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FOUR–DIMENSIONAL BRUSSELATOR MODEL WITH PERIODICAL SOLUTION[1]

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Abstract: In the paper, a four-dimensional model of cyclic reactions of the type Prigogine's Brusselator is considered. It is shown that the corresponding dynamical system does not have a closed trajectory in the positive orthant that will make it inadequate with the main property of chemical reactions of Brusselator type. Therefore, a new modified Brusselator model is proposed in the form of a four-dimensional dynamic system. Also, the existence of a closed trajectory is proved by the DN-tracking method for a certain value of the parameter which expresses the rate of addition one of the reagents to the reaction from an external source.

Keywords: Chemical reaction, Closed trajectory, DN-tracking method, Discrete trajectory, Numerical trajectory.

1. Introduction

Cyclic (oscillating) reactions such as the Brusselator of Prigogine [12, 24, 25] are of importance in the kinetic theory of chemical reactions.

The mechanism of this reaction is described by the following reactions:

$$\begin{aligned} A &\xrightarrow{k_1} X, \\ B + X &\xrightarrow{k_2} Y + D, \\ 2X + Y &\xrightarrow{k_3} 3X, \\ X &\xrightarrow{k_4} E. \end{aligned} \tag{1.1}$$

The mathematical model of such reactions is also called Brusselator and serves as an important tool for their study. In fact, the Brusselator is adequately described by a system of two

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parabolic equations (diffusion and transfer equations) with respect to the concentrations of substances involved in the reaction that occurs in a given region in $\mathbb{R}^3$ (see [20, system (7.11)] and also [1, 2, 30, 34]. In practice, one mainly considers models in the form of a system of ordinary differential equations for averaged concentrations of substances A, B, X, Y, D, and E involved in the reaction

$$\begin{aligned} &\frac{dA}{dt} = -k_1 A, \quad \frac{dB}{dt} = -k_2 BX, \quad \frac{dX}{dt} = k_1 A - k_2 BX + k_3 X^2 Y - k_4 X, \\ &\frac{dY}{dt} = k_2 BX - k_3 X^2 Y, \quad \frac{dD}{dt} = k_2 BX, \quad \frac{dE}{dt} = k_4 X, \end{aligned} \tag{1.2}$$

where the parameters $k_i = \text{const}$ characterize the reaction rate constants of reaction (1.1).

The reagents D and E express the final products of reaction, therefore, their influence on other quantities can be neglected, and so we focus only on the dynamics of the reagents A, B, X, and Y. Assuming that the concentrations of A and B remain unchanged, after substituting $X = \lambda x$, $Y = \lambda y$, and $t = \mu\tau$, model (1.2) reduces to the second-order dynamical system

$$\begin{aligned} \frac{dx}{d\tau} &= a - bx + x^2 y - x, \\ \frac{dy}{d\tau} &= bx - x^2 y, \end{aligned} \tag{1.3}$$

where $\lambda = \sqrt{\dfrac{k_4}{k_3}}$, $\mu = \dfrac{1}{k_4}$, $a = \dfrac{k_1 A}{\lambda}\mu$, and $b = k_2 B\mu$. For system (1.3) and its diffusion form, the constructions of both phase portraits and bifurcations were completely studied [17–19, 22, 26, 28, 29, 31–33].

The three-dimensional model with the positive dynamics of the reagent B was also studied in the case when the corresponding reagent is constantly added to the reaction with the rate β [14]. In this case, the substitution $X = \lambda x$, $Y = \lambda y$, $B = \lambda b$, and $t = \mu\tau$ into system (1.2) gives

$$\begin{aligned} \frac{db}{d\tau} &= -bx + \tilde{\beta}, \\ \frac{dx}{d\tau} &= \tilde{a} - bx + x^2 y - \tilde{c}x, \\ \frac{dy}{d\tau} &= bx - x^2 y, \end{aligned} \tag{1.4}$$

where

$$\lambda = \frac{k_2}{k_3}, \quad \mu = \frac{k_3}{k_2^2}, \quad \tilde{a} = \frac{k_1 A}{\lambda}\mu, \quad \tilde{c} = k_4\mu, \quad \tilde{\beta} = \frac{\beta}{\lambda}\mu.$$

System (1.4) still has a periodic trajectory, for example, for $\tilde{a} = 1$, $\tilde{c} = 1$, and for a certain range of the parameter β. In [11], a full Brusselator model taking into account the diffusion was studied and its mathematical description of a long-term behavior was developed.

In [4, 6], with the use of the discrete-numerical tracking (DN-tracking) method [3], the existence of a closed trajectory was proved for specific values of the parameters of two-dimensional and three-dimensional systems of the Brusselator model, respectively.

Notice that, if the initial concentration of the reagent A is equal to $\lambda/(k_1\mu)$ and it is added to the reaction with the rate λ/μ, then one can provide the equality $\tilde{a} = 1$, and if the reaction rate k_4 of $X \xrightarrow{k_4} E$ is equal to $1/\mu$, then $\tilde{c} = 1$.

In the present paper, we consider the problem of the existence of a periodic regime in the four-dimensional model of Brusselator, where the dynamics of all reagents A, B, X, and Y are of interest. In the classic case, the Brusselator system has the form

$$\begin{aligned} \frac{dA}{dt} &= -k_1 A, \\ \frac{dB}{dt} &= -k_2 BX + \beta, \\ \frac{dX}{dt} &= k_1 A - k_2 BX + k_3 X^2 Y - k_4 X, \\ \frac{dY}{dt} &= k_2 BX - k_3 X^2 Y. \end{aligned} \tag{1.5}$$

Due to the first equation of (1.5), which corresponds to the reaction $A \xrightarrow{k_1} X$, system (1.5) cannot have a closed trajectory in the positive orthant $A > 0, B > 0, X > 0, Y > 0$ for any values of parameters $k_i, i = \overline{1,4}$ and β, since $A(t) \to 0$ as $t \to +\infty$. Based on this circumstance, one may conclude that the model (1.5) does not possess the main property of the Brusselator, that is, there is no an attractor, namely, an asymptotically stable periodic trajectory.

