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Analysis and new simulations of fractional Noyes-Field model using Mittag-Leffler kernel

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ABSTRACT

In this manuscript, the fractional-in-time NoyesField model for Belousov-Zhabotinsky reaction transport is considered with a novel numerical technique, which was used to approximate the Atangana-Baleanu (ABC) operator which models the subdiffusion partial derivative in time. The effect of the ABC operator is observed and captured more interesting physical behavior of some real-life phenomena. Applicability and suitability of the adopted method were carried out on some cases of nonlinear Belousov-Zhabotinsky subreaction-diffusion models, their dynamic behaviors with respect to fractional-order parameters were displayed in figures.

Introduction

Nonlinear phenomena, which are so critical for nature and society, are in contrast to linear systems which cannot be explained by a linear relationship between two variables. Together with its rapid development field in applied physics, it has a noteworthy role in various fields of science and engineering [3–5,11–14,20,28,29,31]. In particular, nonlinear phenomena are observed in the environment or in living organisms such as chemical physics and biology as a Chemical reaction that evolves in time and is observed in the environment or in living organisms such as chemical physics and biology. Specifically, the Belousov-Zhabotinsky reaction is a noteworthy example of the non-linear behavior of chemical reaction systems occurring inhomogeneous media. In the early, 1950s, Belousov-Zhabotinsky's reaction was discovered by Belousov and developed by Zhabotinsky. It is described as autocatalytic oxidation of organic acid by potassium bromate [15,35]. While he was working on the Krebs cycle, he put together bromate and cerium ions with citric acid. After an induction period, the color of the compound oscillated between colorless and pale yellow with a characteristic period. It was a remarkable result affected

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Belousov proudly. Belousov carefully characterized the phenomenon and submitted his results, with recipes included, to a number of journals, all of them rejected his results on the grounds that such a thing could not exist [16,17]. After a decade, Zhabotinsky who is a Soviet scientist worked on the experiments of Belousov and procreate them once more. His researches persuaded more chemists to accept the idea of chemical oscillators. In 1972, the FKN mechanism which is a mechanism describing the Belousov-Zhabotinsky reaction was brought to public attention by Field, K örös and Noyes [18]. The FNK mechanism had a handicapped, it was too complex to do the numerical analysis of the system via computers belonging to those days. After 2 years, namely in 1974, Field and Noyes suggested a reduced model for the FNK system. It was consisting 5 chemical reactions instead of 11 reactions. When the Field-Noyes system, known as Oregonator, is evaluated numerically, The system produces the same oscillatory behavior as the Belousov-Zhabotinsky reaction.

The simplified Noyes–Field fractional model for this Belousov-Zhabotinsky reaction is read as [1]

$$\begin{aligned} {}^{ABC}_{t_0}D^{\alpha}u(x,t) &= \xi_1 u_{xx}(x,t) + \beta\delta v(x,t) + u(x,t) - u^2(x,t) - \delta u(x,t)v(x,t) \\ {}^{ABC}_{t_0}D^{\alpha}v(x,t) &= \xi_2 v_{xx}(x,t) + \gamma v(x,t) + \lambda u(x,t)v(x,t) \end{aligned} \tag{0.1}$$

where $\xi_1, \beta, \delta, \xi_2, \gamma$ and λ are positive parameters. ξ_1 and ξ_2 are the diffusing constant for the concentration u and v,respectively. Before focusing on the motivation of the manuscript, it will be useful to touch on some studies on Noyes-Filed model. Akinyemi [1] have considered the fractional Noyes- Field model and applied q-Homotopy analysis transform method and Laplace transform to obtain efficient numerical solution. Wang et al. [34] have obtained explicit traveling wave front solutions of the Noyes field model. In [32], Stanshine and Howard have used asymptotic methods to obtain solutions of the model. the approximate solutions of time-fractional nonlocal reaction-diffusion equation have been investigated by Arqub et al. [10]

In this manuscript, we are going to bring out a new outlook to fractional Noyes Field model defined using Atangana-Baleanu (AB) fractional derivative which introduced in 2016 by Atangana and Baleanu for the first time [6]. The new genuine fractional derivative based on using the generalized MittagLeffler function as non-local and non-singular kernel and it naturally appears in several physical problems and the field of science and engineering[7–9].It is obvious that many works were done around this new finding with great success. This motivated us to investigate the reaction models with Mittag Leffler kernel and present the effectiveness and efficiency of the new fractional definition to scholars and show off the effect of AB derivative on the fractional Noyes Field model. Atangana Baleanu derivatives having Mittag Leffler kernel captured the attention of many scientists; Qureshi et al. [30] have investigated, and analyzed nonlinear Duffing oscillators via integer and non-integer order differential operators known as the Caputo, CaputoFabrizio, and the AtanganaBaleanu taken in the Caputo sense. Modanlı [21] has obtained numerical solutions of telegraph equation defined by Caputo fractional derivative and by AtanganaBaleanu fractional derivative are obtained using difference scheme method. Heydari et al. [19] have investigated fractional optimal control problems with ABC fractional derivative using Chebyshev cardinal wavelets. Owolabi et al. [26] have considered breast cancer model and extended to a system of fractal fractional partial differential equations and Owolabi and Atangana [27] have formulated fractional version of the Adams-Bashforth method using the Atangana-Baleanu derivative.

Considering the explanations presented above, this manuscript is structured as follows: Section 1 describes a brief introduction to the aim of the manuscript and the model which will be discussed. The existence and uniqueness of the model under AB derivative is going to be proof using Picard-Lindelöf theorem in Section 2. The following section, i.e. Section 3 includes constructing a numerical scheme which is obtained by using polynomials and application to the fractional Noyes field model for analyzing and understanding the behavior of the model. The results of numerical results in different cases are presented in Section 4. Additionally, some stability results are presented in Section 4 as well. In the end, the conclusion and a brief summary of the manuscript take place in Section 5.

Existence and uniqueness of solutions for fractional Noyes-Field model

The goal of this segment is to establish the existence and uniqueness of solutions for the fractional Noyes-Field model. For this purpose, we are going to adapt the major fixed point theorem by Picard named “Picard Lindelöf” theorem. The theorem gives sufficient but not necessary conditions for the existence of the unique solution to initial value problems. The general existence and uniqueness theory describes the features of a differential equation which makes it tractable for computation both numerical and theoretical. Picard Lindelöf theorem establishes conditions under which a differential equation has a solution and guarantees that its solution is unique. Before beginning to adapt the theorem, Let

$$C_{\varepsilon,r} = I_{\varepsilon}(t_0) \times B_r(x_0) \tag{0.2}$$

where

$$\begin{aligned} I_{\varepsilon}(t_0) &= [t_0 - \varepsilon, t_0 + \varepsilon] \\ B_r(x_0) &= [x_0 - b, x_0 + b]. \end{aligned} \tag{0.3}$$

This is a compact cylinder where f is defined. Let

$$M = \sup_{C_{\varepsilon,r}} \|\varrho_i\| \tag{0.4}$$

is equivalent to the supremum norm.

Step 1: Transform Noyes Field model into an integral equation

Now, recall the Noyes Field model given in Eq. (0.1) and apply Atangana-Balenau integral to the two side of model. So, we get

$$\begin{aligned} u(x,t)-u(x,0) &= \tfrac{1-\alpha}{AB(\alpha)}\left[\xi_1 u_{xx}(x,t)+\beta\delta v(x,t)+u(x,t)-u^2(x,t)-\delta u(x,t)v(x,t)\right] \\ &+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\left[\xi_1 u_{xx}(x,\tau)+\beta\delta v(x,\tau)+u(x,\tau)-u^2(x,\tau)-\delta u(x,\tau)v(x,\tau)\right]d\tau, \\ v(x,t)-v(x,0) &= \tfrac{1-\alpha}{AB(\alpha)}[\xi_2 v_{xx}(x,t)+\gamma v(x,t)+\lambda u(x,t)v(x,t)] \\ &+\tfrac{\gamma}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\xi)^{\alpha\gamma-1}[\xi_2 v_{xx}(x,\tau)+\gamma v(x,\tau)+\lambda u(x,\tau)v(x,\tau)]d\xi. \end{aligned} \tag{0.5}$$

For convenience;

$$\begin{aligned} \varrho_1(u,v,t) &= \xi_1 u_{xx}(x,t)+\beta\delta v(x,t)+u(x,t)-u^2(x,t)-\delta u(x,t)v(x,t) \\ \varrho_2(u,v,t) &= \xi_2 v_{xx}(x,t)+\gamma v(x,t)+\lambda u(x,t)v(x,t) \end{aligned} \tag{0.6}$$

and

$$\Lambda(u,v,t)=\begin{bmatrix}\varrho_1(u,v,t)\\ \varrho_2(u,v,t)\end{bmatrix},\qquad U(u,v,t)=\begin{bmatrix}u(x,t)\\ v(x,t)\end{bmatrix},\qquad U_0=\begin{bmatrix}u_0\\ v_0\end{bmatrix}, \tag{0.7}$$

hence we can write;

$$\begin{aligned} u(x,t) &= u_0+\tfrac{1-\alpha}{AB(\alpha)}\varrho_1(u,v,t)+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\varrho_1(u,v,\tau)d\xi, \\ v(x,t) &= v_0+\tfrac{1-\alpha}{AB(\alpha)}\varrho_2(u,v,t)+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\varrho_2(u,v,\alpha)d\xi. \end{aligned} \tag{0.8}$$

Step 2: Applying the Picard-Lindelöf theorem to Noyes-Field model

We define a nonlinear operator

$$\begin{aligned} &\chi: C_{\varepsilon,r}\to C_{\varepsilon,r} \\ &\chi(U(u,v,t)) = U_0+\tfrac{1-\alpha}{AB(\alpha)}\Lambda(u,v,t)+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\Lambda(u,v,\tau)d\tau. \end{aligned} \tag{0.9}$$

