On oscillation appearance in one chemical problem

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Abstract. The paper is devoted to the investigation of the Brusselator model under the assumption that the concentrations of initial substances slowly changing in time. This is the reason for the appearance of the delayed loss of stability effect. The existence of oscillations is studied.

1. Introduction
Mathematical models of complex nonlinear systems naturally depend on many different parameters. These parameters may describe the properties of the model and the influence of the external environment. They can have different absolute values, so the system can be considered as a one with slow and fast motions. Also, the usual approach for the study is that the parameters of the system are constants. However, in real-life models, the parameters can change in time. It could be because of the aging of the system or incompleteness of the mathematical model. So the system’s dimension increases, and behavior can vary dramatically. Therefore it is necessary to study the dependence of the behavior of the system on absolute values and changes of the parameters. Usually, in such cases, the combination of analytical and numerical methods is used (see, e.g. [1]). One of the effective tools among the analytical methods to study such systems is the method of integral manifolds. It is based on the idea of finding the invariant sets of the model and on the separation of motions according to internal speeds of the components.

In the paper at hand, we study the classical Brusselator model. It is a well-known fact that this system for different initial values of the parameters possesses either a stable steady-state or self-exited oscillations. Our crucial assumption is that the concentrations of the substances are slowly changing in time. So, the system has a transition from a stable regime to the oscillatory one. But this transition is determined by the parameters.

In our study, we use some ideas of the method of integral manifolds. In the first part of the paper, we recall the main ideas of this method. Then we describe the use of it to the dynamical Brusselator model.

2. Integral manifolds method
The method of integral manifolds is a good tool to study nonlinear systems with complicated behavior. The base of the method was established by N. Bogolyubov and Yu. Mitropoliski in the 1950s. Then it was developed by many authors. The integral manifold is an invariant set of the system, so it consists of the integral curves of the system. The most useful approach is to use the manifolds of lower
dimension such we can decrease the dimension of the system (see, e.g. [2]). The main ideas of this method are the following.

Consider the slow-fast system

$$\begin{align*}
\frac{dx}{dt} &= f(x, y, a, \varepsilon), \\
\varepsilon \frac{dy}{dt} &= g(x, y, a, \varepsilon),
\end{align*}$$

(1)

with $x \in \mathbb{R}^n, y \in \mathbb{R}^m, t \in \mathbb{R}, a$ is a parameter, $0 < \varepsilon \ll 1$. Here $x$ is a slow variable, $y$ is a fast variable. We are interested in the integral manifolds of the form $y = h(x, a, \varepsilon)$, or the so-called slow integral manifolds. It is supposed that the function $h$ depends smoothly on $x$ and $\varepsilon$. The motion on the integral manifold is due to the relation

$$\dot{x} = f(x, h(x, a, \varepsilon), a, \varepsilon).$$

Taking $\varepsilon = 0$ in the system (1) we get the so-called degenerated system. Suppose that the second equation of it

$$g(x, y, a, 0) = 0$$

has an isolated root $y = h_0(x, a)$. Then the surface $\Gamma$ described by this relation $y = h_0(x, a)$ is called a slow manifold of the system (1). The part of the slow manifold is attracting if the eigenvalues of the linearization matrix $\partial g / \partial y(y(x, h_0(x, a), a))$ have negative real parts. In case that there exists at least one eigenvalue with a positive real part, the slow manifold is repelling. In the $\varepsilon$-neighborhoods of the attracting and repelling parts of the slow manifolds there exist attracting and repelling slow integral manifolds. All other solutions starting in the small neighborhood of the attracting (repelling) part of the slow integral manifold will ends to it for $t \to +\infty$ ($t \to -\infty$).

The surface with the condition that the eigenvalues of the Jacobi matrix $\partial g / \partial y_y(x, h_0(x, a), a)$ are on the imaginary axis is called the surface of change of attractivity or break-down surface. Due to the presence of the additional parameter $a$ we are able to glue together attracting and repelling slow integral manifolds at one point [3]. Thus we obtain the solution that follows first an attractive slow manifold and then repelling slow manifold. Such a solution is called a canard solution.

Also, there exists another type of change of attractivity. Suppose that in the spectrum of the Jacobi matrix there exists a pair of complex conjugated eigenvalues that cross an imaginary axis from the left to the right with nonvanishing speed. In this case, the trajectories of the system starting in the small neighborhood of the attracting part of the slow manifold follow it until the point of change of attractivity. But after crossing this point the trajectories do not leave this small neighborhood immediately. The loss of attractivity is delayed: for some time the trajectories stay near repelling part of the slow manifold and then jump away. This phenomenon was described in [4]. Let us mention that the presence of the additional parameter allows us to change the time of the attractivity loss delay [5].