The simplest way to correct this is to replace the equation

$$\frac{dA}{dt} = -k_1 A$$

by the equation

$$\frac{dA}{dt} = -k_1 A + \alpha,$$

where $\alpha > 0$, i.e., to add some compensation of the reagent A from an external source with the rate α. However, in this case, it is easy to see that $A(t) \to \alpha/k_1$ as $t \to +\infty$ for any initial concentration of A unless it is equal to 0, meaning that there is no a closed trajectory. Moreover, the restriction of the new system to the invariant hyperplane $A = \alpha/k_1$ coincides with system (1.4).

The other way to compensate the concentration of A is to replace the reagent D with A in the bimolecular reaction $B + X \xrightarrow{k_2} Y + D$, i.e., to consider the new mechanism of reaction as

$$\begin{aligned} A &\xrightarrow{k_1} X, \\ B + X &\xrightarrow{k_2} Y + A, \\ 2X + Y &\xrightarrow{k_3} 3X, \\ X &\xrightarrow{k_4} E. \end{aligned}$$

Then, a modified 4-dimensional Brussellator model corresponding to the above reaction is

$$\begin{aligned} \frac{dA}{dt} &= -k_1 A + k_2 BX, \\ \frac{dB}{dt} &= -k_2 BX + \beta, \\ \frac{dX}{dt} &= k_1 A - k_2 BX + k_3 X^2 Y - k_4 X, \\ \frac{dY}{dt} &= k_2 BX - k_3 X^2 Y. \end{aligned} \tag{1.6}$$

In the study of the qualitative behaviour of trajectories of system (1.6), it was established that system (1.6) has a closed trajectory, which will be proved in the next section.

One can use other approaches to obtain a modified Brusselator model with the cyclical regime provided such a model exists. However, our purpose is to get a modified Brusselator model such that its two- and three-dimensional models are the same with the models (1.3) and (1.4), respectively.

Thus, unlike the model (1.5), the dynamics of the component A in (1.6) is determined by the influence of the reagents X and B.

Substituting $X = \lambda x$, $Y = \lambda y$, $B = \lambda b$, $A = \lambda a$, and $t = \mu\tau$, we can write model (1.6) as follows:

$$\begin{aligned} \frac{da}{d\tau} &= -\alpha a + bx, \\ \frac{db}{d\tau} &= -bx + \tilde{\beta}, \\ \frac{dx}{d\tau} &= \alpha a - bx + x^2 y - \gamma x, \\ \frac{dy}{d\tau} &= bx - x^2 y, \end{aligned} \tag{1.7}$$

where

$$\lambda = \frac{k_2}{k_3}, \quad \mu = \frac{k_3}{k_2^2}, \quad \alpha = k_1\mu, \quad \gamma = k_4\mu, \quad \tilde{\beta} = \frac{\beta}{\lambda}\mu.$$

2. Main result

The rest of the paper is devoted to the proof of below given Theorem 1, which states that model (1.7) has a periodic trajectory for certain values of $\tilde{\beta}$ and $\alpha = \gamma = 1$ (meaning that $k_1 = k_4 = 1/\mu$).

In vector form, system (1.7) is

$$\dot{z} = f(z), \tag{2.1}$$

where

$$z = (z_1, z_2, z_3, z_4), \quad f = (f_1, f_2, f_3, f_4), \quad f_1(z) = -z_1 + z_2 z_3,$$
$$f_2(z) = -z_2 z_3 + \tilde{\beta}, \quad f_3(z) = z_1 - z_2 z_3 - z_3 + {z_3}^2 z_4, \quad f_4(z) = z_2 z_3 - {z_3}^2 z_4.$$

A computer experiment allows us to formulate the following conjecture: for $\beta = 1.17$, system (2.1) has a closed trajectory $z(t)$ of the period $T \approx 8.36$ passing near the point $z_0^{(1)} = (1.11692,\ 0.99112,\ 1.09485,\ 0.80461)$.

System (2.1) does not have an internal symmetry; moreover, it is impossible to find its integral in explicit form. One may conclude that the only way to prove the existence of a closed trajectory is to apply the method of Poincaré map. To construct the Poincaré map, we use the DN-tracking method [3, 5]. To this end, first, it is necessary to choose the starting point as close to the proposed closed trajectory as possible. The point $z_0^{(1)}$ defined above is selected as the starting point.

Theorem 1. *For $\tilde{\beta} = 1.17$, system (2.1) has a closed trajectory in the region*

$$\Pi_4 = \left\{(z_1, z_2, z_3, z_3) \mid 1.07 \le z_1 \le 1.26,\ 0.85 \le z_2 \le 1.15,\ 0.98 \le z_3 \le 1.38,\ 0.65 \le z_4 \le 1.1\right\}.$$

3. Proof of Theorem 1

3.1. Preliminaries

Let

$$m_0 = \max_{z\in\Pi_4} \|f(z)\|, \quad m_1 = \max_{z\in\Pi_4} \left\|f'(z)\right\|, \quad m_2 = \max_{z\in\Pi_4} \left\|f''(z)\right\|, \quad m_3 = \max_{z\in\Pi_4} \left\|f'''(z)\right\|,$$

where $\|\cdot\|$ is the Euclidean norm of tensor quantities of type $(1,0), (1,1), (1,2)$, and $(1,3)$, respectively [10].