In order to make sure that $\Lambda(u,v,t)$ maps $C_{\varepsilon,r}$ into itself, we make sure that κ is small enough to quarantenee that $\chi(U(u,v,t))\in C_{\varepsilon,r}$ for all $t\in I_\varepsilon$. If we use bound M to obtain; we get

$$\begin{aligned} \|\chi(U(u,v,t))-U(u,v,t_0)\|_{C_{\varepsilon,r}} &= \left\|U_0+\tfrac{1-\alpha}{AB(\alpha)}\Lambda(u,v,t)+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\Lambda(u,v,\tau)d\tau.\right\| \\ &\le \left\|\tfrac{1-\alpha}{AB(\alpha)}\Lambda(u,v,t)\right\|+\left\|\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\Lambda(u,v,t)d\tau\right\| \\ &\le \tfrac{1-\alpha}{AB(\alpha)}\|\Lambda(u,v,t)\|+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\left\|\int_{t_0}^{t}(t-\tau)^{\alpha-1}\Lambda(u,v,t)d\tau\right\| \\ &< \tfrac{1-\alpha}{AB(\alpha)}M+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}MT_{\max}^{\alpha-1} \\ &= \tfrac{M}{AB(\alpha)}\left((1-\alpha)+\tfrac{\alpha T_{\max}^{\alpha-1}}{\Gamma(\alpha)}\right)=\kappa \end{aligned} \tag{0.10}$$

Thus;

$$\|\chi(U(u,v,t))-U(u,v,t_0)\|_{C_{\varepsilon,r}}<\frac{M}{AB(\alpha)}\left((1-\alpha)+\frac{\alpha T_{\max}^{\gamma-1}}{\Gamma(\alpha)}\right) \tag{0.11}$$

we need

$$\|\chi(U(u,v,t))-U(u,v,t_0)\|_{C_{\varepsilon,r}}<b \tag{0.12}$$

thus;

$$\frac{M}{AB(\alpha)}\left((1-\alpha)+\frac{\alpha T_{\max}^{\alpha-1}}{\Gamma(\alpha)}\right)<b$$
$$T_{\max}<\left\{\frac{\Gamma(\alpha)}{\alpha}\left(\frac{bAB(\alpha)}{M}+\alpha-1\right)\right\}^{1-\alpha} \tag{0.13}$$

This means; χ maps $C_{\varepsilon,r}$ into itself. Furthermore; we get for

$$\begin{aligned}\|\chi(U_1(u,v,t))-\chi(U_2(u,v,t))\|_{C_{\varepsilon,r}} &= \Bigg\|\left(U_0^1+\frac{1-\alpha}{AB(\alpha)}\Lambda_1(u,v,t)+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\xi)^{\alpha-1}\Lambda_1(u,v,\tau)d\tau\right)\\ &\quad-\left(U_0^2+\frac{1-\alpha}{AB(\alpha)}\Lambda_2(u,v,t)+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\Lambda_2(u,v,\tau t)d\tau\right)\Bigg\|\\ &\le \left\|U_0^1-U_0^2\right\|+\frac{1-\alpha}{AB(\alpha)}\|\Lambda_1(u,v,t)-\Lambda_2(u,v,t)\|\\ &\quad+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\left\|\int_{t_0}^{t}(t-\tau)^{\alpha-1}(\Lambda_1(u,v,\tau)-\Lambda_2(u,v,\tau))\right\|d\tau\\ &\le \frac{1-\alpha}{AB(\alpha)}\omega+\frac{\alpha\gamma}{AB(\alpha)\Gamma(\alpha)}T_{\max}^{\alpha-1}\omega\\ &= \frac{\omega}{AB(\alpha)}\left((1-\alpha)+\frac{\gamma T_{\max}^{\alpha-1}}{\Gamma(\alpha)}\right)\end{aligned} \tag{0.14}$$

Any such ω is referred to as a Lipschitz constant for the function $\Lambda(u,v,t)$.
Here, we need

$$\frac{\omega}{AB(\alpha)}\left((1-\alpha)+\frac{\gamma T_{\max}^{\alpha-1}}{\Gamma(\alpha)}\right)<1 \tag{0.15}$$

So the equation has unique solution if

$$T_{\max}\le\left\{\frac{\Gamma(\alpha)}{\alpha}\left(\frac{AB(\alpha)}{w}+\alpha-1\right)\right\}^{1-\alpha} \tag{0.16}$$

Application of numerical scheme to Noyes-Field model

In this segment, the application of numerical method to Noyes-Field model is considered. At the first stage, Let us recall the model in the sense of the Atangana-Balenau derivative definition as follow [3]

$$\begin{aligned}{}^{ABC}_{t_0}D^{\alpha}u(x,t)&=\xi_1u_{xx}(x,t)+\beta\delta v(x,t)+u(x,t)-u^2(x,t)-\delta u(x,t)v(x,t)\\ {}^{ABC}_{t_0}D^{\alpha}v(x,t)&=\xi_2v_{xx}(x,t)+\gamma v(x,t)+\lambda u(x,t)v(x,t)\end{aligned} \tag{0.17}$$

using the fundamental theory of calculus, we get;

$$\begin{aligned}u(x,t)-u(x,t_0)&=\frac{1-\alpha}{AB(\alpha)}\left[\xi_1u_{xx}(x,t)+\beta\delta v(x,t)+u(x,t)-u^2(x,t)-\delta u(x,t)v(x,t)\right]\\ &\quad+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}\left[\xi_1u_{xx}(x,\tau)+\beta\delta v(x,\tau)+u(x,\tau)-u^2(x,\tau)-\delta u(x,\tau)v(x,\tau)\right]d\tau\end{aligned} \tag{0.18}$$

and

$$\begin{aligned}v(x,t)-v(x,t_0)&=\frac{1-\alpha}{AB(\alpha)}[\xi_2v_{xx}(x,t)+\gamma v(x,t)+\lambda u(x,t)v(x,t)]\\ &\quad+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}[\xi_2v_{xx}(x,\tau)+\gamma v(x,\tau)+\lambda u(x,\tau)v(x,\tau)]d\tau.\end{aligned} \tag{0.19}$$

For convenience, we can rewrite above integral as

$$u(x,t)=u_0+\frac{1-\alpha}{AB(\alpha)}[\varrho_1(u,v,t)]+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}[\varrho_1(u,v,\tau)]d\tau \tag{0.20}$$

and

$$v(x,t)=v_0+\frac{1-\alpha}{AB(\alpha)}[\varrho_2(u,v,t)]+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t}(t-\tau)^{\alpha-1}[\varrho_2(u,v,\tau)]d\tau \tag{0.21}$$

where $\varrho_1(u,v,t)=\xi_1 u_{xx}(x,t)+\beta\delta v(x,t)+u(x,t)-u^2(x,t)-\delta u(x,t)v(x,t)$ $\varrho_2(u,v,t)=\xi_2 v_{xx}(x,t)+\gamma v(x,t)+\lambda u(x,t)v(x,t)$ and $u(x,t_0)=u_0, v(x,t_0)=v_0$ are initial conditions. At the point $t=t_{n+1}=(n+1)\Delta t,$ we get

$$\begin{aligned} u(x,t_{n+1}) &= u_0+\tfrac{1-\alpha}{AB(\alpha)}[\varrho_1(u,v,t_n)]+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t_{n+1}}(t_{n+1}-\tau)^{\alpha-1}[\varrho_1(u,v,\tau)]d\tau \\ v(x,t_{n+1}) &= v_0+\tfrac{1-\alpha}{AB(\alpha)}[\varrho_2(u,v,t_n)]+\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\int_{t_0}^{t_{n+1}}(t_{n+1}-\tau)^{\alpha-1}[\varrho_2(u,v,\tau)]d\tau \end{aligned} \tag{0.22}$$

Therefore, we can rewrite above integrals as

$$u(x,t_{n+1})=u_0+\frac{1-\alpha}{AB(\alpha)}[\varrho_1(u,v,t_n)]+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=2}^{n}\int_{t_j}^{t_{j+1}}(t_{n+1}-\tau)^{\alpha-1}[\varrho_1(u,v,\tau)]d\tau \tag{0.23}$$

and

$$v(x,t_{n+1})=v_0+\frac{1-\alpha}{AB(\alpha)}[\varrho_2(u,v,t_n)]+\frac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=2}^{n}\int_{t_j}^{t_{j+1}}(t_{n+1}-\tau)^{\alpha-1}[\varrho_2(u,v,\tau)]d\tau. \tag{0.24}$$

Now, we can construct an approximate values for functions under the integrals, that is $\varrho_1(u,v,t)$ and $\varrho_2(u,v,t)$, respectively

$$\begin{aligned} P_n^1(\tau) &= \varrho_1(u,v,t_{n-2})+((\varrho_1(u,v,t_{n-1})-\varrho_1(u,v,t_{n-2}))/\Delta t)(\tau-t_{n-2}) \\ &\quad +\Big((\varrho_1(u,v,t_n)-2\varrho_1(u,v,t_{n-1})+\varrho_1(u,v,t_{n-2}))/2(\Delta t)^2\Big)(\tau-t_{n-2})(\tau-t_{n-1}) \end{aligned} \tag{0.25}$$

and

$$\begin{aligned} P_n^2(\tau) &= \varrho_2(u,v,t_{n-2})+((\varrho_2(u,v,t_{n-1})-\varrho_2(u,v,t_{n-2}))/\Delta t)(\tau-t_{n-2}) \\ &\quad +\Big((\varrho_2(u,v,t_n)-2\varrho_2(u,v,t_{n-1})+\varrho_2(u,v,t_{n-2}))/2(\Delta t)^2\Big)(\tau-t_{n-2})(\tau-t_{n-1}) \end{aligned} \tag{0.26}$$

when Eqs. (0.25) and (0.26) substitute into Eqs. (0.23) and (0.24), we get

$$\begin{aligned} v(x,t_{n+1}) &= v_0+\tfrac{1-\alpha}{AB(\alpha)}[\varrho_2(u,v,t_n)] \\ &\quad +\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=2}^{n}\varrho_2\big(u,v,t_{j-2}\big)\Delta t\int_{t_j}^{t_{j+1}}(t_{n+1}-\tau)^{\alpha-1}d\tau \\ &\quad +\tfrac{\alpha}{AB(\alpha)\Gamma(\alpha)}\sum_{j=2}^{n}\Big(\big(\varrho_2\big(u,v,t_{j-1}\big)-\varrho_2\big(u,v,t_{j-2}\big)\big)/\Delta t\Big)\int_{t_j}^{t_{j+1}}\big(\tau-t_{j-2}\big)(t_{n+1}-\tau)^{\alpha-1}d\tau \\ &\quad +\tfrac{\gamma}{AB(\gamma)\Gamma(\gamma)}\sum_{j=2}^{n}\Big(\big(\varrho_2\big(u,v,t_j\big)-2\varrho_2\big(u,v,t_{j-1}\big)+\varrho_2\big(u,v,t_{j-2}\big)\big)/2(\Delta t)^2\Big) \\ &\qquad \times\int_{t_j}^{t_{j+1}}\big(\tau-t_{j-2}\big)\big(\tau-t_{j-1}\big)(t_{n+1}-\tau)^{\alpha-1}d\tau. \end{aligned} \tag{0.27}$$

