

STABILITY AND A NUMERICAL SOLUTION OF FRACTIONAL-ORDER BRUSSELATOR CHEMICAL REACTION SYSTEM

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ABSTRACT. In this paper, we focus on the local stability of the fractional-order Brusselator chemical reaction system (FOBS) with incommensurate order for the first time, which is a famous model of chemical reactions. Then, we apply the piecewise constant arguments (PWCA) for obtaining numerical solution of FOBS. This method is an approximation for the right-hand side of the fractional-order system (FOS). It is different from the usual discretization process for FOS. And fortunately, once again it can be confirmed that some amazing phenomena are quite similar to limit cycle. Through graph comparison and statistical analysis, these show that the numerical solutions are consistent with existing results. These also show that the PWCA is an effective method for solving FOS. Finally, some discussions of limit cycles are given.

1. INTRODUCTION

Fractional calculus has a longer history than integer calculus. However, the application of fractional derivatives and integrals has been infrequent until the last century. Insofar as it concerns the application of fractional derivative operator, there have many areas such as viscoelastic damping, anomalous diffusion process, signal processing, electrochemistry, fluid flow, chemistry and so on [1, 2, 3, 4]. In many previous studies, the existence or no-existence of periodic solution and limit cycle of fractional-order equation (system) are important research directions [5, 6, 7, 8, 9, 10, 11]. These references shown that FOS cannot generate exactly periodic signals and limit cycle. But, the fractional derivative of a periodic signal is periodic if it is defined on the whole real line. The limit cycle observed in numerical simulations of FOS cannot be an exact periodic solution. It is just a kindred limit cycle, not really limit cycle.

In other relevant references, many numerical observations show that some FOS exhibits limit cycle. However, it can only be observed after long-term refined simulations. That means an asymptotic periodicity can be observed as t increases to

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infinity, i.e., $\lim_{t \rightarrow \infty} [f(t+T) - f(t)] = 0$ with an asymptotic period $T > 0$ [12, 13]. In process of numerical simulation, the obtained results of discretization of FOS are approximation. Thus, the observed limit cycle is a phenomenon of approximation. It is just very similar to limit cycle.

The Brusselator system is a famous model of chemical reaction with oscillations. It is different from most chemical reaction, where, a state of homogeneity and equilibrium is quickly reached. The reaction is a remarkable chemical reaction that maintains a prolonged state of non-equilibrium leading to macroscopic temporal oscillations. The partial differential equation form of Brusselator chemical reaction system is as following[14, 15, 16, 17, 18, 19, 20].

$$\begin{aligned}\frac{\partial u}{\partial t} &= a - (\mu + 1)u + u^2v + k_1 \frac{\partial^2 u}{\partial x^2}, \\ \frac{\partial v}{\partial t} &= \mu u - u^2v + k_2 \frac{\partial^2 v}{\partial x^2},\end{aligned}\quad (1)$$

where a, μ, k_1, k_2 are constants. When we consider the case of the absence of diffusion, i.e., $k_1 = k_2 = 0$ and rewrite $u(t), v(t)$ as $x(t), y(t)$ respectively. The system (1) reduce to the following ordinary differential equation form[21, 22, 23, 24].

$$\begin{aligned}\frac{dx(t)}{dt} &= a - (\mu + 1)x(t) + x(t)^2y(t), \\ \frac{dy(t)}{dt} &= \mu x(t) - x(t)^2y(t),\end{aligned}\quad (2)$$

This system has a unique limit cycle when $\mu > a^2 + 1$ and it has a stable limit cycle for $(a - 1)^2 < \mu < a^2 + 1$ [25].