It is easy to establish the following exact estimates:

$$0.83 < m_0 < 0.85, \quad 4.8 < m_1 < 4.9, \quad 6.9 < m_2 < 7, \quad m_3 = 2\sqrt{6}. \tag{3.1}$$

Let $P = \{z \in \mathbb{R}^d | -0.001 \le z_i \le 0.001, \ i = \overline{1,4}\}$. Using the Minkowski–Pontryagin difference [21], we construct the parallelepipeds $\Pi_j = \Pi_4 \dot{-} (4-j)\,P, \ j = 0,1,2,3$.

Obviously, $\Pi_0 \subset \Pi_1 \subset \Pi_2 \subset \Pi_3 \subset \Pi_4$ and $\operatorname{dist}(\Pi_j, \ \partial\Pi_{j+1}) = 0.001, \ j = 0,1,2,3$.

Let $\Sigma^{(1)}$ be a hyperplane passing through the point $z_0^{(1)}$ and orthogonal to the vector $f\big(z_0^{(1)}\big)$. On the hyperplane $\Sigma^{(1)}$, we introduce the Cartesian coordinate system (u,v,w) with the origin $z_0^{(1)}$.

As a basis on $\Sigma^{(1)}$, we take the vectors $u, \ v, \ w \in \mathbb{R}^4$ with the coordinates

$$\begin{gathered} u_1 = n_2, \quad u_2 = -n_1, \quad u_3 = n_4, \quad u_4 = -n_3, \\ v_1 = \sqrt{n_3^2 + n_4^2}, \quad v_2 = 0, \quad v_3 = -\frac{n_1 n_3 + n_2 n_4}{v_1}, \quad v_4 = \frac{n_2 n_3 - n_1 n_4}{v_1}, \\ w_1 = 0, \quad w_2 = v_1, \quad w_3 = -v_4, \quad w_4 = v_3, \end{gathered} \tag{3.2}$$

where $n_i = f_i(z_0^{(1)}) / \big|f(z_0^{(1)})\big| \big|f(z_0^{(1)})\big|, \ i = \overline{1,4}$. It is easy to verify that the vectors $u, \ v, \ w$ defined by (3.2) really form an orthonormal basis on $\Sigma^{(1)}$.

As the domain of the Poincaré map, we take the parallelepiped

$$S^{(1)} = \Big\{\xi = (\xi_1, \, \xi_2, \, \xi_3) \, \Big| \, \xi \in \Sigma^{(1)}, \, -325\delta \le \xi_1 \le 325\delta, -20\delta \le \xi_2 \le 20\delta, \, -24\delta \le \xi_3 \le 24\delta \Big\} \subset \Sigma^{(1)}.$$

Next, we construct a grid

$$K_\delta^{(1)} = \delta M_\delta^{(1)} \subset S^{(1)},$$

where $\delta = 4 \cdot 10^{-6}$, $M_\delta^{(1)} = \big\{(i, \, j, \, k) \in \mathbb{Z}^3 \, | \, -325 \le i \le 325, \, -20 \le j \le 20, \, -24 \le k \le 24\big\}$. Note that the grid $K_\delta^{(1)}$ contains exactly 1307859 nodes.

It is known that, if analytical and topological methods are not enough for studying the nonlocal qualitative properties of dynamical systems, then one has to involve the methods of numerical integration and computer visualization. The corresponding approach was given the special name "Computational Dynamics" [13].

For numerical integration of system (2.1), we apply the Runge–Kutta method [7, 9, 15]. For our purpose, a second-order accuracy scheme is sufficient:

$$\tilde{z}^{(n+1)} = \tilde{z}^{(n)} + F\big(k_1(\tilde{z}^{(n)}, \ h), \, k_2(\tilde{z}^{(n)}, \ h)\big), \quad n = 0, \, 1, \, \ldots, \tag{3.3}$$

where $F\,(k_1, \ k_2) = 0.5\,(k_1 + k_2)\,, \ k_1 = hf(z), \ k_2 = hf(z + k_1)$, and $\tilde{z}^{(0)} \in K_\delta^{(1)}$.

We call the approximate solution $\tilde{z}^{(n)}$ obtained by formula (3.3) the *discrete trajectory* of system (2.1). Note that one cannot find the discrete trajectory explicitly as well as the trajectory of the Cauchy problem, despite the fact that system (2.1) is polynomial. Therefore, one has to work with another sequence of vectors $\tilde{\zeta}^{(n)}$ to be obtained by rounding the values of $\tilde{z}^{(n)}$ by a computer [8, 16].

Indeed, in real calculations, due to rounding of the results of arithmetic operations by a computer (in our case, we used a computer with IntelCore i5 processor, frequency of 2.50 GHz and with extended accuracy), instead of the sequence $\tilde{z}^{(n)}$, we get another sequence of vectors $\tilde{\zeta}^{(n)}$. We call this solution a *numerical trajectory* of system (2.1).

Let $z_{uvw}(t)$ be the trajectory starting from the point $z_{uvw}(0) \in S^{(1)}$, and let $\tilde{z}_{ijk}(t)$ be the trajectory corresponding to the trajectory $z_{uvw}(t)$ and starting from the point $\tilde{z}_{ijk}(0) \in K_\delta^{(1)}$ close to $z_{uvw}(0)$, i.e., $i = [u/h + 1/2]$, $j = [v/h + 1/2]$, and $k = [w/h + 1/2]$. It is easy to see that $|z_{uvw}(0) - \tilde{z}_{ijk}(0)| \le \sqrt{3}/2\delta$.

In [27], an algorithm based on a partitioning process and using the interval arithmetics with directed rounding is proposed for computing rigorous solutions to a large class of ordinary differential equations. As an application, it was proved that the Lorenz system supports a strange attractor.