It is almost finished. Now, we need to calculate integrals

$$\begin{aligned} I_1 &= \int_{t_j}^{t_{j+1}}(t_{n+1}-\tau)^{\alpha-1}d\tau \\ I_2 &= \int_{t_j}^{t_{j+1}}\big(\tau-t_{j-2}\big)(t_{n+1}-\tau)^{\alpha-1}d\tau \\ I_3 &= \int_{t_j}^{t_{j+1}}\big(\tau-t_{j-2}\big)\big(\tau-t_{j-1}\big)(t_{n+1}-\tau)^{\alpha-1}d\tau. \end{aligned} \tag{0.28}$$

For calculation we need an auxiliary variable such as $y=t_{n+1}-\tau$, so we get $dy=-d\tau$;

$$\begin{aligned} I_1 &= \int_{t_{n+1}-t_j}^{t_{n+1}-t_{j+1}}y^{\alpha-1}(-dy)=\Big(\tfrac{1}{\alpha}y^{\alpha}\Big)_{t_{n+1}-t_{j+1}}^{t_{n+1}-t_j} \\ &= \tfrac{1}{\alpha}\Big(\big(t_{n+1}-t_j\big)^{\alpha}-\big(t_{n+1}-t_{j+1}\big)^{\alpha}\Big) \\ &= \tfrac{1}{\alpha}\big(((n+1)\Delta t-j\Delta t)^{\alpha}-((n+1)\Delta t-(j+1)\Delta t)^{\alpha}\big) \\ &= \tfrac{(\Delta t)^{\alpha}}{\alpha}((n-j+1)^{\alpha}-(n-j)^{\alpha}). \end{aligned} \tag{0.29}$$

When we use same auxiliary variable for I_2, we obtain;

$$\begin{aligned} I_2 &= \int_{t_j}^{t_{j+1}} \left(\tau - t_{j-2}\right)(t_{n+1}-\tau)^{\alpha-1} d\tau \\ &= \int_{t_j}^{t_{j+1}} \left(\tau - t_{j-2}\right)(t_{n+1}-\tau)^{\alpha-1} d\tau \\ &= \int_{t_{n+1}-t_j}^{t_{n+1}-t_{j+1}} \left(t_{n+1} - y - t_{j-2}\right) y^{\alpha-1}(-dy) \\ &= \int_{t_{n+1}-t_j}^{t_{n+1}-t_{j+1}} ((n+1)\Delta t - y - (j-2)\Delta t) y^{\alpha-1}(-dy) \\ &= \int_{t_{n+1}-t_j}^{t_{n+1}-t_{j+1}} ((n-j-3)\Delta t - y) y^{\alpha-1}(-dy) \end{aligned} \tag{0.30}$$

after some calculations, we obtain

$$I_2 = \frac{(\Delta t)^{\alpha+1}}{\alpha(\alpha+1)}\Big((n-j+1)^\alpha(n-j+3+2\alpha) - (n-j)^\alpha(n-j+3+3\alpha)\Big) \tag{0.31}$$

If integral I_3 calculate using auxiliary variable y, we obtain

$$\begin{aligned} I_3 &= \int_{t_j}^{t_{j+1}} \left(\tau - t_{j-2}\right)\left(\tau - t_{j-1}\right)(t_{n+1}-\tau)^{\alpha-1} d\tau. \\ &= \int_{t_{n+1}-t_j}^{t_{n+1}-t_{j+1}} \left(t_{n+1} - y - t_{j-2}\right)\left(t_{n+1} - y - t_{j-1}\right) y^{\alpha-1}(-dy). \\ &= \int_{t_{n+1}-t_j}^{t_{n+1}-t_{j+1}} ((n+1)\Delta t - y - (j-2)\Delta t)((n+1)\Delta t - y - (j-1)\Delta t) y^{\alpha-1}(-dy). \\ &= \int_{t_{n+1}-t_j}^{t_{n+1}-t_{j+1}} ((n-j+3)\Delta t - y)((n-j+2)\Delta t - y) y^{\alpha-1}(-dy). \end{aligned} \tag{0.32}$$

after calculating above integral, I_3can be obtained as

$$\begin{aligned} I_3 = \frac{(\Delta t)^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)} & (n-j+1)^\alpha\Big[2(n-j)^2 + (3\alpha+10)(n-j) + 2\alpha^2 + 9\alpha + 12\Big] \\ & -(n-j)^\alpha\Big[2(n-j)^2 + (5\alpha+10)(n-j) + 6\alpha^2 + 18\alpha + 12\Big]. \end{aligned} \tag{0.33}$$

substituting I_1, I_2 and I_3 into Eqs. (11) and (12), we can obtain the following

$$\begin{aligned} u(x,t_{n+1}) = u_0 &+ \frac{1-\alpha}{AB(\alpha)}[\varrho_1(u,v,t_n)] \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=2}^{n} \varrho_1\big(u,v,t_{j-2}\big)\Delta t\left(\frac{(\Delta t)^\alpha}{\alpha}((n-j+1)^\alpha - (n-j)^\alpha).\right) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=2}^{n} \Big(\big(\varrho_1\big(u,v,t_{j-1}\big) - \varrho_1\big(u,v,t_{j-2}\big)\big)/\Delta t\Big) \\ &\times\left(\frac{(\Delta t)^{\alpha+1}}{\alpha(\alpha+1)}\Big((n-j+1)^\alpha(n-j+3+2\alpha) - (n-j)^\alpha(n-j+3+3\alpha)\Big)\right) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=2}^{n} \Big(\big(\varrho_1\big(u,v,t_j\big) - 2\varrho_1\big(u,v,t_{j-1}\big) + \varrho_1\big(u,v,t_{j-2}\big)\big)/2(\Delta t)^2\Big) \\ &\times\Bigg[\frac{(\Delta t)^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}(n-j+1)^\alpha\Big(2(n-j)^2 + (3\alpha+10)(n-j) + 2\alpha^2 + 9\alpha + 12 \\ &\ -(n-j)^\alpha 2(n-j)^2 + (5\alpha+10)(n-j) + 6\alpha^2 + 18\alpha + 12.\Big)\Bigg] \end{aligned} \tag{0.34}$$

and

$$\begin{aligned} v(x,t_{n+1}) = v_0 &+ \frac{1-\alpha}{AB(\alpha)}[\varrho_2(u,v,t_n)] \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=2}^{n} \varrho_2\big(u,v,t_{j-2}\big)\Delta t\left(\frac{(\Delta t)^\alpha}{\alpha}((n-j+1)^\alpha - (n-j)^\alpha).\right) \\ &+ \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \sum_{j=2}^{n} \Big(\big(\varrho_2\big(u,v,t_{j-1}\big) - \varrho_2\big(u,v,t_{j-2}\big)\big)/\Delta t\Big) \\ &\times\left(\frac{(\Delta t)^{\alpha+1}}{\alpha(\alpha+1)}\Big((n-j+1)^\alpha(n-j+3+2\alpha) - (n-j)^\alpha(n-j+3+3\alpha)\Big)\right) \\ &+ \frac{\gamma}{AB(\gamma)\Gamma(\gamma)} \sum_{j=2}^{n} \Big(\big(\varrho_2\big(u,v,t_j\big) - 2\varrho_2\big(u,v,t_{j-1}\big) + \varrho_2\big(u,v,t_{j-2}\big)\big)/2(\Delta t)^2\Big) \\ &\times\Bigg[\frac{(\Delta t)^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}(n-j+1)^\alpha\Big(2(n-j)^2 + (3\alpha+10)(n-j) + 2\alpha^2 + 9\alpha + 12 \\ &\ -(n-j)^\alpha 2(n-j)^2 + (5\alpha+10)(n-j) + 6\alpha^2 + 18\alpha + 12\Big)\Bigg] \end{aligned} \tag{0.35}$$

During above process, time discretization is completed. The space discretization process can be done using finite difference approximation easily, see [22–25]. We refer our readers to [2,18,33] for detailed analytical studies for a class of diffusive Noyes-Field model for the Belousov-Zhabotinskii reaction where the global existence, boundedness and the asymptotic behaviors of the solutions have been considered.

