, y_i + \frac{1}{2}\vec{k_2} \right),$$

$$\vec{k_5} = h\vec{f}\left( x_i + \frac{3}{4}h, y_i + \frac{5}{32}\vec{k_1} + \frac{7}{32}\vec{k_2} + \frac{13}{32}\vec{k_3} - \frac{1}{32}\vec{k_4} \right).$$

here

$$\vec{y}_i = (y_1(x), y_2(x))$$

Results of computational experiment of Zonneveld method (Fig. 6-8):

**Impact Factor:**

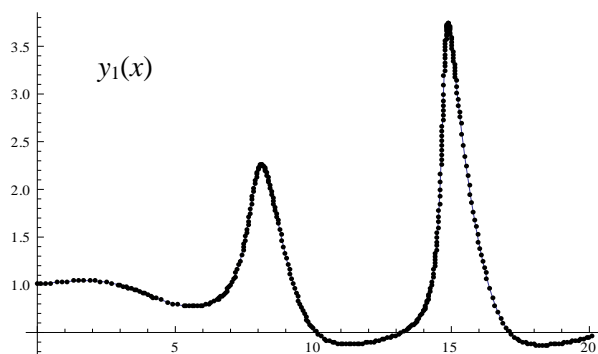| | | | | | |
|---|---|---|---|---|---|
| **ISRA** (India) | = **4.971** | **SIS** (USA) | = **0.912** | **ICV** (Poland) | = **6.630** |
| **ISI** (Dubai, UAE) = **0.829** | | **РИНЦ** (Russia) = **0.126** | | **PIF** (India) | = **1.940** |
| **GIF** (Australia) | = **0.564** | **ESJI** (KZ) | = **8.716** | **IBI** (India) | = **4.260** |
| **JIF** | = **1.500** | **SJIF** (Morocco) = **5.667** | | **OAJI** (USA) | = **0.350** |

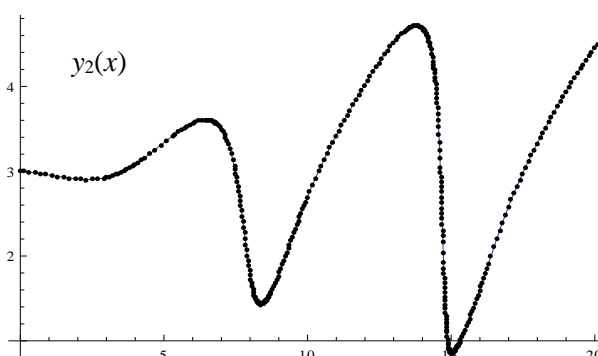**Fig. 6. Graph of approximate solution of function $y_1(x)$.**



**Fig. 7. Graph of approximate solution of function $y_2(x)$.**
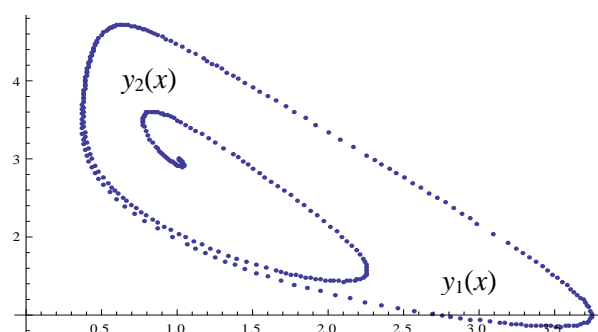


**Fig. 8. Phase portrait.**

**Example 3.** The interactions of six substances in the three-dimensional case were studied. According to the law of inter-influencing masses for simplicity, these two substances do not affect the reaction of the rest of the substance; the amount of one substance is constant; three substances are involved in the reaction. In this case, the Cauchy problem will be represented by a system of three nonlinear ordinary first-order differential equations [5,7,8]:

$$y_1' = 1 + y_1^2 y_2 - (y_3 + 1)y_1, \tag{3}$$
$$y_2' = y_1 y_3 - y_1^2 y_2, \quad y_3' = -y_1 y_3 + \alpha.$$

The initial conditions for this problem are of the form: $y_1(0)=1$ ; $y_2(0)=1+\alpha$ ; $y_3(0)=1+\alpha$ .