In the present paper, the DN-tracking method is used as the method of proof of the existence of a closed trajectory. It is based on the estimations of the accuracy of numerical and discrete solutions approximating the solution of system (2.1). This requires rigorous proof of the inequalities establishing the accuracy of the estimate. Therefore, it is necessary to derive the required estimate with deductive rigour. The estimations given below were derived in [6] for the considering scheme (3.3) based on two preliminary assumptions.

Assumption 1. *The trajectory $z_{uvw}(t)$ exists on a time interval $0 \le t \le T$ and $z_{uvw}(t) \in \Pi_4$.*

Assumption 2. *The inclusion $\tilde{z}^{(n)} \in \Pi_1$ holds for all $n = 0, 1, \dots, N$.*

Estimation 1.

$$\left|\tilde{\zeta}^{(n+1)} - \tilde{\zeta}^{(n)}\right| < m_0 h + \Delta_*, \quad n = \overline{0, N},$$

where Δ_* is the local round-off error that produced by scheme (3.3). In our case, the inequality $\Delta_* < 10^{-14}$ holds.

Estimation 2.

$$\left|\tilde{z}^{(n)} - \tilde{\zeta}^{(n)}\right| < \frac{e^{LT} - 1}{Lh}\Delta_*, \quad n = \overline{0, N}, \tag{3.4}$$

where $L = m_1 + 0.5m_1^2 h$.

Estimation 3.

$$\left|\tilde{z}_{ijk}(nh) - \tilde{z}^{(n)}\right| < \frac{m_0^2 m_2 + 4m_0 m_1^2}{12m_1}\left(e^{m_1 T} - 1\right)h^2, \quad n = \overline{0, N}, \tag{3.5}$$

where $\tilde{z}_{ijk}(0) = \tilde{z}^{(0)}$.

Estimation 4.

$$|\tilde{z}_{ijk}(t) - \tilde{z}_{ijk}(nh)| < \frac{m_0 h}{2},$$

where $n = [t/h + 1/2]$.

Estimation 5.

$$|z_{uvw}(t) - \tilde{z}_{ijk}(t)| < \frac{\sqrt{3}}{2}e^{m_1 T}\delta. \tag{3.6}$$

By estimate (3.1), $m_1 > 4.8$; hence, $e^{m_1 T} > 3 \cdot 10^{17}$. This inequality means that estimates (3.4), (3.5), and (3.6) are not effective for tracking the trajectories of $z_{uvw}(t)$ on the time interval $[0,\ 8.37]$. Therefore, to overcome this difficulty, we use the technique of dividing the interval into 23 subintervals:

$$J^{(m)} = [0.37(m-1),\ 0.37m + 0.03], \quad m = 1, 2, \dots, 22$$

(of length 0.40) and the last one is

$$J^{(23)} = [8.14,\ 8.37]$$

(of length 0.23).

In this case, on each time interval $J^{(m)}$, estimates (3.4)–(3.6) are acceptable to apply the DN-tracking.

3.2. Constructing a map on the first segment

Further, we continue the reasoning on the first segment $J^{(1)} = [0,\, 0.4]$. Let $\tilde{z}_*(t)$ be one of the trajectories $\tilde{z}_{ijk}(t)$, let $\tilde{z}_*^{(n)}$ be the discrete trajectory corresponding to $\tilde{z}_*(t)$, i.e., a solution of system (2.1) with the initial condition $\tilde{z}_*^{(0)} = \tilde{z}_*(0) \in K_\delta^{(1)}$, and let $\zeta_*^{(n)}$ be the numerical trajectory corresponding to $\tilde{z}_*^{(n)}$. We put $h = 2^{-16}$, $T = 0.40$, and $N = [T/h] = 26214$.

Using Estimations 1–5 and the method of proof by contradiction, the following Lemmas can be proved in the same way as in [6]. Therefore, here we restrict ourselves to proving Lemma 3.

Lemma 1. *For all $n = 0,\, 1,\, \ldots,\, N$,*

$$\zeta_*^{(n)} \in \Pi_0 \quad \textit{and} \quad \left|\tilde{\zeta}_*^{(n+1)} - \tilde{\zeta}_*^{(n)}\right| < 1.4 \cdot 10^{-5}. \tag{3.7}$$

Since $\zeta_*^{(n)}$ is a numerical solution kept in the memory of a computer, the validity of the first inclusion in (3.7) is verified by the computer, while the inequality in (3.7) is derived by means of Estimation 1.

Lemma 2. *The estimate*

$$\left|\tilde{z}_*^{(n)} - \tilde{\zeta}_*^{(n)}\right| < 8.2 \cdot 10^{-10} \tag{3.8}$$

holds as long as $\tilde{z}_*^{(k)} \in \Pi_1$, $k = 0, 1, 2, \ldots, n$.

Estimate (3.8) can be easily obtained by using estimates (3.1) and substituting the values $T = 0.40$ and $h = 2^{-16}$ into the right hand side of (3.4) in Estimation 3.