Applications

In this part, application of the suggested method is carried-out on the fractional Noyes-Field (Belousov-Zhabotinsky) model (0.17) and its variants are considered in the following cases:

Case 1

With $\gamma = 0$ and $\beta = 0$ in nonlinear time-fractional Belousov-Zhabotinsky reaction-diffusion system (0.17) reduces to

$$\begin{aligned} {}^{ABC}_{t_0}D^{\alpha}u(x,t) &= \xi_1 u_{xx}(x,t) + u(x,t) - u^2(x,t) - \delta u(x,t)v(x,t) \\ {}^{ABC}_{t_0}D^{\alpha}v(x,t) &= \xi_2 v_{xx}(x,t) + \lambda u(x,t)v(x,t) \end{aligned} \tag{0.36}$$

using the initial conditions

$$\begin{aligned} u(x,t=0) &= \frac{1}{\left(e^{\sqrt{\frac{\lambda}{6}}x}+1\right)^2}, \\ v(x,t=0) &= \frac{(1-\lambda)e^{\sqrt{\frac{\lambda}{6}}x}\left(e^{\sqrt{\frac{\lambda}{6}}x}+2\right)}{\delta\left(e^{\sqrt{\frac{\lambda}{6}}x}+1\right)^2}. \end{aligned} \tag{0.37}$$

When $\alpha = 1$, the exact solution of Eq. (0.36) is given as

$$\begin{aligned} u(x,t) &= \frac{e^{\frac{5\lambda}{3}t}}{\left(e^{\sqrt{\frac{\lambda}{6}}x}+e^{\frac{5\lambda}{6}t}\right)^2}, \\ v(x,t) &= \frac{(1-\lambda)e^{\sqrt{\frac{\lambda}{6}}x}\left(e^{\sqrt{\frac{\lambda}{6}}x}+2e^{\frac{5\lambda}{6}t}\right)}{\delta\left(e^{\sqrt{\frac{\lambda}{6}}x}+e^{\frac{5\lambda}{6}t}\right)^2}, \end{aligned} \tag{0.38}$$

where $\delta > 0$ and $\lambda > 0$, but $\lambda \neq 1$. It should also be mentioned that the exact solution (0.38) can be written as:

$$\begin{aligned} u(x,t) &= \frac{e^{\frac{5\lambda}{3}t}}{\left(e^{\sqrt{\frac{\lambda}{6}}x}+e^{\frac{5\lambda}{6}t}\right)^2} = \frac{1}{4}\left(\tanh^2\left[\sqrt{\frac{\lambda}{24}}x - \frac{5\lambda}{12}t\right] - 1\right)^2, \\ v(x,t) &= \frac{(1-\lambda)e^{\sqrt{\frac{\lambda}{6}}x}\left(e^{\sqrt{\frac{\lambda}{6}}x}+2e^{\frac{5\lambda}{6}t}\right)}{\delta\left(e^{\sqrt{\frac{\lambda}{6}}x}+e^{\frac{5\lambda}{6}t}\right)^2} \\ &= \frac{\lambda-1}{4\delta}\left(\tanh^2\left[\sqrt{\frac{\lambda}{24}}x - \frac{5\lambda}{12}t\right] - 2\tanh\left[\sqrt{\frac{\lambda}{24}}x - \frac{5\lambda}{12}t\right] - 3\right). \end{aligned} \tag{0.39}$$

In the numerical experiment, we set $\Delta x = 0.25$ and $\Delta t = 0.01, \xi_1 = 1.00$ and $\xi_2 = 1.00$. The corresponding numerical results for various value of α and other parameters is shown in Figs. 1–3. The dynamic evolution in Figs. 2 and 3 are obtained with initial conditions

$$\begin{aligned} u(x,t=0) &= 1 - \exp(-10(x-\mu/2)^2), \\ v(x,t=0) &= \exp(-10(x-\mu/2)^2). \end{aligned} \tag{0.40}$$

Case 2

Consider the case $\gamma = \lambda$ and $\beta = 1$, so that the time-fractional Belousov-Zhabotinsky reaction-diffusion system in the sense of Atangana-Baleanu derivative of order $0 < \alpha \leq 1$ becomes

$$\begin{aligned} {}^{ABC}_{t_0}D^{\alpha}u(x,t) &= \xi_1 u_{xx}(x,t) + \delta v(x,t) + u(x,t) - u^2(x,t) - \delta u(x,t)v(x,t) \\ {}^{ABC}_{t_0}D^{\alpha}v(x,t) &= \xi_2 v_{xx}(x,t) + \lambda v(x,t) - u(x,t)v(x,t), \end{aligned} \tag{0.41}$$

subject to the initial conditions

$$\begin{aligned} u(x,t=0) &= \frac{1}{\left(e^{\sqrt{\frac{\lambda}{6}}x}+1\right)^2}, \\ v(x,t=0) &= \frac{(1-\lambda)}{\delta\left(e^{\sqrt{\frac{\lambda}{6}}x}+1\right)^2}. \end{aligned} \tag{0.42}$$

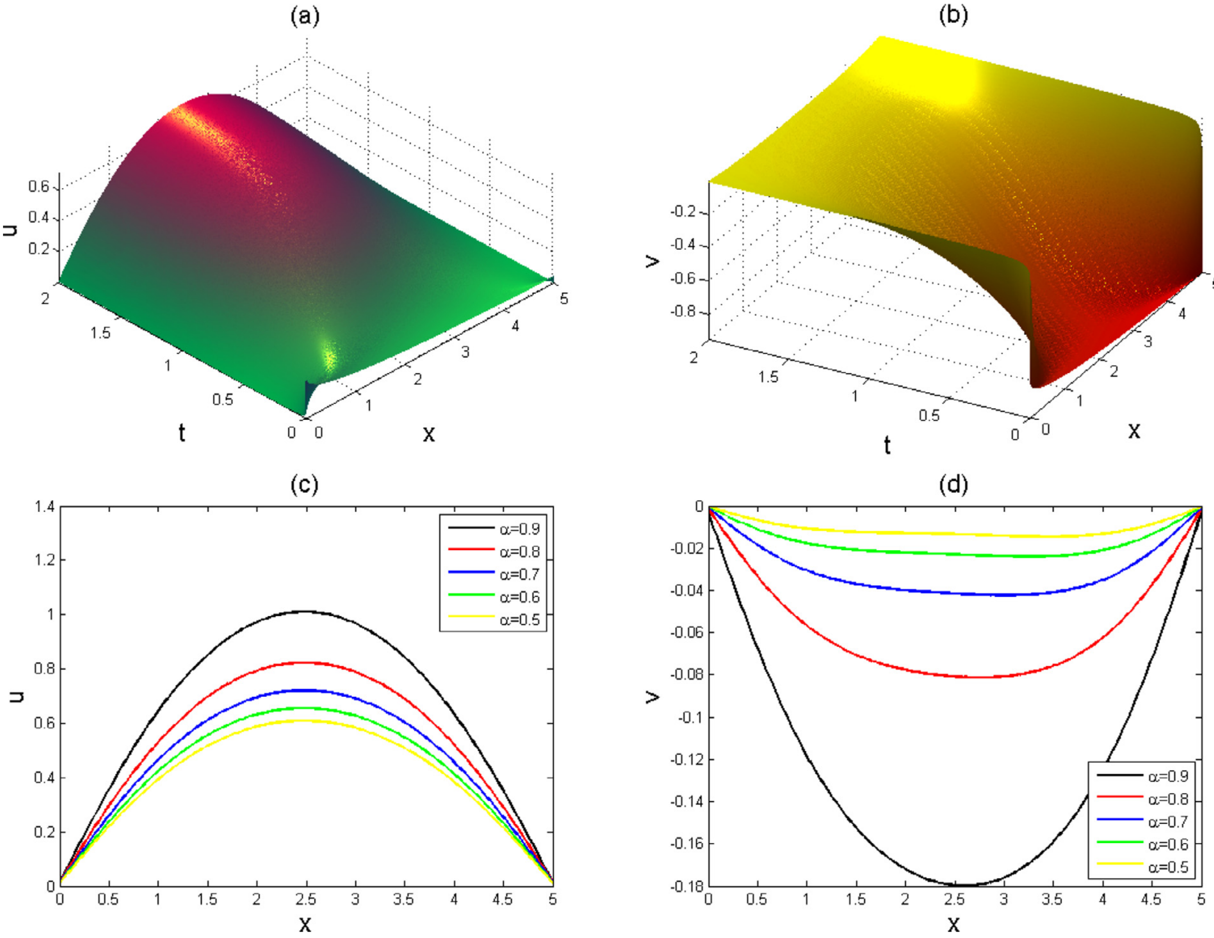

Fig. 1. Fractional distribution of system (0.36) with $\delta = 2$ and $\lambda = 2$ for different α.

The exact solution of (0.41) when $\alpha = 1$ is given as

$$\begin{aligned} u(x,t) &= \frac{e^{\frac{5\lambda}{3}t}}{\left(e^{\sqrt{\frac{\lambda}{6}}x} + e^{\frac{5\lambda}{6}t}\right)^2} = \frac{1}{4}\left(\tanh\left[\sqrt{\frac{\lambda}{24}}x - \frac{5\lambda}{12}t\right] - 1\right)^2, \\ v(x,t) &= \frac{(\lambda-1)e^{\sqrt{\frac{5\lambda}{3}}t}}{\delta\left(e^{\sqrt{\frac{\lambda}{6}}x} + e^{\frac{5\lambda}{6}t}\right)^2} = \frac{\lambda-1}{4\delta}\left(\tanh\left[\sqrt{\frac{\lambda}{24}}x - \frac{5\lambda}{12}t\right] - 1\right)^2, \end{aligned} \tag{0.43}$$

where $\lambda \neq 1$. The simulation experiment results for two values of α are reported in Figs. 4 and 5. Other parameters are given in the captions.

Case 3

Here, consider the solution nonlinear fractional reaction-diffusion model (0.17) using the initial conditions in (0.40) and the computer random initial condition computed as $u0 = 0.1 * ones(N, 1), v0 = 0.2 * ones(N, 1)$, with $N = 200$ and zero-flux boundary conditions. The corresponding results are given in Figs. 6 and 7, respectively. In Fig. 7, Rows 1 to 3 correspond to $\alpha = 0.45, 0.55, .0.65, 1.00$, respectively.