**Solution.** This system (3) at $y_1 = 1$, $y_2 = y_3 = \alpha$ has one singular point:

$$\frac{\partial f}{\partial y} = \begin{pmatrix} \alpha - 1 & 1 & -1 \\ -\alpha & -1 & 1 \\ -\alpha & 0 & -1 \end{pmatrix}$$

The characteristic polynomial of this matrix has the form

$$\lambda^3 + (3-\alpha)\lambda^2 + (3-2\alpha)\lambda + 1 = 0$$

and it satisfies the stability condition only when condition $\alpha < (9-\sqrt{17})/4 = 1.21922$ is satisfied (that is, the real part of the root of the polynomial is less than zero).

If we continue to study the field of study, we will see that there is a limit cycle only if the value of α increases from 1.0 to 1.5. The proof of the above considerations in the MATLAB program by the Runge-Kutta method is shown in Fig. 9 ($x = 20$, $\alpha = 1$) [1,4,10].
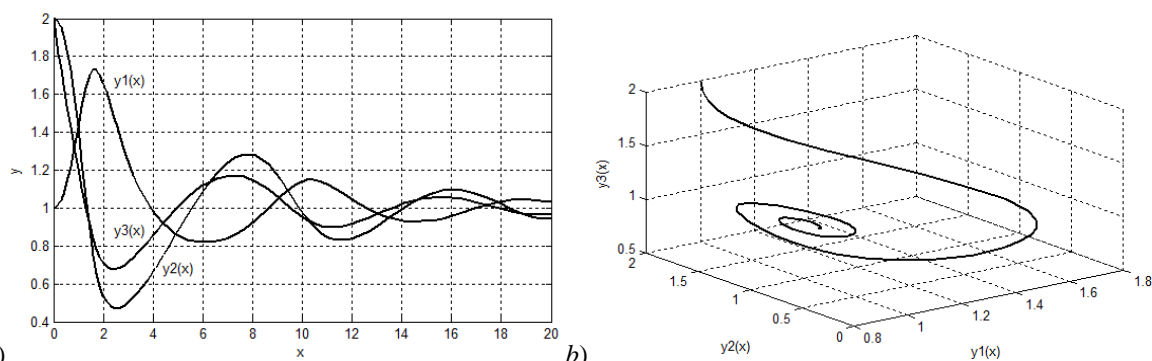
**Fig. 9. Graphs of the results approximate solution of the system (3) at x=20, α=1 (a – graphs of functions $y_1(x)$, $y_2(x)$ and $y_3(x)$; b – phase portrait).**