Lemma 3. *Assumption 2 holds.*

P r o o f. By Lemma 2, we obtain

$$\left|\tilde{z}_*^{(n)} - \tilde{\zeta}_*^{(n)}\right| < 8.2 \cdot 10^{-10},$$

when the inclusion $\tilde{z}_*^{(n)} \in \Pi_1$ holds. We now show that this inclusion holds for all $n = 0,\, 1,\, \ldots,\, N$. We assume the contrary, let for some minimal $n_* \geq 1$, we have $\tilde{z}_*^{(n_*-1)} \in \Pi_1$, but $\tilde{z}_*^{(n_*)} \notin \Pi_1$. Then

$$\left|\tilde{z}_*^{(n_*)} - \tilde{\zeta}_*^{(n_*)}\right| < \left|\tilde{z}_*^{(n_*)} - \tilde{z}_*^{(n_*-1)}\right| + \left|\tilde{z}_*^{(n_*-1)} - \tilde{\zeta}_*^{(n_*-1)}\right| + \left|\tilde{\zeta}_*^{(n_*-1)} - \tilde{\zeta}_*^{(n_*)}\right|.$$

Since by the scheme (3.3) one has the estimation

$$\left|\tilde{z}_*^{(n_*)} - \tilde{z}_*^{(n_*-1)}\right| \leq \max_{z \in \Pi_1} |F(k_1(z), k_2(z))| < m_0 h < 1.3 \cdot 10^{-5},$$

and by assumption, we have $\tilde{z}_*^{(n_*-1)} \in \Pi_1$ so one can apply Lemma 2 and get the estimation $\left|\tilde{z}_*^{(n_*-1)} - \tilde{\zeta}_*^{(n_*-1)}\right| < 8.2 \cdot 10^{-10}$. As for the estimation $\left|\tilde{\zeta}_*^{(n_*-1)} - \tilde{\zeta}_*^{(n_*)}\right| < 1.4 \cdot 10^{-5}$, it follows from Lemma 1.

Therefore,

$$\left|\tilde{z}_*^{(n_*)} - \tilde{\zeta}_*^{(n_*)}\right| < 2.8 \cdot 10^{-5}. \tag{3.9}$$

Since $\tilde{\zeta}_*^{(n_*)} \in \Pi_0$ and $\operatorname{dist}(\Pi_0,\, \partial\Pi_1) = 0.001$, therefore, (3.9) implies that $\tilde{z}_*^{(n_*)} \in \Pi_1$. This contradicts the above assumption $\tilde{z}_*^{(n_*)} \notin \Pi_1$. Thus, the inclusion $\tilde{z}_*^{(n)} \in \Pi_1$ holds for all $n = 0,\, 1,\, \ldots,\, N$, i.e., Assumption 2 holds. □

Lemma 4. *For all* $n = 0,\, 1,\, \ldots,\, N$,

$$\tilde{z}_*\,(nh) \in \Pi_2 \ \textit{and}\ \left|\tilde{z}_*\,(nh) - \tilde{z}_*^{(n)}\right| < 2.1 \cdot 10^{-9}.$$

Lemma 5. *Let* $t \in J^{(1)}$ *and* $n = [t/h + 1/2]$. *Then*

$$\tilde{z}_*(t) \in \Pi_3 \ \textit{and}\ |\tilde{z}_*(t) - \tilde{z}_*(nh)| < 6.49 \cdot 10^{-6}.$$

Lemma 6. *Let* $t \in J^{(1)}$ *and* $(u, \vartheta, w) \in S^{(1)}$. *Then*

$$z_{u\vartheta w}(t) \in \Pi_4 \ \textit{and}\ |z_{u\vartheta w}(t) - z_{ijk}(t)| < 2.46 \cdot 10^{-5}.$$

Lemmas 1–6 imply that Assumption 1 holds on the first segment $J^{(1)}$ and the following theorem is true.

Theorem 2. *Let* $t \in J^{(1)}$. *Then*

$$z_{uvw}(t) \in \Pi_4 \quad \textit{and} \quad \left|z_{uvw}(t) - \tilde{\zeta}_{ijk}^{(n)}\right| < 3.11 \cdot 10^{-5} = \varepsilon. \tag{3.10}$$

The estimation (3.10) means that one can track any real trajectory $z_{uvw}(t)$ of system (2.1) by means of the numerical trajectory $\tilde{\zeta}_{ijk}^{(n)}$ with accuracy ε.

Let $z_0^{(2)} = \tilde{\zeta}_{000}^{(N-1966)}$, and let $\Sigma^{(2)}$ be a hyperplane with normal $f\big(z_0^{(2)}\big)$ and passing through the point $z_0^{(2)}$.

Theorem 3. *Each trajectory* (2.1) *intersects the hyperplane* $\Sigma^{(2)}$ *at some time* $t_{uvw} \in (T - 0.06,\, T) = (0.34,\, 0.4)$.

The proof of this theorem is directly verified by a computer by showing that the points $\tilde{\zeta}_{ijk}^{(N-3932)}$ and $\tilde{\zeta}_{ijk}^{(N)}$ lie in the half-spaces

$$\Omega_+ = \left\{ z \,\middle|\, \big\langle z - z_0^{(2)},\, f\big(z_0^{(2)}\big)\big\rangle > 0 \right\}, \quad \Omega_- = \left\{ z \,\middle|\, \big\langle z - z_0^{(2)},\, f\big(z_0^{(2)}\big)\big\rangle < 0 \right\},$$

respectively. Moreover, the distances between these points and $\Sigma^{(2)}$ are not less than ε (Fig. 1).

Therefore, every trajectory $z_{uvw}(t)$ crosses the plane $\Sigma^{(2)}$ at some $t_{uvw} \in (0.34,\, 0.4)$ and by the implicit function theorem it follows that the function t_{uvw} is continuous in $(u,\, v,\, w) \in S^{(1)}$.

Thus, we obtain a map $\Phi_{(1)}^{(2)}$ of the parallelepiped $S^{(1)}$ onto the plane $\Sigma^{(2)}$, which relates each point $(u,\, v, w) \in S^{(1)}$ to a point $z_{uvw}\,(t_{uvw})$ where $z_{uvw}(t)$ intersects the plane $\Sigma^{(2)}$. We denote the set of these points by $S^{(2)}$. The continuity of the map $\Phi_{(1)}^{(2)}$ follows from the theorem on the continuous dependence of solutions on the initial point.