Case 4

In this case, consideration is given to the spatially homogeneous Belousov-Zhabotinskii fractional-order reaction model

$$\begin{aligned} {}^{ABC}_{t_0}D^{\alpha}u &= f_1(u,v,w) = u(1-u-\sigma v), \quad t>0, \\ {}^{ABC}_{t_0}D^{\alpha}v &= f_2(u,v,w) = \phi w - v - \varphi uv, \quad t>0 \\ {}^{ABC}_{t_0}D^{\alpha}w &= f_3(u,v,w) = \psi(u-w), \quad t>0, \end{aligned} \tag{0.44}$$

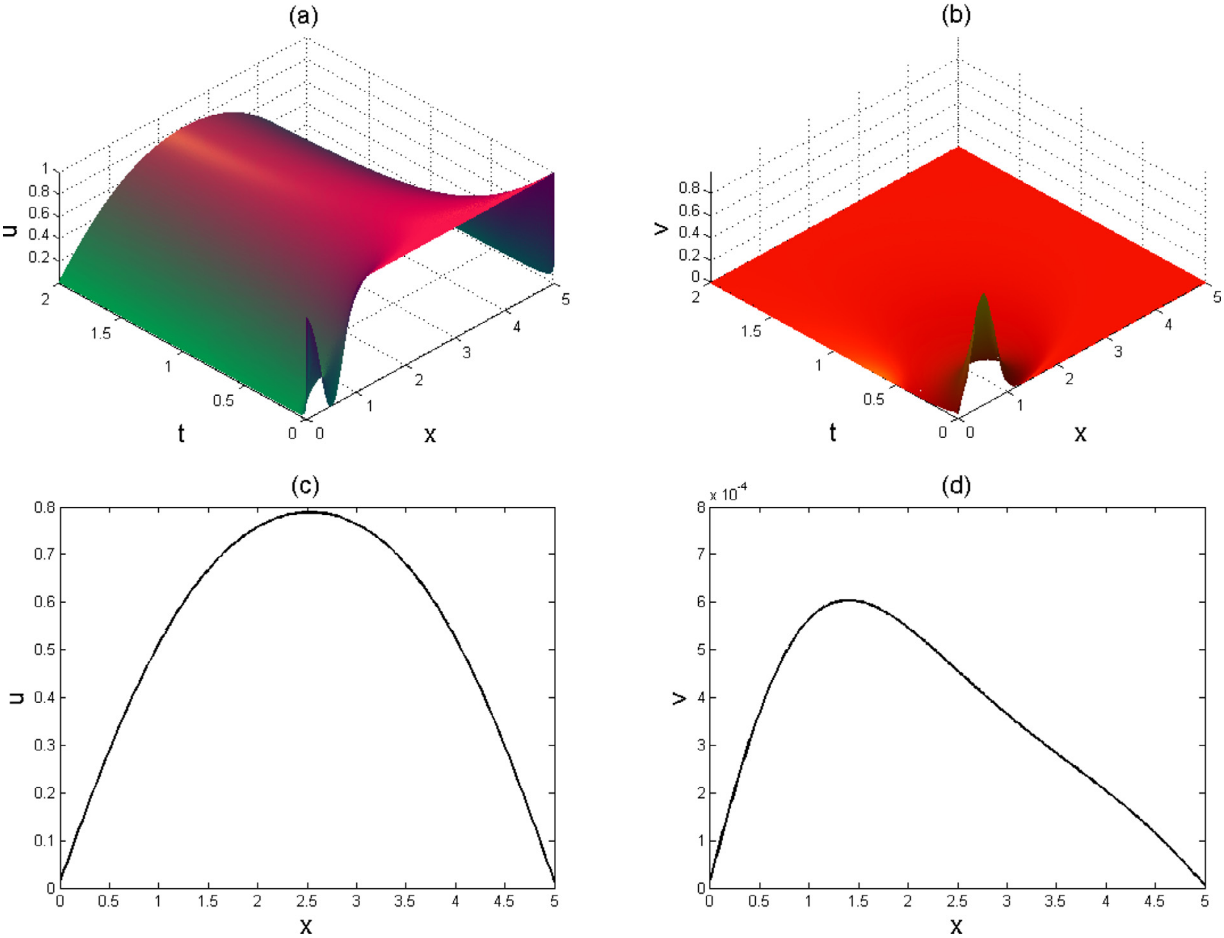

Fig. 2. Fractional evolution of system (0.36) with $\mu = 0.5, \delta = 2, \lambda = 2, \alpha = 0.93$ and initial conditions in (0.40).

where $f_i, i = 1, 2, 3$ is nonlinear local kinetic or simply the reaction terms, σ, ϕ, φ and ψ are positive parameters related to the speed of species reactions, and $u > 0, v > 0, w > 0$ denote the concentration of chemical reactants or biological populations. In the presence of diffusion, Eq. (0.44) becomes

$$\begin{array}{l} {}_{t_0}^{ABC}D^{\alpha}u(x,t) = u(1-u-\sigma v) + d_1\Delta u, \quad x\in\Omega, t>0,\\ {}_{t_0}^{ABC}D^{\alpha}v(x,t) = \phi w - v - \varphi uv + d_2\Delta v, \quad x\in\Omega, t>0\\ {}_{t_0}^{ABC}D^{\alpha}w(x,t) = \psi(u-w) + d_3\Delta w, \quad x\in\Omega, t>0,\\ \frac{\partial u}{\partial \nu}=0,\ \frac{\partial v}{\partial \nu}=0,\ \frac{\partial w}{\partial \nu}=0, \quad x\in\partial\Omega,\ \ t\geq 0,\\ (u,v,w)=(u_0,v_0,w_0), \quad x\in\bar{\Omega},\ \ t=0, \end{array} \tag{0.45}$$

where $d_i, i = 1, 2, 3$ are diffusion constants, $\Omega \subset \mathbb{R}^n$ is bounded domain with boundary $\partial\Omega$. The no-flux boundary condition is applied to assume no external flux into the domain. The stationary problem which corresponds to (0.45) is given as

$$\begin{array}{l} 0 = u(1-u-\sigma v) + d_1\Delta u, \quad x\in\Omega,\\ 0 = \phi w - v - \varphi uv + d_2\Delta v, \quad x\in\Omega,\\ 0 = \psi(u-w) + d_3\Delta w, \quad x\in\Omega,\\ \frac{\partial u}{\partial \nu}=0,\ \frac{\partial v}{\partial \nu}=0,\ \frac{\partial w}{\partial \nu}=0, \quad x\in\partial\Omega. \end{array} \tag{0.46}$$

Let $E = (u, v, w)$ be the solution of (0.46), it is not difficult to see that model (0.46) has just a solution $\hat{E} = (\hat{u}, \hat{v}, \hat{w})$:

$$\begin{array}{l} \hat{u} = \hat{w} = 1 - \sigma\hat{v},\\ \hat{v} = \frac{\phi\sigma+\varphi+1-\sqrt{(\phi\sigma+\varphi+1)^2-4\sigma\phi\varphi}}{2\sigma\varphi}. \end{array} \tag{0.47}$$

Though we are primarily concerned with the evolution of diffusive system, but many chemists or biologists are interested to see the dynamic behaviour of system (0.44). Hence, we set the parameters as $\sigma = 4, \phi = 1.5, \varphi = 1$ and $\psi = 0.5$ to obtain the time series plots and attractors for chemical species in Fig. 8 for different values of α. It was observed all states of reaction oscillates in phase regardless of the chosen value of α or computational time.

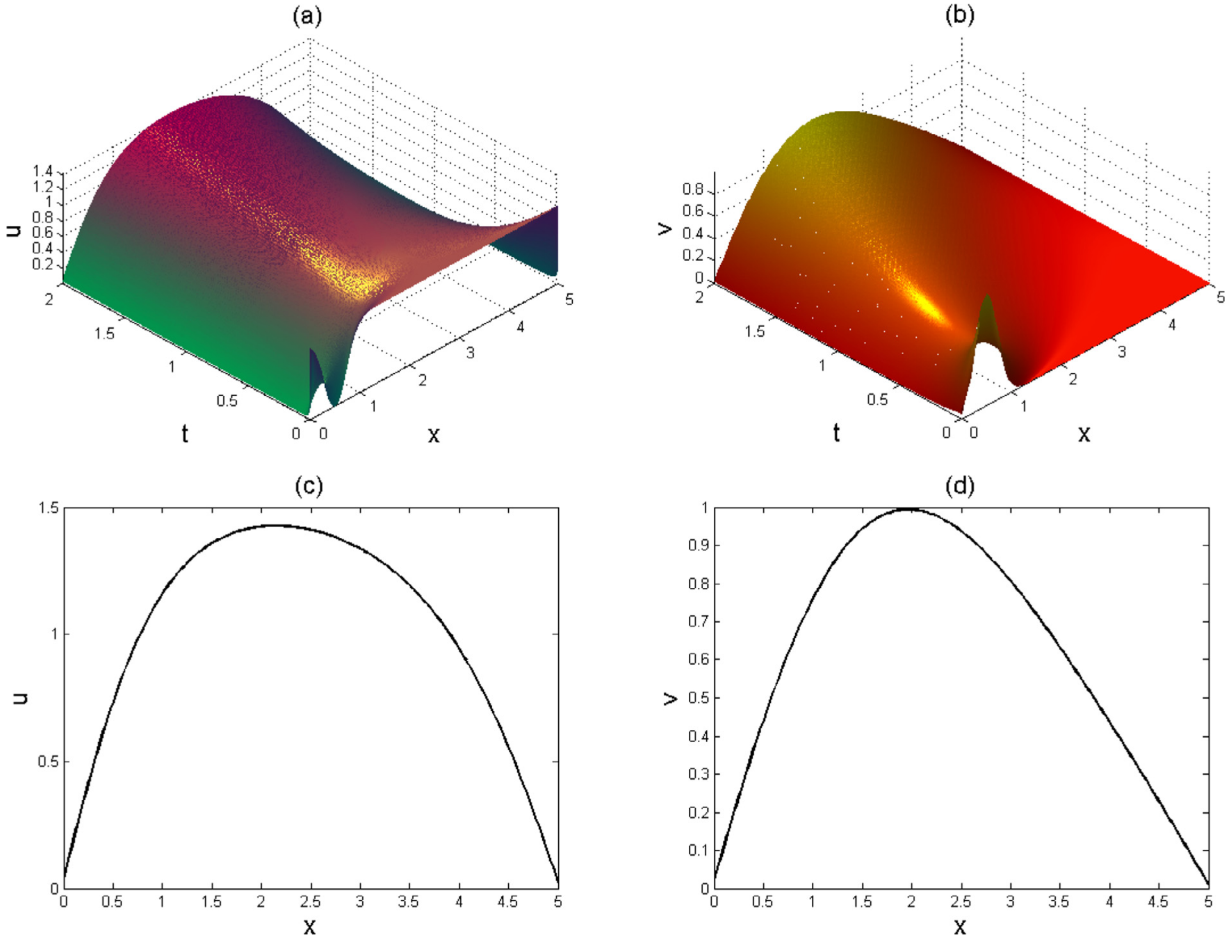

Fig. 3. Fractional evolution of system (0.36) with $\mu = 0.5, \delta = 2, \lambda = 2, \alpha = 0.75$ and initial conditions in (0.40).