Taking into account (3), we construct the trajectory of the system of ordinary first-order differential equations ($y_1$, $y_2$, $y_3$) in space, its projections ($y_1$, $y_2$), ($y_2$, $y_3$), ($y_1$, $y_3$) in the planes at $\alpha = 1.5$, $x = 50, 100, 500, 1000, 5000$. The results remained virtually unchanged (Fig. 10). If we increase the value of $\alpha$, then we will see that the mentioned limit cycle "explodes", that is, $y_1 \to 0$, $y_2, y_3 \to \infty$ as $x \to \infty$.
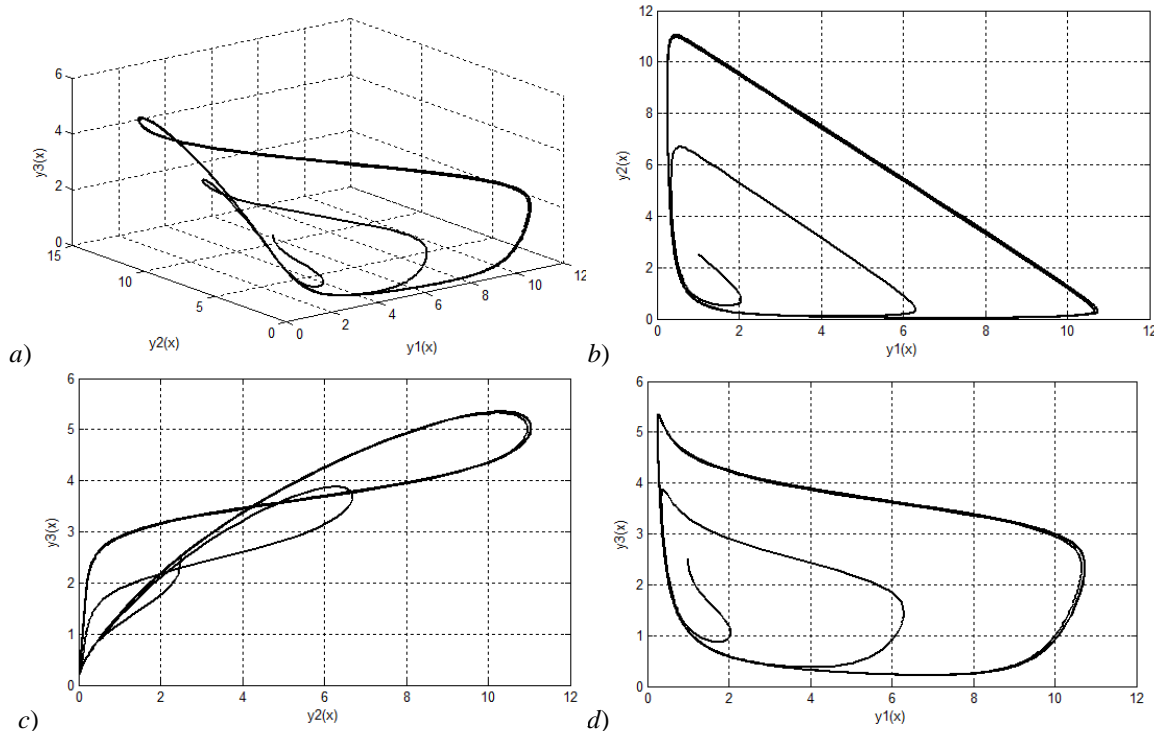


**Fig. 10. Graphs of the results approximate solution of the system (3) at x=12, α=1.5 (a – phase portrait; b, c, d – graphs of functions ($y_1$, $y_2$), ($y_2$, $y_3$), ($y_1$, $y_3$) in the planes).**

Thus, numerical calculations show that the entire solution of this system has a limit cycle at $\alpha < 2$; If we increase the value of a, we will see that the limit cycle disappears.

**Example 4.** Assume that according to Example 3, a solution to the following DDE is required [2,5,10]:

$$\begin{cases} y_1'(t) = 1 + y_1(t)\,y_1(t-\tau)\,y_2(t) - y_1(t)(y_3(t)+1), \\ y_2'(t) = y_1(t)\,y_3(t) - y_1(t)\,y_1(t-\tau)\,y_2(t), \\ y_3'(t) = -y_1(t)\,y_3(t) + \alpha. \end{cases} \quad (4)$$

Here functions $y_1(t)$, $y_2(t)$ and $y_3(t)$ are time-dependent $t$ changes in the amount of substances, and $\tau$ denotes time delay. The initial conditions for this problem are of the form: $y_1(0)=1$; $y_2(0)=1+\alpha$; $y_3(0)=1+\alpha$.

**Solution**. For $\tau = 0$, we obtain a solution to Example 3. The proof of the above considerations in the MATLAB program by the Runge-Kutta method is shown in Fig. 11 ($\alpha$=1.0, $t$=50: $\tau = 0$ (a) and $\tau = 2$ (b))

and Fig. 12 ($\alpha$=1.5: $t$=50 (a) and $t$=500 (b)) [1,4,6,10]. Here the same thing, the conclusions of Example 3 are repeated.



