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A fractional model of a dynamical Brusselator reaction-diffusion system arising in triple collision and enzymatic reactions

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Abstract: In this paper, we study a dynamical Brusselator reaction-diffusion system arising in triple collision and enzymatic reactions with time fractional Caputo derivative. The present article involves a more generalized effective approach, proposed for the Brusselator system say q -homotopy analysis transform method (q -HATM), providing the family of series solutions with nonlocal generalized effects. The convergence of the q -HATM series solution is adjusted and controlled by auxiliary parameter \hbar and asymptotic parameter n . The numerical results are demonstrated graphically. The outcomes of the study show that the q -HATM is computationally very effective and accurate to analyze nonlinear fractional differential equations.

Keywords: Fractional reaction-diffusion Brusselator system; Laplace transform method; q -homotopy analysis transform method; \hbar and n -curves

1 Introduction

Fractional order differential equations have been proved to be an important and useful tool to show the hidden aspects in many phenomena occurring from real world, such as physical sciences, signal processing, electromagnetic, earthquake, traffic flow, measurement of viscoelastic ma-

terial properties and many more processes [1–7]. The concept of fractional differential coefficients is considered as the history and nonlocal distributed effects, an excellent literature of this can be found in various monographs [8–11].

In this article, we consider a fractional dynamical Brusselator model is a simple reaction-diffusion equations occurring in various physical problems, referred to the formation of ozone by atomic oxygen via triple collision and enzymatic reactions. This dynamical system holds a pivotal role in study of chemical kinetics, or biochemical reactions, and biological systems. The dynamical Brusselator reaction-diffusion system involves controlled concentration of paired variables intermediates with reactants and product chemicals with nonlinear oscillations [12–15]. Considerable significant investigations of solutions of the Brusselator model have been done earlier with various schemes [16–25] which have their local point effects. The present research entails a more generalized effective approach, proposed for the Brusselator system say q -HATM, providing the family of series solutions with nonlocal generalized effects. The q -HATM basically shows how the Laplace transform can be employed to find the approximate series solutions of the time fractional Brusselator reaction-diffusion equations by manipulating the q -homotopy analysis method. The q -HAM initially given by El-Tavil and Huseen [26, 27], is more generalized computational approach than the classical homotopy analysis method (HAM) introduced by Liao in his PhD thesis in 1992 [28–31] and contains the HAM as a special case. The comparisons between both the approaches are shown by graphically. The HAM is an analytical algorithm to solve various kinds of nonlinear problems of integer and fractional order and is free from any restriction, perturbations, complicated integrals calculations and polynomials, uniformly valid for both large/small physical parameters [32–35]. In recent scenario analytical techniques have also been employed to investigate various scientific and technological problems such as unsteady two-dimensional and axisymmetric squeezing flows between parallel plates [36], three-dimensional Navier Stokes equa-

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tions [37], magneto-hemodynamic flow in a semi-porous channel [38], micropolar flow in a porous channel with mass injection [39], unsteady MHD flow past a stretching permeable surface in nano-fluid [40], Jeffery-Hamel flow with high magnetic field and nano-particle [41], squeezing unsteady nanofluid flow [42], three-dimensional problem of condensation film on inclined rotating disk [43], nanofluid flow and heat transfer between parallel plates considering Brownian motion [44], effects of heat transfer in flow of nanofluids over a permeable stretching wall in a porous medium [45]. In now a days numerical techniques has also been discussed such as numerical simulation of two dimensional hyperbolic equations with variable coefficients [46], numerical solution of Burgers' equation [47], numerical simulation of two-dimensional sine-Gordon solitons [48], etc.