3.3. Constructing Poincaré map

For the time segments $J^{(m)}$, $m = \overline{2, 22}$, we choose the values of h, T, and δ the same as for the first segment. Therefore, the estimation (3.10) does not change, that is, ε remains unchanged.

On the hyperplane $\Sigma^{(2)}$, we introduce again the Cartesian coordinate system (u, v, w) with the origin $z_0^{(2)}$ taking the basis on it the vectors defined by (3.2).

Let $S_\varepsilon^{(2)} = \bigcup\limits_{p \in S^{(2)}} B_\varepsilon(p)$ be the ε-neighborhood of the set $S^{(2)}$, where $B_\varepsilon(p)$ is a ball with centre p and radius ε. We denote again the trajectory starting from the point $(u, v, w) \in S_\varepsilon^{(2)}$ and the corresponding numerical trajectory by $z_{uvw}(t)$ and $\tilde{\zeta}^{(n)}_{ijk}$, respectively, where $i = [u/h + 1/2]$, $j = [v/h + 1/2]$, and $k = [w/h + 1/2]$.

For the segment $J^{(2)}$, the existence of a map $\Phi^{(3)}_{(2)}$ of the domain $S^{(2)}_{\varepsilon} \subset \Sigma^{(2)}$ to the plane $\Sigma^{(3)}$ passing through the point $z^{(3)}_0 = \tilde{\zeta}^{(N-1966)}_{00}$ and orthogonal to the vector $f\big(z^{(3)}_0\big)$ is established similar to the construction for the first segment.

Repeating a similar reasoning and calculations, we obtain 21 continuous mappings

$$\Phi^{(m+1)}_{(m)} : S^{(m)}_{\varepsilon} \to \Sigma^{(m+1)}, \quad m = 2, 3, \ldots, 22.$$

The last segment $J^{(23)} = [8.14, 8.37]$ requires a special consideration. Consider an ensemble of trajectories $z_{uvw}(t)$ with starting points in $S^{(23)}_{\varepsilon}$. Putting $h = 2^{-16}$, $T = 0.23$, and $N = [T/h] = 15073$, we find numerical trajectories $\tilde{\zeta}^{(n)}_{ijk}$ approximating the ensemble of trajectories $z_{uvw}(t)$.

Then, for the time interval $J^{(23)}$, we prove the following statement.

Theorem 4. *Let $t \in J^{(23)}$. Then*

$$z_{uvw}(t) \in \Pi_4 \quad \textit{and} \quad \left|z_{uvw}(t) - \tilde{\zeta}^{(n)}_{ijk}\right| < 1.72 \cdot 10^{-5} = \varepsilon. \tag{3.11}$$

Theorem 5. *Let Π^+ and Π^- be open half-spaces defined by the hyperplane $\Sigma^{(1)}$; more precisely,*

$$\Pi^+ = \Big\{z \in R^4 | \big\langle z - z^{(1)}_0, f\big(z^{(1)}_0\big)\big\rangle > 0\Big\} \quad \textit{and} \quad \Pi^- = \Big\{z \in R^4 | \big\langle z - z^{(1)}_0, f\big(z^{(1)}_0\big)\big\rangle < 0\Big\}.$$

Then $\tilde{\zeta}^{(N-3932)}_{ijk} \in \Pi^-$ and $\tilde{\zeta}^{(N)}_{ijk} \in \Pi^+$ for all i, j, k.

Corollary 1. *Every trajectory*

$$z_{uvw}(t) \ \textit{with} \ (u, v, w) \in S^{(23)}_{\varepsilon}$$

reaches the hyperplane $\Sigma^{(1)}$ at some time $t_{uvw} \in (8.34, 8.37)$.

Mapping a point $(u, v, w) \in S^{(23)}_{\varepsilon}$ to the point $z_{uvw}(t_{uvw})$, we get a continuous mapping $\Phi^{(1)}_{(23)}$: $S^{(23)}_{\varepsilon} \to \Sigma^{(1)}$. Next, we set

$$\Phi = \Phi^{(1)}_{(23)} \circ \Phi^{(23)}_{(22)} \circ \ldots \circ \Phi^{(2)}_{(1)}.$$

As a result, we obtain the required Poincaré map (Fig. 2).

Let $S^{\omega} = \Phi\left(S^{(1)}\right)$ and, for fixed i, j, k, let n_{ijk} be the number of the term of the sequence $\tilde{\zeta}^{(n)}_{ijk}$ closest to the hyperplane $\Sigma^{(1)}$. We denote the set of all points $\tilde{\zeta}^{(n_{ijk})}_{ijk}$ by $\widetilde{Z}$. It can be easily checked by computer that the following inequalities hold for every $\tilde{\zeta}^{(n_{ijk})}_{ijk} = \left(\tilde{\zeta}^*_1, \tilde{\zeta}^*_2, \tilde{\zeta}^*_3\right) \in \widetilde{Z}$:

$$-316.6\,\delta < \tilde{\zeta}^*_1 < 316.74\,\delta, \quad -11.17\,\delta < \tilde{\zeta}^*_2 < 11.49\,\delta, \quad -15.70\,\delta < \tilde{\zeta}^*_3 < 15.25\,\delta.$$

(The range of all projections of numerical trajectories $\tilde{\zeta}^{(n_{ijk})}_{ijk} = \left(\tilde{\zeta}^*_1, \tilde{\zeta}^*_2, \tilde{\zeta}^*_3\right)$ to the hyperplane $\Sigma^{(m)}$, $m = 1, 2, \ldots, 23$, is provided in Table 1.)