In recent years, the corresponding fractional-order Brusselator chemical reaction system is mathematically described as follows.

$$\begin{aligned}D^{\alpha_1} x(t) &= a - (\mu + 1)x(t) + x(t)^2y(t), \\ D^{\alpha_2} y(t) &= \mu x(t) - x(t)^2y(t),\end{aligned}\quad (3)$$

where $0 < \alpha_1, \alpha_2 \leq 1$, $x(t), y(t)$ are activator and inhibitor variables, a and μ are external parameters(the relationship between them determines the system dynamics)[25, 26, 27, 28, 29, 30, 31]. If $(\alpha_1, \alpha_2) = (1, 1)$, then the system (3) is the classical Brusselator system. If $0 < \alpha_1 = \alpha_2 = \alpha < 1$, the system (3) is commensurate order. Otherwise, it is incommensurate order ($\alpha_1 \neq \alpha_2$).

In this paper, we mainly study two problems. One is the local stability of FOBS with incommensurate order. This is complementary of the previous study. On the other hand, PWCA is firstly applied to solve FOBS. The obtained numerical results (including kindred (false) phenomenon of limit cycle) are in agreement with previous findings in the literatures.

The rest of the paper is organized as follows. In Section 2, the basic concepts of fractional derivative are presented. In Section 3, local stable and numerical solutions of FOBS are investigated based on theory of stability and PWCA. In the last Section, possible reasons for generating kindred (false) limit cycles are discussed and conclusions are drawn.

2. PRELIMINARIES AND NOTATIONS

There are several definitions of fractional derivative. The Grunwald-Letnikov, Riemann-Liouville and Caputo definitions are used for the general fractional differential equation. Here and throughout, the Caputo-type definition is used[2, 3, 4].

Definition 1. A real function $f(t), t > 0$ is said to be in space $C_\alpha, \alpha \in R$ if there exists a real number $p(> \alpha)$, such that $f(t) = t^p f_1(t)$ where $f_1(t) \in C[0, \infty]$.

Definition 2. A real function $f(t), t > 0$ is said to be in space $C_\alpha^m, m \in \mathbb{N} \cup \{0\}$ if $f^{(m)}(t) \in C_\alpha$.

Definition 3. The function $\Gamma : (0, \infty) \rightarrow \mathbb{R}$, defined by $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$, is called Euler's Gamma function.

Definition 4. The Riemann-Liouville integral operator of order $\beta > 0$ is defined as

$$J^\beta z(t) = \frac{1}{\Gamma(\beta)} \int_0^t (t - \tau)^{\beta-1} z(\tau) d\tau, \quad (4)$$

where $\Gamma(\cdot)$ is the Euler's Gamma function.

Definition 5. The Caputo fractional derivative of $y(t), y(t) \in C_{-1}^m, m \in \mathbb{N} \cup \{0\}$, is defined as

$$D^\alpha y(t) = J^{m-\alpha} y^{(m)}(t), \quad \alpha > 0, \quad (5)$$

where $m = [\alpha]$, i.e., m is the first integer which is no less than α , $y^{(m)}$ is the ordinary m th derivative of y , J is the Riemann-Liouville integral operator.

Note that for $m - 1 < \alpha \leq m$ ($m \in \mathbb{N}$), $J^\alpha D_*^\alpha y(t) = y(t) - \sum_{k=0}^{m-1} \frac{d^k y}{dt^k}(0) \frac{t^k}{k!}$, and for $\alpha \rightarrow m$, the Caputo fractional derivative of (5) becomes a conventional m th derivative. In this paper, the α is limited in $(0, 1]$. Since it is integral form, the Caputo derivative has a relationship with all of the function history information and a chemical reaction model described by FOS will possess memory.

Definition 6. Limit cycle is a closed trajectory in phase space of a dynamical system having the property that at least one other trajectory spirals into it either as time approaches infinity or as time approaches minus-infinity.

Isolated periodic solutions of the systems are called limit cycles[5].

Definition 7. [32] A non-constant solution $x(t)$ of any system is said to be a periodic solution if there exists $T > 0$ such that $x(t) = x(t + T)$ for all $t \in \mathbb{R}$.