a)                                                                         b)
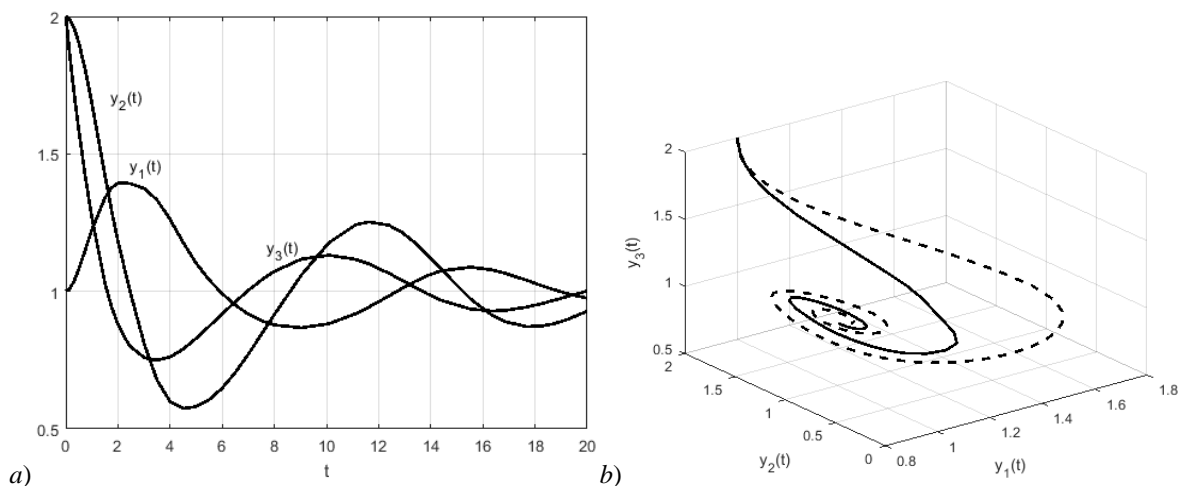
**Fig. 11. Graphs of the results approximate solution of the system (4) at $\alpha$=1 (a – graphs of functions $y_1(t)$, $y_2(t)$ and $y_3(t)$ ($\tau = 2$); b – phase portrait ($\tau = 2$ - solid line, $\tau = 0$ - dashed line)).**



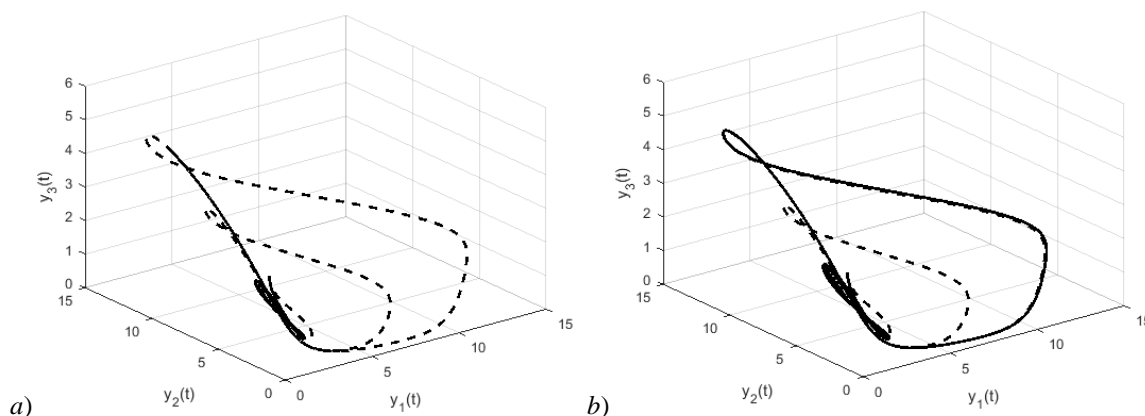a)                                                                         b)

**Fig. 12. Graphs phase portrait of the results approximate solution of the system (4) at $\alpha$=1.5: $t$=50 (a) and $t$=500 (b) ($\tau = 2$ - solid line, $\tau = 0$ - dashed line).**

**Conclusion.**

In this paper, we applied the numerical method for solving nonlinear ODE and DDE. It was shown that this metod provides an approximate solution which is closer to the real solution. We offer a procedure that is simple and clear, and illustrative examples demonstrate that the applied numerical method is valid and effective. In the same way, more complex tasks with ODE or DDE can be solved further [2,4,7,8,10].

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