Next, we carry out the linear stability of problem (0.44) at point $\hat{E}$. With $E = (u, v, w)$ independent of variable x, one writes model (0.44) in the general form

$$E_t = F(E), \tag{0.48}$$

where

$$F(E) = F(u, v, w) = \begin{pmatrix} u(1 - u - \sigma v) \\ \phi w - v - \varphi uv \\ \psi (u - w) \end{pmatrix}. \tag{0.49}$$

Obviously,

$$\begin{aligned} F_E(\hat{E}) &= \begin{pmatrix} 1 - 2\hat{u} - \sigma\hat{v} & -\sigma\hat{u} & 0 \\ -\varphi\hat{v} & -(1 + \varphi\hat{u}) & \phi \\ \psi & 0 & -\psi \end{pmatrix} \\ &= \begin{pmatrix} \frac{(\phi\sigma - \varphi + 1) - \vartheta}{2\varphi} & \frac{\sigma[(\phi\sigma - \varphi + 1) - \vartheta]}{2\sigma} & 0 \\ \frac{-(\phi\sigma + \varphi + 1) + \vartheta}{2\varphi} & \frac{\sigma[(\phi\sigma - \varphi - 1) - \vartheta]}{2} & 0 \\ \psi & 0 & -\psi \end{pmatrix}, \end{aligned} \tag{0.50}$$

where $\vartheta = \sqrt{(\phi\sigma + \varphi + 1)^2 - 4\sigma\phi\varphi}$. With ease, one can verify that the corresponding characteristic equation of $F_E(\hat{E})$ is

$$\rho(r) = r^3 + \mathcal{A}r^2 + \mathcal{B}r + \mathcal{C}, \tag{0.51}$$

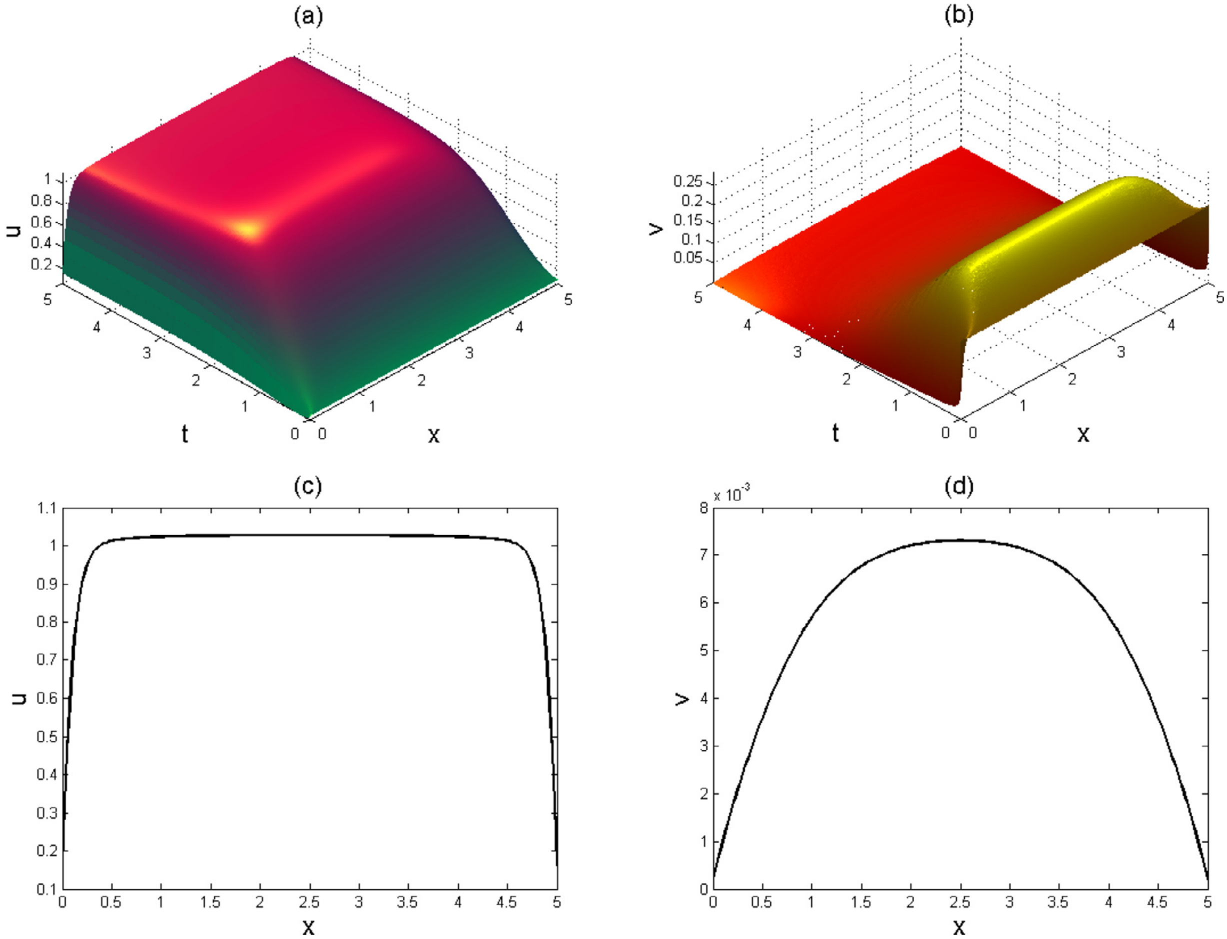

Fig. 4. Simulation results for system (0.41) with $\delta = 2$, $\lambda = 2.3$ and $\alpha = 0.48$.

where

$$\begin{aligned} \mathcal{A} &= \tfrac{[(\varphi^2+2\varphi-1)-(\varphi+1)\phi\sigma+2\varphi\psi+(\varphi+1)\vartheta]}{2\varphi} > 0, \\ \mathcal{B} &= [(\varphi+1)^2+(3+2\sigma\phi-3\varphi)\sigma\phi+[\varphi^2+2\varphi-1-\phi\sigma(\varphi+1)]\psi \\ &\quad +[\varphi-2\phi\sigma-1+(\varphi+1)\psi]\vartheta]\tfrac{1}{2\varphi}, \\ \mathcal{C} &= \tfrac{\psi[\phi^2\sigma^2-2\sigma\phi(\varphi-1)+(\varphi+1)^2+(\varphi-\sigma\phi-1)\vartheta]}{2\varphi} > 0. \end{aligned} \tag{0.52}$$

The roots of polynomial $\rho(r) = 0$ satisfies the following inequalities

$$\mathcal{A} = -(r_1 + r_2 + r_3) > 0, \quad \mathcal{B} = r_2 r_3 + r_3 r_1 + r_1 r_2, \quad \mathcal{C} = -r_1 r_2 r_3 > 0. \tag{0.53}$$

Based on the Routh-Hurwitz criteria, necessary and sufficient conditions for the solution E to be stable is that $\mathcal{AB} - \mathcal{C} > 0$. Other stability conditions are omitted here.

To observe the dynamic behaviour of full fractional system (0.45) under the Atangana-Baleanu derivative in the Caputo sense, we utilize the zero-flux boundary conditions and the random initial condition

`u0=u*(ones(N,1)),`

`v0=v*(ones(N,1)),`

`w0=w*(ones(N,1)),` where $N = 200$ with small noise $(u*, v*, w*) = (0.5, 0.1, 0.1)$. Other parameters used are; $\sigma = 3.5, \phi = 1.5, \varphi = 1.2, \psi = 0.05, d_1 = 0.007, d_2 = 0.001, d_3 = 0.002$. Simulation runs for $t = 100$ to obtain the results in Figs. 9 and 10. A number of spatiotemporal oscillations were observed.

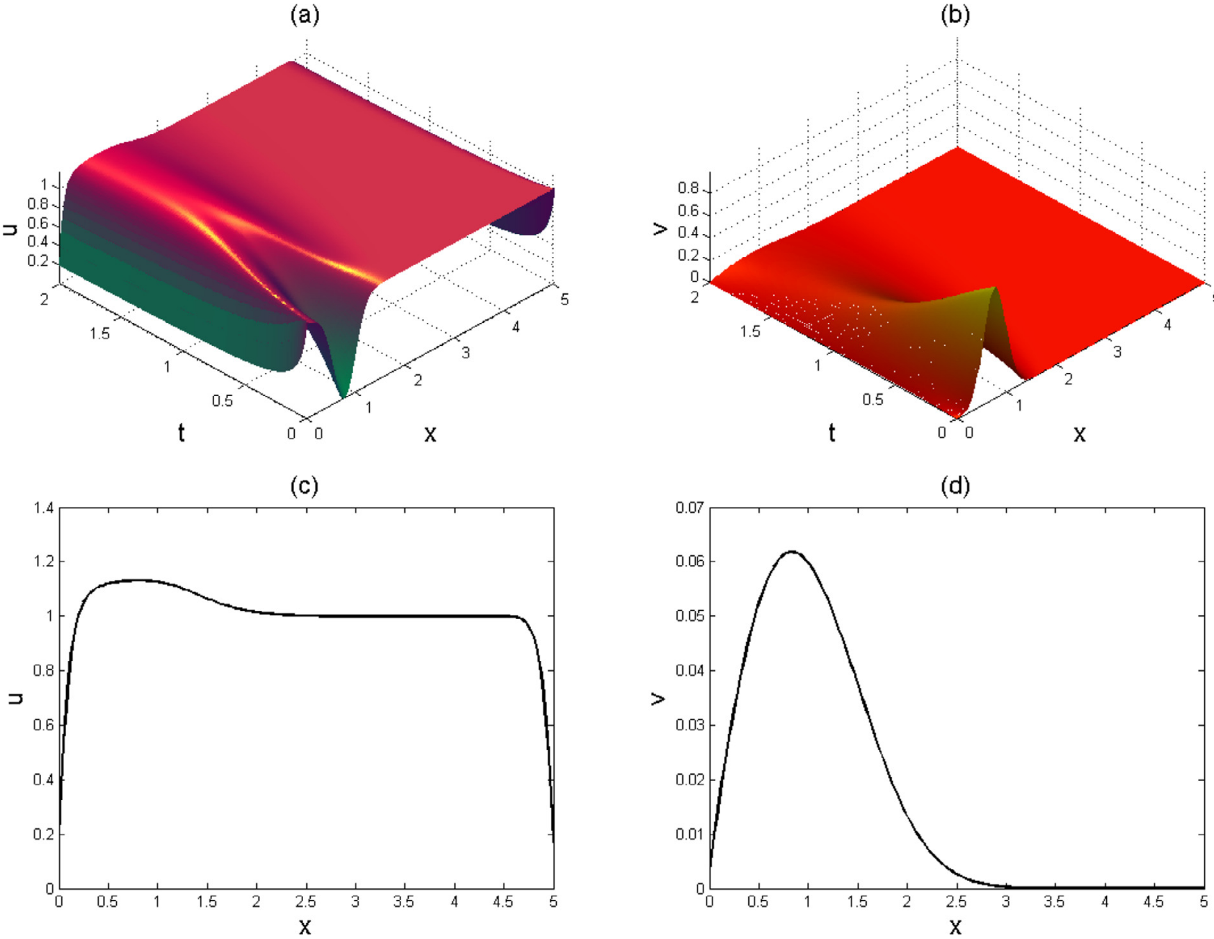

Fig. 5. Simulation results for system (0.41) with $\delta = 2$, $\lambda = 2.3$ and $\alpha = 0.65$.