3. FRACTIONAL-ORDER BRUSSELATOR SYSTEM

3.1. Stability analysis. The system (3) has a unique equilibrium point $E = (a, \frac{\mu}{a})$. For the commensurate case, there have the following local stable results. "There exists a marginal value α_0 such that the equilibrium E is locally asymptotically stable if $\alpha < \alpha_0$ and it is unstable if $\alpha > \alpha_0$ " (See the equations (4)-(6) in [25]). For further analysis, it is necessary to have the following lemma.

Lemma 1. [33] Suppose that α_i 's are rational numbers between 0 and 1, for $i = 1, 2, \dots, n$. Let $\gamma = 1/m$ where m is the least common multiple of the denominators m_i of α_i 's, where $\alpha_i = k_i/m_i, k_i, m_i \in \mathbb{N}, i = 1, 2, \dots, n$. Then the system $D^\alpha x(t) = Ax(t), x(0) = x_0$ is asymptotically stable if all roots λ of the equation $\det(\text{diag}(\lambda^{m\alpha_1}, \lambda^{m\alpha_2}, \dots, \lambda^{m\alpha_n}) - A) = 0$ satisfy $|\arg(\lambda)| > \gamma\pi/2$.

Based on the Lemma 1 and extended condition $\mu \geq 0$, we have the following result.

Theorem 1. For the incommensurate case, when $\mu = 0$, α_i 's are rational numbers and lie in $(0, 1)$, then the equilibrium E of the system (3) is locally asymptotically stable.

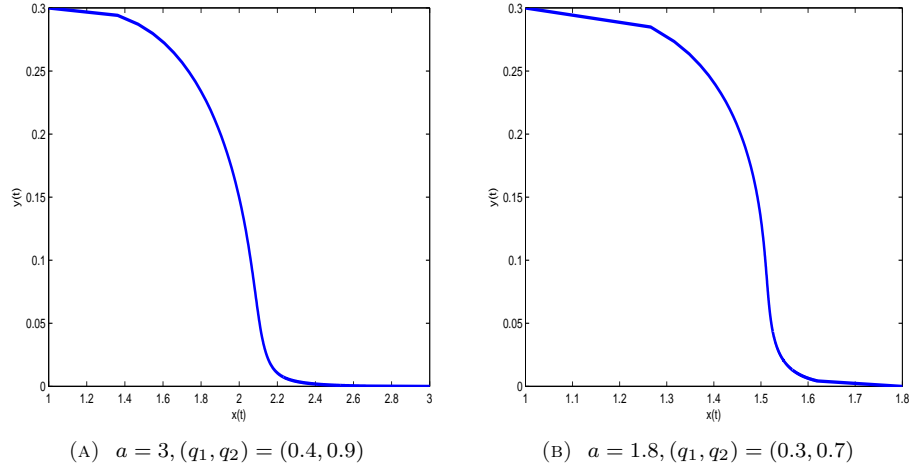


FIG. 1. Locally asymptotically stable of the equilibrium point $E = (a, 0)$ in the system (3).

Proof. Since α_i 's are rational numbers, we assume that $\alpha_1 = \frac{k_1}{m_1}$, $\alpha_2 = \frac{k_2}{m_2}$, $\gamma = \frac{1}{m}$, m is the least common multiple of the m_1 and m_2 , and $m = n_1 m_1$, $m = n_2 m_2$. The Jacobian matrix of the system (3) at the equilibrium point is

$$J|_E = \begin{bmatrix} -(\mu + 1) + 2xy & x^2 \\ \mu - 2xy & -x^2 \end{bmatrix}_{(x,y)=(a,\frac{\mu}{a})} = \begin{bmatrix} \mu - 1 & a^2 \\ -\mu & -a^2 \end{bmatrix}.$$