It follows then from estimate (3.11) and the inequalities

$$|z_1^*| < \left|z_1^* - \tilde{\zeta}_1^*\right| + \left|\tilde{\zeta}_1^*\right| < \varepsilon + 316.74\,\delta < 322\,\delta,$$
$$|z_2^*| < \left|z_2^* - \tilde{\zeta}_2^*\right| + \left|\tilde{\zeta}_2^*\right| < \varepsilon + 11.49\,\delta < 16\,\delta,$$
$$|z_3^*| < \left|z_3^* - \tilde{\zeta}_3^*\right| + \left|\tilde{\zeta}_3^*\right| < \varepsilon + 15.70\,\delta < 21\,\delta,$$

that (Fig. 3)

$$S^\omega \subset \operatorname{Int} S^{(1)},$$

where $(z_1^*, z_2^*, z_3^*) = z_{uvw}(t_{uvw}) - z_0^{(1)}$.

Therefore, it follows from Brouwer's fixed point theorem [23] that the map Φ has a fixed point $z^* \in S^{(1)}$ that is $\Phi(z^*) = z^*$ and therefore, the trajectory passing through this point will be closed.

Applying the DN-tracking method for each fixed value of $\tilde{\beta} \in (0.431,\ 1.173)$, one can prove the following theorem.

Theorem 6. *For $\tilde{\beta} \in (0.431,\ 1.173)$, system (2.1) has a closed trajectory.*

4. Conclusion

In the present paper, a Brusselator model has been studied. The main contribution of the paper is as follows:

(1) a new modified four-dimensional Brusselator model, having cyclical property, has been proposed;

(2) the existence of a closed trajectory for this model has been established.

To prove the existence of a closed trajectory, the DN-tracking method has been applied.

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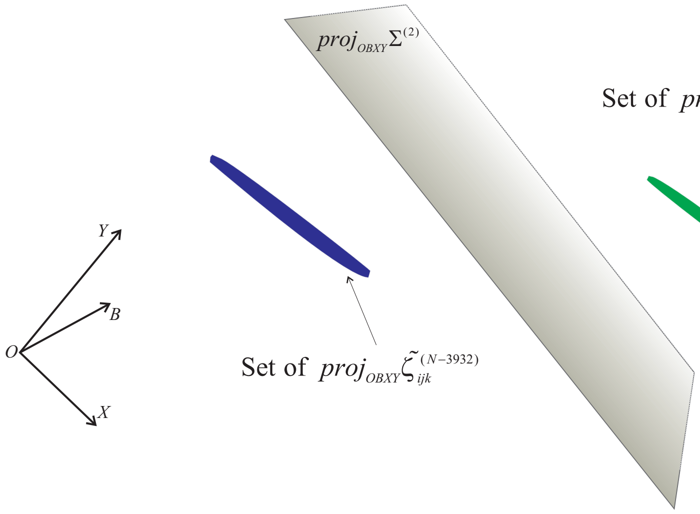

Figure 1. Parallel projection set of points $\tilde{\zeta}_{ijk}^{(N-3932)}$ and $\tilde{\zeta}_{ijk}^{(N)}$ onto the space $OBXY$ with parallel projection direction which is perpendicular to the normal $f\left(z_0^{(2)}\right)$.

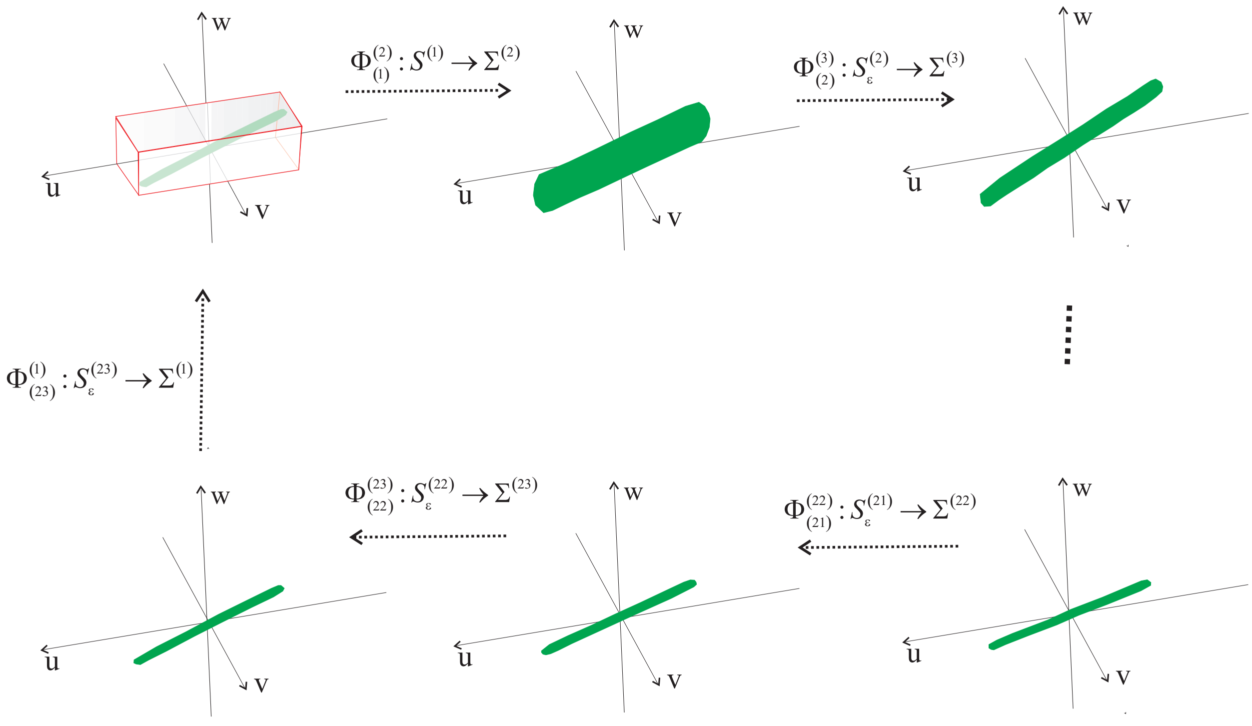

Figure 2. Some components of the Poincaré map. Scale u:v:w=1:5:5.