3. The Brusselator model

Consider the Brusselator model. This model is a base to study different real-life processes in chemical systems (periodical reactions, spiral reactions), in biology, economy, etc (for example [6], [7]). In the beginning, the mathematical model describes the oscillating chemical reaction (I. Prigogine, 1968). This model arises in the study of 4 conjugated chemical reactions

$$A \rightarrow A, \quad B \rightarrow B,$$

$$A + 2B \rightarrow 3A, \quad 2A + B \rightarrow 2A + B.$$
By linearizing the system in the small neighborhood of the steady-state we get the following matrix

$$L = \begin{pmatrix} B - 1 & A^2 \\ -B & -A^2 \end{pmatrix}.$$ 

Its characteristic equations

$$\lambda^2 + \lambda (A^2 + 1 - B) + A^2 = 0$$

has the roots

$$\lambda = -\frac{1}{2} (A^2 + 1 - B) \pm \sqrt{(A^2 + 1 - B) - 4A^2}.$$ 

Thus we get that for $B < A^2 + 1$ the steady-state is attracting and for $B > A^2 + 1$ the steady-state is repelling. For $(A - 1)^2 < B < A^2 + 1$ the steady-state is an attractive focal point. For $B > A^2 + 1$ the steady-state is an unstable focal point. It is known that in this case there exists an attractive limit cycle. So, the parameter $B$ is a bifurcation parameter, and its critical value is $B = A^2 + 1$.

In Figure 1 there are different trajectories of the system with different initial values of the bifurcation parameter $B$. The graphs are shown in order of increase of the parameter $B$. It could be seen that the trajectories approach the attracting focal point. The last graph is for the value of $B$ more than the critical one. So, the appearance of the oscillations can be observed.

**Figure 1.** The dependence of the concentration of the substance $X_1$ on the value of parameter $B$.

Consider the model under the assumption that the concentrations of the substances are not constant. For example, irregular delivery of the reacting species may be the cause of such an assumption. Suppose that the concentration of $B$ slowly grows. Thus, we obtain the slow-fast system of differential equations

$$\begin{align*}
\dot{x}_1 &= A - (B + 1)x_1 + x_1^2x_2, \\
\dot{x}_2 &= Bx_1 + x_1^2x_2, \\
\dot{B} &= \varepsilon,
\end{align*}$$
with $0 < \varepsilon \ll 1$. Here $x_1, x_2$ are fast variables, $B$ is a slow variable. This system has a slow manifold $x_1 = A, \quad x_2 = B/A$. Taking into account previous analysis we conclude that for different values of the slow variable $B$ the slow manifold changes its attractivity in time: it is attracting for $B < A^2 + 1$ and repelling for $B > A^2 + 1$. The eigenvalues of the linearization matrix have a pair of complex conjugate eigenvalues depending on the slowly changing value of $B$, the eigenvalues are crossing the imaginary axis from left to right with non-zero speed. It is known that in this case in analytical systems the effect of delayed loss of stability occurs [3].

The behavior of the solutions depends on the initial point. Starting at the initial point with $B(0) > A^2 + 1$. We get the growth of the amplitude of the oscillations. But for $B(0) < A^2 + 1$ we get very interesting behavior. Solutions starting for $B(0) < A^2 + 1$ in a small neighborhood of the slow manifold approach it and follow it until for $B = A^2 + 1$. But after the moment $B$ crossing the value for $B = A^2 + 1$, solutions do not leave the small neighborhood of the repelling part of the slow manifold. They follow it for some time of order $O(1)$ and then jump away. So the system possesses a delayed loss of stability [3].

Using results of [4] we conclude that the slow manifold of the system $x_1 = A, x_2 = B/A$ is a slow manifold with variable attractivity. So it has an infinite time of delayed loss of stability. All other trajectories starting for $B(0) < A^2 + 1$, approach the small neighborhood of the attractive part of the slow manifold and follow it until the point of change of attractivity. But after that, they do not leave the small neighborhood of the slow manifold and follow it for some time and then jump away. We note that the more time solutions spend in the small neighborhood of the attracting part of the slow manifold, the longer they spend in the neighborhood of the repelling part [4].

Figure 2. The dependence of the concentration of the substance $X_1$ on the initial value of slowly changing parameter $B$. 
Thus, in the Brusselator model, we can observe the delayed loss of stability effect. We can consider the concentration of the substances taking part in the reaction as a control parameter. The more time the solution spends near the attraction part of the slow manifold, the further it jumps away, so the oscillation arising at the end will have a bigger amplitude. It could be the reason for dramatical consequences. So, such behavior should be studied and expected.

Figure 2 shows different trajectories with the same initial values for substances and different initial values of bifurcation parameter $B$. It is well seen that the more time the solution spends near the attraction part of the slow manifold, the further it jumps away.

4. References

[1] Perevaryukha A Yu 2017 Izvestiya Vysshikh Uchebnykh Zavedeniy. Prikladnaya Nelineynaya Dinamika 25(2) 51-62
[2] Strygin V V and Sobolev V A 1988 Separation of motion by the integral manifolds method (Moscow: Nauka)
[3] Shchepakin E A and Sobolev V A 2010 Model reduction and critical phenomena in macrokinetics (Moscow: Physmatlit)
[4] Neishtadt A I 1987 Diff. Equations 23 1385-1390
[5] Shchetinina E V 2010 Vestnik SamGU 6(80) 93-105
[6] Kostet B 2018 Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 376
[7] Tlidi M, Gandica Y, Sonnino G, Averlant E and Panajotov K 2016 Entropy 18 64