Thus,

$$\det(\text{diag}(\lambda^{m\alpha_1}, \lambda^{m\alpha_2}) - J|_E) = 0, \quad (6)$$

i.e., $(\lambda^{m\alpha_1} - \mu + 1)(\lambda^{m\alpha_2} + a^2) + a^2\mu = 0$. That is

$$(\lambda^{n_1 k_1} - \mu + 1)(\lambda^{n_2 k_2} + a^2) + a^2\mu = 0, \quad (7)$$

i.e., $\lambda^{n_1 k_1} \lambda^{n_2 k_2} + a^2 \lambda^{n_1 k_1} + (1 - \mu)\lambda^{n_2 k_2} + a^2 = 0$. Just with the condition $\mu = 0$, then this equation has solution in \mathbb{C}^2 . i.e.,

$$(\lambda^{n_1 k_1} + 1)(\lambda^{n_2 k_2} + a^2) = 0, \quad (8)$$

Suppose that $\lambda = r(\cos \theta + i \sin \theta)$, put it to the equation (8), then, $r^{n_1 k_1} (\cos(n_1 k_1 \theta) + i \sin(n_1 k_1 \theta)) = -1 = \cos \pi + i \sin \pi$. i.e., $\theta = \frac{\pi}{n_1 k_1} > \frac{\pi}{n_1 m_1} > \frac{\pi}{2m} = \frac{\gamma \pi}{2}$ or $r^{n_2 k_2} (\cos(n_2 k_2 \theta) + i \sin(n_2 k_2 \theta)) = -a^2 = a^2 (\cos \pi + i \sin \pi)$, so, $\theta = \frac{\pi}{n_2 k_2} > \frac{\pi}{n_2 m_2} > \frac{\pi}{2m} = \frac{\gamma \pi}{2}$. Generally, the condition $|\arg(\lambda)| > \frac{\gamma \pi}{2}$ is satisfied. The equilibrium E is locally asymptotically stable. \square

3.2. Simulations of locally asymptotically stable. Based on the Theorem 1, the system (3) with $\mu = 0$ is reduced to

$$\begin{aligned} D^{\alpha_1} x(t) &= a - x(t) + x(t)^2 y(t), \\ D^{\alpha_2} y(t) &= -x(t)^2 y(t). \end{aligned} \quad (9)$$

For the incommensurate case, the equilibrium point is $E = (a, 0)$. When we fix $a = 3$ and $(q_1, q_2) = (0.4, 0.9)$, the convergence process is shown in Fig.1(a). Fix $a = 1.8$ and $(q_1, q_2) = (0.3, 0.7)$, the convergence processes are shown in Fig.1(b).

These simulations are based on the predictor-corrector (P-C) approach[34]. Numerical simulations are consistent with theoretical results. All these show that the equilibrium point $E = (a, 0)$ is locally asymptotically stable.

Remark 1. *The equilibrium point $E = (a, 0)$ is only locally asymptotically stable, not globally asymptotically stable. But, the convergence radius of the equilibrium point is not known. In the process of numerical simulations, it is not known how far the distance between the initial point (x_0, y_0) and the equilibrium point is appropriate. How close is close enough? Only the proper distance can guarantee that the orbits will be attracted to the equilibrium point. Otherwise, the orbits may be divergent.*

3.3. A numerical solution. In this subsection, we apply the discretization process represented in reference[35, 36, 37, 38, 39] for the FOBS (3). Assume that $(x(0), y(0)) = (x_0, y_0)$ is the initial condition, then a numerical solution of FOBS (3) with PWCA method is given as following.

$$\begin{aligned} D^{\alpha_1}x(t) &= a - (\mu + 1)x([t/s]s) + x([t/s]s)^2y([t/s]s), \\ D^{\alpha_2}y(t) &= \mu x([t/s]s) - x([t/s]s)^2y([t/s]s). \end{aligned} \quad (10)$$