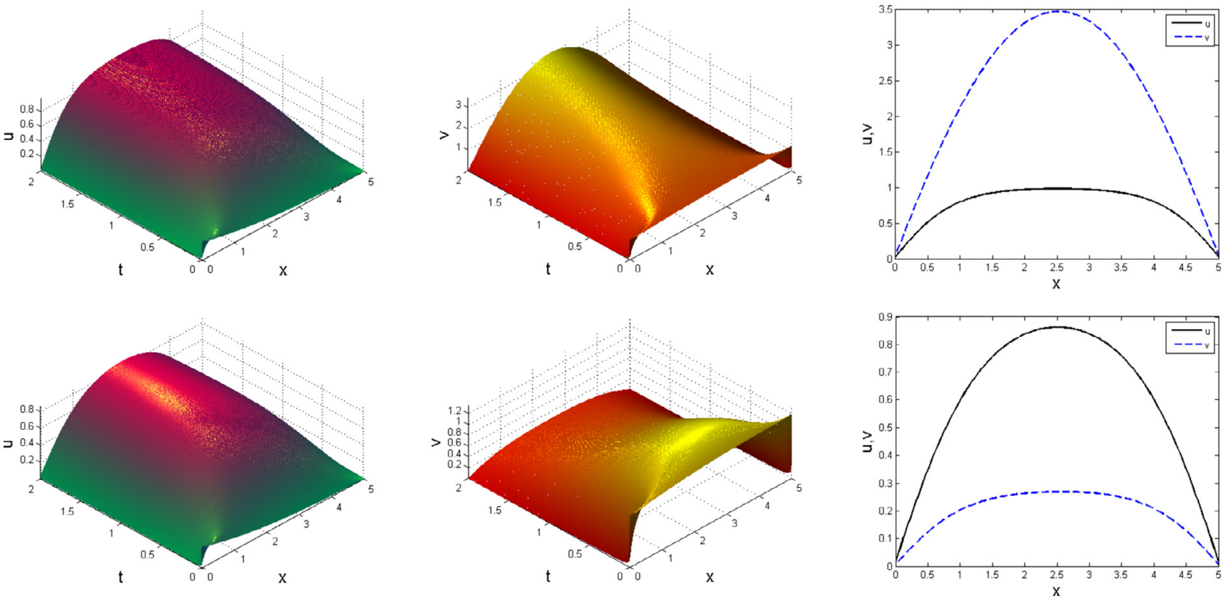

Fig. 6. Evolution of fractional model (0.17) with The upper and lower rows correspond to $\alpha = 0.82$ and $\alpha = 0.89$, respectively.

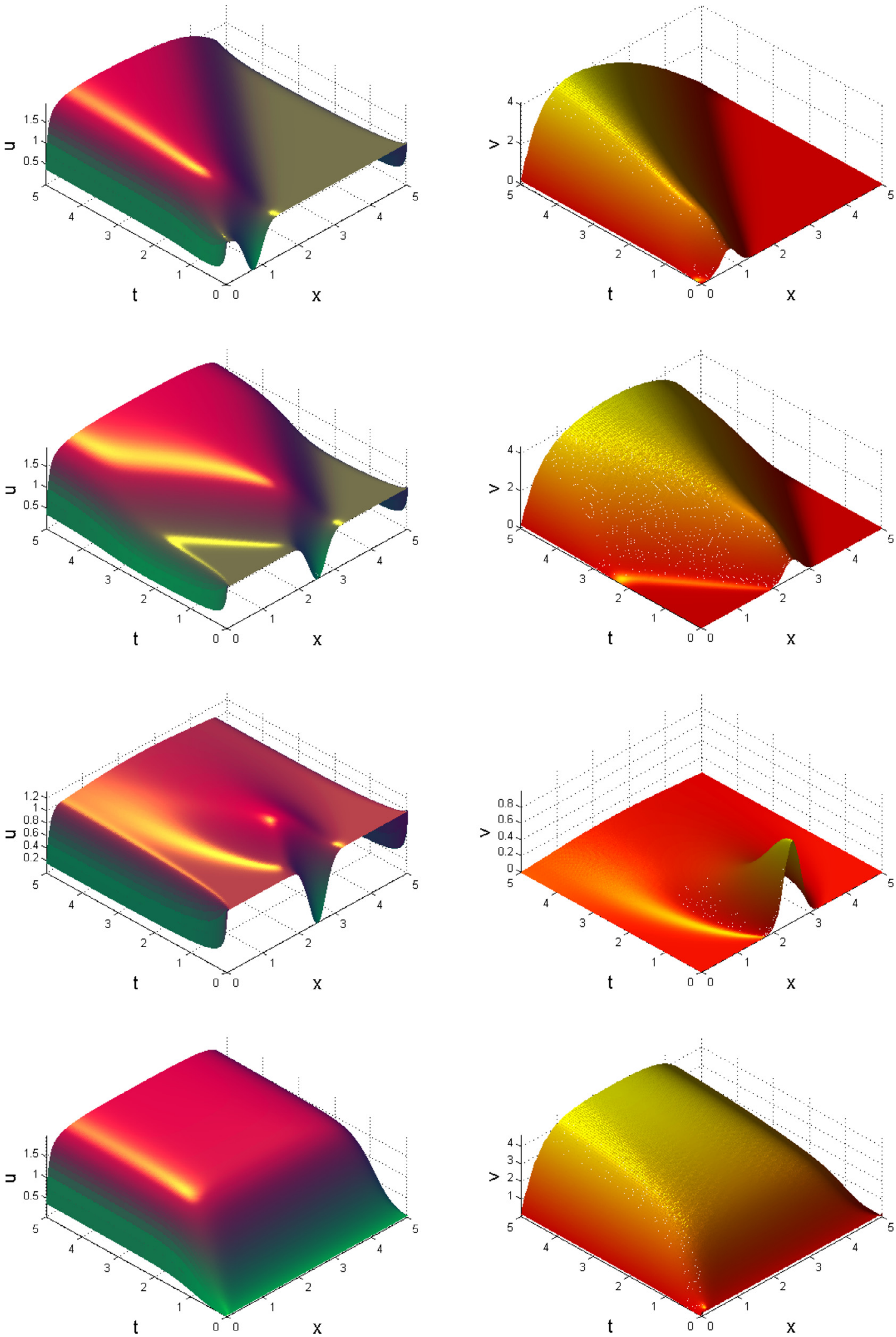

Fig. 7. Simulation results for system (0.41) the computer random initial condition for different α.