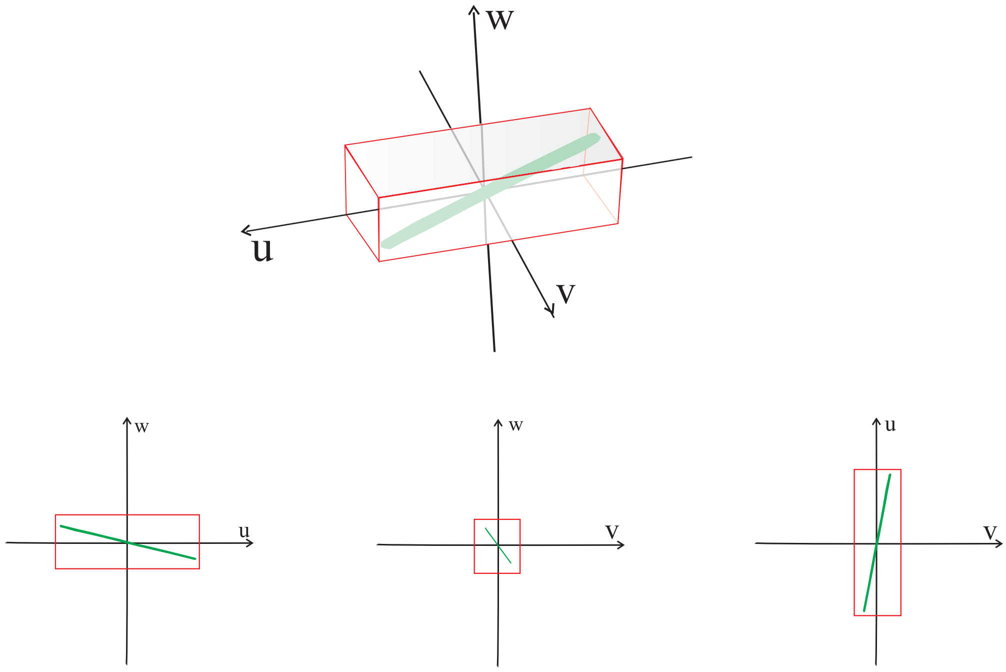

Figure 3. Poincaré map $\Phi : S^{(1)} \to \Sigma^{(1)}$ in axonometric and 2d-projections. Scale u:v:w=1:5:5.

Table 1. The range of all orthogonal projections of numerical trajectories $\tilde{\zeta}_{ijk}^{(n_{ijk})}$ to the hyperplane $\Sigma^{(m)}$.

m	min $\tilde{\zeta}_1^*$	max $\tilde{\zeta}_1^*$		min $\tilde{\zeta}_2^*$	max $\tilde{\zeta}_2^*$		min $\tilde{\zeta}_3^*$	max $\tilde{\zeta}_3^*$
1	-325δ	325δ		-20δ	20δ		-25δ	25δ
2	-346.69δ	347δ		-28.58δ	28.56δ		-29.28δ	29.39δ
3	-378.63δ	379.78δ		-30.23δ	30.06δ		-35.87δ	36.01δ
4	-437.25δ	440.32δ		-33.60δ	33.39δ		-44.64δ	44.70δ
5	-538.99δ	546.29δ		-44.24δ	44.24δ		-55.30δ	55.16δ
6	-714.57δ	729.62δ		-70.09δ	70.86δ		-63.22δ	62.94δ
7	-977.87δ	989.04δ		-117.06δ	117.88δ		-42.42δ	43.18δ
8	-1090.88δ	1087.21δ		-122.66δ	122.04δ		-38.73δ	38.60δ
9	-890.64δ	896.91δ		-56.55δ	56.70δ		-72.00δ	72.36δ
10	-704.54δ	705.84δ		-14.71δ	14.53δ		-56.05δ	56.24δ
11	-599.26δ	597.09δ		-8.01δ	8.01δ		-35.44δ	35.46δ
12	-552.71δ	549.30δ		-14.02δ	13.90δ		-17.81δ	17.87δ
13	-552.12δ	548.61δ		-18.26δ	18.16δ		-2.43δ	2.61δ
14	-600.14δ	597.67δ		-20.19δ	20.00δ		-12.66δ	12.99δ
15	-716.87δ	717.77δ		-18.51δ	18.12δ		-31.28δ	31.71δ
16	-928.67δ	932.88δ		-7.67δ	7.77δ		-55.90δ	56.48δ
17	-1066.81δ	1063.65δ		-43.75δ	43.42δ		-56.06δ	56.34δ
18	-821.69δ	837.41δ		-54.46δ	54.83δ		-17.07δ	16.16δ
19	-583.27δ	592.99δ		-38.93δ	39.02δ		-1.67δ	1.35δ
20	-450.01δ	454.21δ		-27.18δ	27.05δ		-0.84δ	0.69δ
21	-378.01δ	379.81δ		-19.75δ	19.57δ		-3.14δ	3.07δ
22	-340.45δ	341.26δ		-15.07δ	14.90δ		-7.40δ	7.38δ
23	-325.12δ	325.59δ		-12.38δ	12.23δ		-12.63δ	12.64δ