First, let $t \in [0, s)$, i.e., $t/s \in [0, 1)$. Thus, we obtain

$$\begin{aligned} D^{\alpha_1}x(t) &= a - (\mu + 1)x(0) + x(0)^2y(0), \\ D^{\alpha_2}y(t) &= \mu x(0) - x(0)^2y(0), \end{aligned} \quad (11)$$

and the solution of (11) is reduced to

$$\begin{aligned} x_1(t) &= x_0 + J_s^{\alpha_1}(a - (\mu + 1)x(0) + x(0)^2y(0)), \\ &= x_0 + \frac{t^{\alpha_1}}{\alpha_1\Gamma(\alpha_1)}(a - (\mu + 1)x(0) + x(0)^2y(0)), \\ y_1(t) &= y_0 + J_s^{\alpha_2}(\mu x(0) - x(0)^2y(0)), \\ &= y_0 + \frac{t^{\alpha_2}}{\alpha_2\Gamma(\alpha_2)}(\mu x(0) - x(0)^2y(0)). \end{aligned} \quad (12)$$

Second, let $t \in [s, 2s)$, i.e., $t/s \in [1, 2)$. Hence, we get

$$\begin{aligned} D^{\alpha_1}x(t) &= a - (\mu + 1)x_1 + x_1^2y_1, \\ D^{\alpha_2}y(t) &= \mu x_1 - x_1^2y_1, \end{aligned} \quad (13)$$

which has the following solution

$$\begin{aligned} x_2(t) &= x_1(s) + J_s^{\alpha_1}(a - (\mu + 1)x_1(s) + x_1(s)^2y_1(s)), \\ &= x_1(s) + \frac{(t-s)^{\alpha_1}}{\alpha_1\Gamma(\alpha_1)}(a - (\mu + 1)x_1(s) + x_1(s)^2y_1(s)), \\ y_2(t) &= y_1(s) + J_s^{\alpha_2}(\mu x_1(s) - x_1(s)^2y_1(s)), \\ &= y_1(s) + \frac{(t-s)^{\alpha_2}}{\alpha_2\Gamma(\alpha_2)}(\mu x_1(s) - x_1(s)^2y_1(s)), \end{aligned} \quad (14)$$

where $J_s^{\alpha_i} = \frac{1}{\Gamma(\alpha_i)} \int_s^t (t - \tau)^{\alpha_i - 1} d\tau$, $0 < \alpha_i \leq 1$ and $i = 1, 2$. Thus, after repeating the discretization process n times, we obtain the discretized FOBS as following

$$\begin{aligned} x_{n+1}(t) &= x_n(ns) + \frac{(t-ns)^{\alpha_1}}{\alpha_1\Gamma(\alpha_1)}(a - (\mu + 1)x_n(ns) + x_n(ns)^2y_n(ns)), \\ y_{n+1}(t) &= y_n(ns) + \frac{(t-ns)^{\alpha_2}}{\alpha_2\Gamma(\alpha_2)}(\mu x_n(ns) - x_n(ns)^2y_n(ns)), \end{aligned} \quad (15)$$

where $t \in [ns, (n+1)s)$. For $t \rightarrow (n+1)s$, the system (15) is reduced to

$$\begin{aligned} x_{n+1} &= x_n + \frac{s^{\alpha_1}}{\alpha_1\Gamma(\alpha_1)}(a - (\mu + 1)x_n + x_n^2y_n), \\ y_{n+1} &= y_n + \frac{s^{\alpha_2}}{\alpha_2\Gamma(\alpha_2)}(\mu x_n - x_n^2y_n). \end{aligned} \quad (16)$$

It should be notice that if $\alpha_i \rightarrow 1$ ($i = 1, 2$) in (16), we obtain the corresponding Euler discretization of FOBS with commensurate order. It is different from P-C