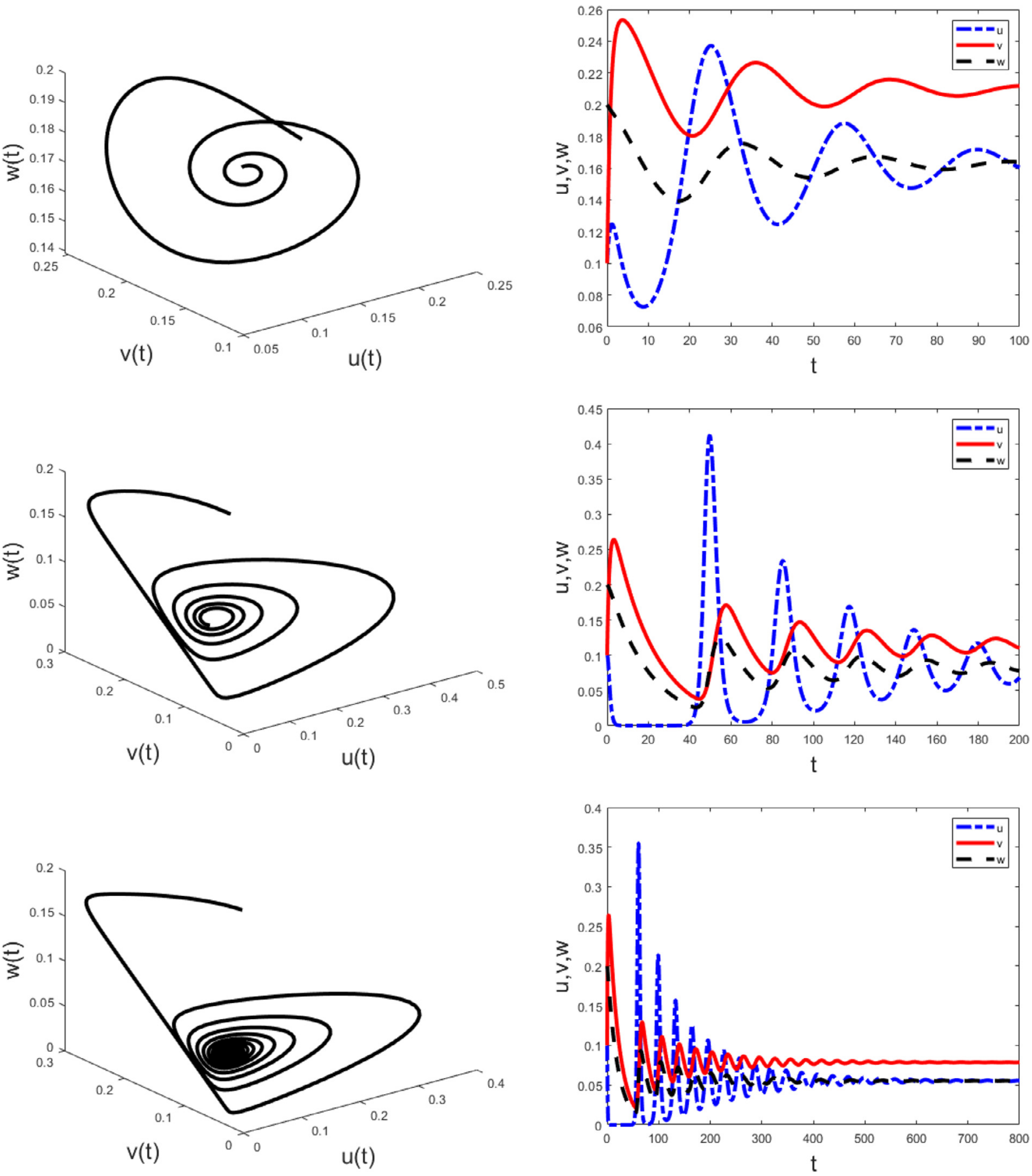

Fig. 8. Chaotic attractors and time-series solution for system (0.44). Rows 1-3 correspond to $\alpha = (0.45, 0.65, 0.85)$, respectively.

Conclusion

Finding the numerical solution to fractional-in-time reaction-diffusion equations is one of the major challenges in the field of applied mathematics. This manuscript suggests a reliable technique for analyzing and investigating the time-fractional Noyes-Field model for the Belousov-Zhabotinskii reaction which is defined in the sense of the Atangana-Baleanu fractional operator. Primarily, the existence and uniqueness of the model are investigated via Picard-Lindelöf theorem. Afterward, we constructed a numerical scheme to investigate the numerical behavior of the solution of the time-fractional Noyes-Field model and the stability conditions are presented. The significant impact of fractional-order parameters was justified via graphical results. Observation from numerical results in Figs. 9 and 10 shows that the variant of the Noyes-Field model can give rise to chaotic and spatiotemporal distribution under certain conditions and parameters. The methodology reported in this paper can be extended to solve other real-life phenomena. In future researches, numerical methods will be use in order to improve the approximation to Reaction-diffusion models, especially we will focus on two-dimensional fractional order diffusion models.

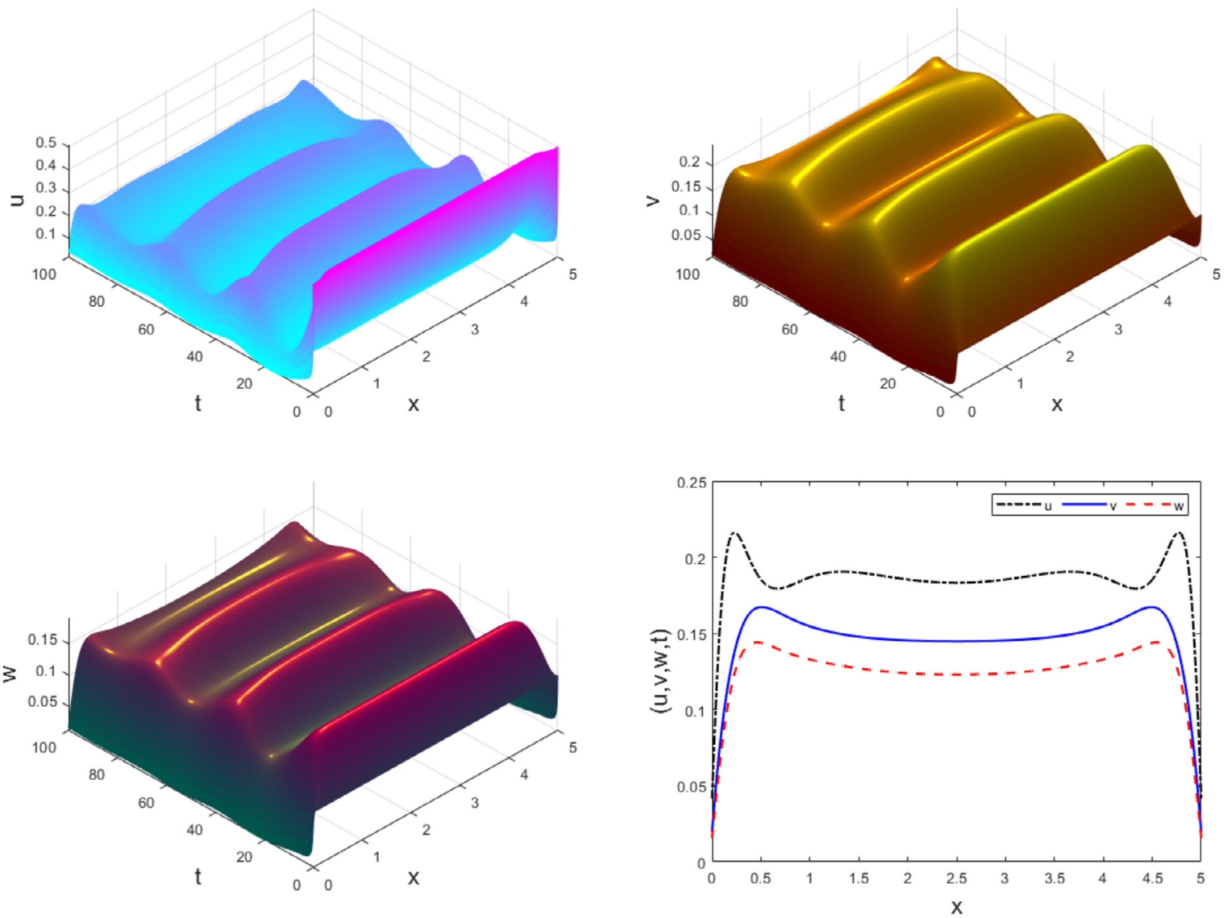

Fig. 9. Dynamic evolution of model (0.45) with $\alpha = 0.53$.

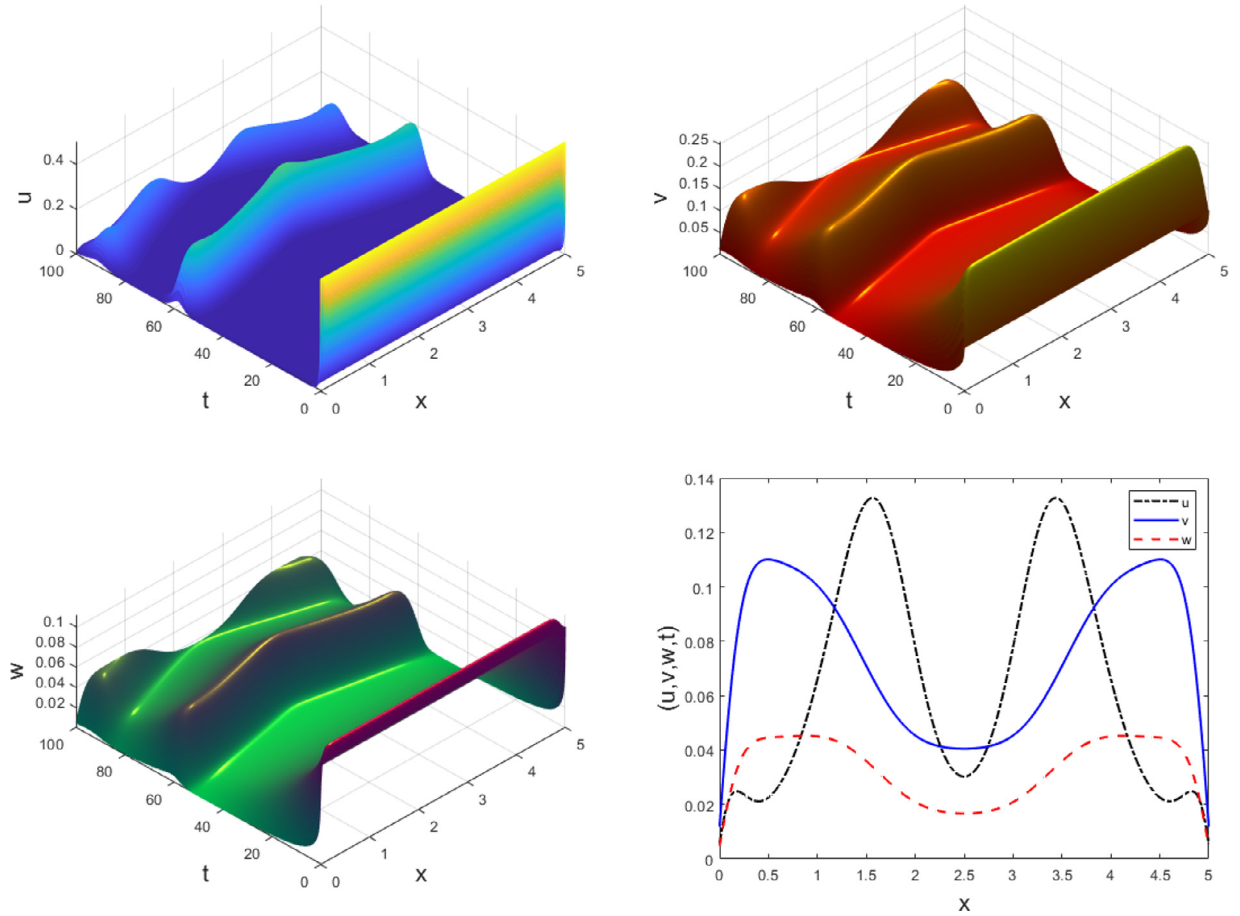

Fig. 10. Dynamic evolution of model (0.45) with $\alpha = 0.76$.

Credit author statement

All authors conceived the idea, BK carried out the initial draft, KMO carried out the numerical experiments, EP supervised the paper and will be responsible for paying the APC, all authors approve the final draft for submission.

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EP Edson Pindza

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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