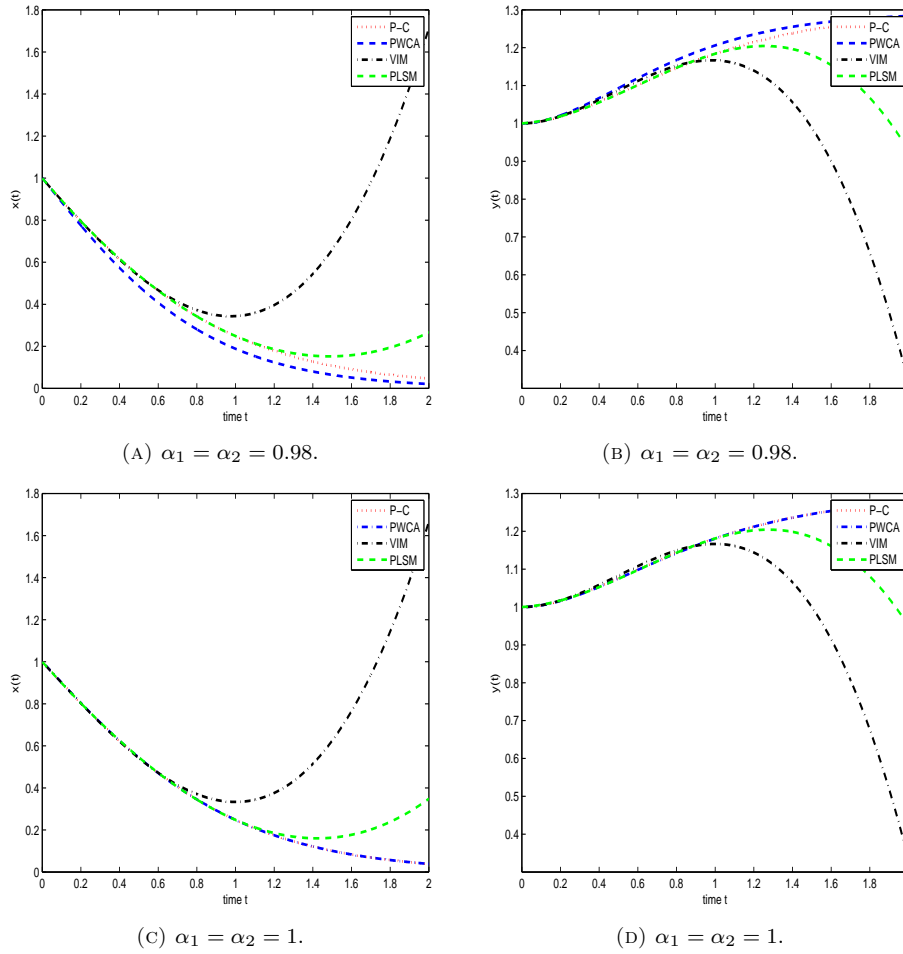


FIG. 2. Numerical solution comparison between PWCA , P-C, VIM and PLSM respectively in the system (3), where $a = 0, \mu = 1$, initial value $(x_0, y_0) = (1, 1)$ (example 1 in [31] and subsection 3.1 in [30]).

algorithm. The obtained result is a two-dimension discrete system. Given the initial condition (x_0, y_0) and s , then through the discrete system (16), we can get another numerical solution of the FOBS (3).

Now, we give an example to show this method is effective through comparing the existing methods.

Example 1. Consider the fractional-order Brusselator system (3) with $a = 0, \mu = 1$ as following:

$$\begin{aligned} D^{\alpha_1} x(t) &= -2x(t) + x(t)^2 y(t), \\ D^{\alpha_2} y(t) &= x(t) - x(t)^2 y(t), \end{aligned} \tag{17}$$

with the initial conditions $(x_0, y_0) = (1, 1)$.

Using the polynomial least squares method (PLSM), the 3-order approximate solutions of (17) are as following[30]. For the case $(\alpha_1, \alpha_2) = (0.98, 0.98)$,

$$\begin{aligned} x_{PLSM}(t) &= 0.0243682t^3 + 0.311138t^2 - 1.08655t + 1, \\ y_{PLSM}(t) &= -0.184414t^3 + 0.333424t^2 + 0.0349127t + 1, \end{aligned} \quad (18)$$

and for the case $(\alpha_1, \alpha_2) = (1, 1)$,

$$\begin{aligned} x_{PLSM}(t) &= 0.0750974t^3 + 0.201028t^2 - 1.02827t + 1, \\ y_{PLSM}(t) &= -0.180088t^3 + 0.334087t^2 + 0.0271107t + 1. \end{aligned} \quad (19)$$

According to the variational iteration method (VIM)[31], the 2-order approximate solutions of (17) are

$$\begin{aligned} x_{VIM}(t) &= 1 - \frac{t^\alpha}{\Gamma(\alpha+1)} + \frac{t^{3\alpha+1}\Gamma(2\alpha+1)}{\Gamma(1+\alpha)^2\Gamma(1+3\alpha)}, \\ y_{VIM}(t) &= 1 + \frac{t^{\alpha_1+\alpha_2}}{\Gamma(\alpha_1+\alpha_2+1)} - \frac{t^{2\alpha_1+\alpha_2}\Gamma(2\alpha_1+1)}{\Gamma(\alpha_1+1)^2\Gamma(1+2\alpha_1+\alpha_2)}. \end{aligned} \quad (20)$$

The comparison between PWCA, P-C, VIM and PLSM are shown in Fig.2. These numerical results show that the introduced approach (PWCA) is a promising tool for solving fractional-order differential equations.

Statistical analysis–correlation coefficient (CC)

In addition to comparison results of the Fig.2, we also introduce correlation coefficient method as following to test the effect of the above numerical methods.

$$r = \frac{\sum_{i=1}^n (\mu_i - \bar{\mu})(\nu_i - \bar{\nu})}{n\sigma_\mu\sigma_\nu}, \quad i = 1, 2, \dots, n, \quad (21)$$

where, σ_μ and σ_ν are the standard deviation of time series μ_i and ν_i respectively. $\bar{\mu}$ and $\bar{\nu}$ are the average value of time series μ_i and ν_i . The expression (21) can be simplified as following.

$$r = \frac{n \sum_{i=1}^n \mu_i \nu_i - \sum_{i=1}^n \mu_i \sum_{i=1}^n \nu_i}{\sqrt{n \sum_{i=1}^n \mu_i^2 - (\sum_{i=1}^n \mu_i)^2} \sqrt{n \sum_{i=1}^n \nu_i^2 - (\sum_{i=1}^n \nu_i)^2}}, \quad (22)$$

where $-1 \leq r \leq 1$. The correlation coefficient r measures the relativity of two time series μ_i and $\nu_i (i = 1, 2, \dots, n)$. If these two time series are highly correlated, the correlation coefficient $|r|$ is close to 1. That is, the larger $|r|$, the more relevant of the two time series.

Denote the time series of P-C method by $\nu_i (i = 1, 2, \dots, n)$. Other time series are denoted by $\mu_i (i = 1, 2, \dots, n)$ respectively. Then, the results of correlation coefficient are as following Table 1.

P-C method is a mature and reliable algorithm for fractional-order differential equation(FODE). Thus, it is used as the object of comparison. From the Table 1, we can find that the PWCA for FODE is the most effective comparing to the other two methods(VIM, PLSM). Furthermore, this method (CC) is more intuitive and direct than the graphical comparison.

Remark 2. *PWCA is different from the usual methods (P-C, VIM, PLSM), which are based on corresponding integral equation of FODE. But, the PWCA deals with FODE at its right part directly. When $\alpha_1 = \alpha_2 = 1$, PWCA method is consistent with P-C method, i.e., Euler-discretization method.*

μ_i	ν_i	α_k	data	r	effect	α_k	data	r	effect
VIM	P-C	0.98	x(t)	-0.1178	weaker	1	x(t)	-0.0743	weaker
			y(t)	-0.4555	weaker		y(t)	-0.4395	common
PLSM			x(t)	0.9829	better		x(t)	0.9649	better
			y(t)	0.4590	common		y(t)	0.5307	common
PWCA			x(t)	0.9987	best		x(t)	1.0000	best
			y(t)	0.9979	best		y(t)	1.0000	best

TABLE 1. Comparison of numerical results ($i = 1, 2, \dots, n$. $k = 1, 2$.)

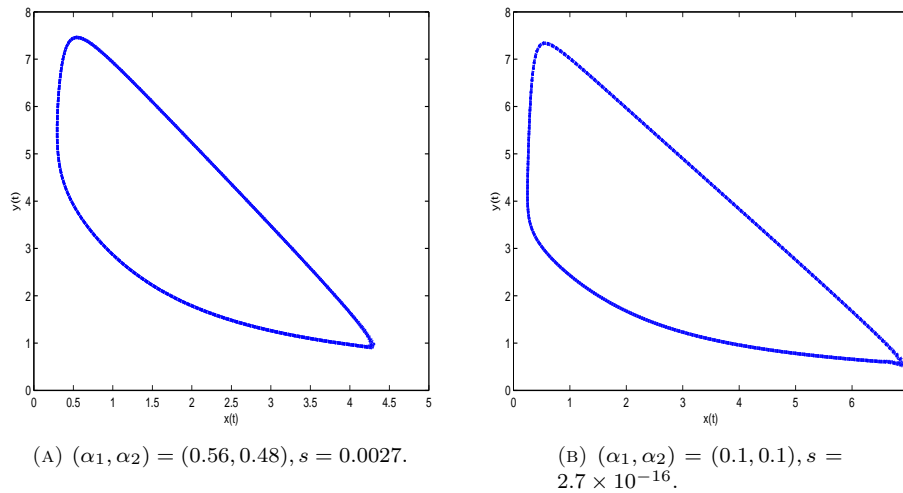


FIG. 3. Numerical solution using PWCA for the system (3) with $a = 1, (x_0, y_0) = (0.2, 0.03), \mu = 4$ and 3.98 respectively.

4. DISCUSSIONS OF LIMIT CYCLES

Similar to references [25, 26], we also can get some phenomena of limit cycles based on PWCA method. We only simulate two special cases as shown in Fig.3. Other cases are similar. From the Fig.3, we can find that the “limit cycles” are still retained. However, it was even strictly proved that the nonexistence of limit cycles in fractional-order differential equation[5, 6, 7, 8, 9, 10, 11]. Here, the numerical simulations and the theory is contradictory. However, numerical simulation is just an approximation of the exact solution by a two-dimension discrete system (16). What is the way to produce these false limit cycle? These similar phenomena of limit cycles have been observed in many literatures[12, 13, 25, 26, 27, 28, 30, 31] through various numerical simulations. We guess the phenomena of limit cycle may be generated by Neimark-Sacker bifurcation in corresponding discrete system of fractional-order system. Neimark-Sacker bifurcation always forms a invariant curve, which is similar to limit cycle. Another possibility is that these “limit cycles” may be eventually periodic orbits (Let $F : J \rightarrow J$. For $x \in J, F^0(x)$ denotes x and $F^{n+1}(x)$ denotes $F(F^n(x))$ for $n = 0, 1, \dots$. we say q is eventually periodic if for some positive integer $m, p = F^m(q)$ is periodic [40]). These “limit cycles”

actually are obtained by throwing away some points. Of course, perhaps there are other reasons for these phenomena of limit cycle. These doubts are interesting and deserve further consideration and discussion.

Here, we mainly have done following things. Firstly, stability of FOBS is studied. Secondly, a numerical solution of FOBS is obtained using PWCA method. It is compared with P-C, VIM and PLSM methods. By comparison (Figures and Statistical analysis), we find that the PWCA method is effective and optimal. Finally, possible reasons for the phenomenon of “limit cycles” are analyzed. Some key matlab codes of Fig.2(a)-2(b) are listed in <http://ylgdiy.bokee.com/504158376.html>. All these analysis will improve understanding of the fractional-order Brusselator chemical reaction system.

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