2 A dynamical Brusselator reaction-diffusion system

In this work, we analyze the following dynamical Brusselator fractional reaction-diffusion equations with time fractional derivative

$$\left. \begin{aligned} \frac{\partial^\alpha u}{\partial t^\alpha} &= u^2 v - (A+1)u + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + B, \\ \frac{\partial^\beta v}{\partial t^\beta} &= -u^2 v + Au + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \\ 0 < \alpha, \beta &\leq 1, (x, y) \in \Omega, t > 0, \end{aligned} \right\} \quad (1)$$

with the appropriate initial conditions

$$\left. \begin{aligned} u(x, y, 0) &= \xi(x, y) \\ v(x, y, 0) &= \zeta(x, y) \end{aligned} \right\} \quad (x, y) \in \Omega. \quad (2)$$

In the above equations $u(x, y, t)$ and $v(x, y, t)$ represent dimensionless concentrations of two reactants, A and B be constants concentrations of the two reactants, $\Omega \subset \mathbb{R}^2$ denotes the domain set and $\partial\Omega$ indicates the boundary of the domain set Ω , $0 < \alpha, \beta \leq 1$ are parameters representing the order of the time fractional derivatives. It is well known that for small values of the diffusion coefficient μ , the steady state solution of the Brusselator system (1) converges to equilibrium point $(B, A/B)$, if $1 - A + B^2 \geq 0$ [49]. In this article we select the constant values of $A = 1$, $B = 0$ and $\mu = 0.25$.

3 Basic definitions

Definition 1. The fractional derivative of $f(t)$ in the Caputo sense is defined and represented in the following manner [50]:

$$D^\alpha f(t) = J^{n-\alpha} D^n f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} f^n(\tau) d\tau, \quad (3)$$

for $n-1 < \alpha \leq n$, $n \in \mathbb{N}$, $t > 0$, $f \in C_{-1}^n$.

Lemma: If $n-1 < \alpha \leq n$, $n \in \mathbb{N}$, $f \in C_\mu^n$, $\mu \geq -1$, then

$$D^\alpha J^\alpha f(t) = f(t) - \sum_{r=0}^{n-1} f^{(r)}(0^+) \frac{t^r}{\Gamma(r+1)}, \quad t > 0. \quad (4)$$

The fractional derivative given by Caputo is employed here because it permits traditional initial and boundary conditions to be included in the modelling of the problem.

Definition 2. For r to be the smallest integer that exceeds α , the Caputo-fractional derivative operator of order $\alpha > 0$ is explained as

$$D^\alpha v(x, t) = \frac{\partial^\alpha v(x, t)}{\partial t^\alpha} = \begin{cases} \frac{1}{\Gamma(r-\alpha)} \int_0^t (t-y)^{r-\alpha-1} \frac{\partial^r v(x, t)}{\partial y^r} dy, & \text{for } r-1 < \alpha < r \\ \frac{\partial^r v(x, t)}{\partial t^r}, & \text{for } \alpha = r \in \mathbb{N} \end{cases} \quad (5)$$

Definition 3. The Laplace transform (LT) of a function $f(t)$, denoted by $F(s)$, is defined by the equation

$$L\{f(t), s\} = F(s) = \int_0^\infty e^{-st} f(t) dt. \quad (6)$$

If $n \in \mathbb{N}$, then Laplace transform is given as

$$L\left\{\frac{d^n}{dx^n}; f; s\right\} = s^n F(s) - \sum_{r=0}^{n-1} s^{n-r-1} f^{(r)}(0^+), \quad (7)$$

and the LT of fractional order, the Caputo derivative is given by [50] see also [51] in the form

$$L[D^\alpha f(t)] = s^\alpha L[f(t)] - \sum_{r=0}^{n-1} s^{\alpha-r-1} f^{(r)}(0^+), \quad n-1 < \alpha \leq n. \quad (8)$$

Definition 4. The Laplace transform of the Riemann-Liouville fractional derivative is defined and explained as

$$L[I_t^\alpha f(t)] = s^{-\alpha} F(s). \quad (9)$$

4 Basic idea of q -HATM

To present the basic idea and concept of this scheme, we consider a general nonlinear non-homogeneous partial differential equation of fractional order written in the following form:

$$D_t^\alpha u(x, y, t) + R u(x, y, t) + N u(x, y, t) = w(x, y, t), \quad n-1 < \alpha \leq n. \quad (10)$$

In the above equation $D_t^\alpha u(x, y, t)$ is the famous Caputo fractional derivative of the function $u(x, y, t)$, R is representing the linear differential operator, N is depicting the general nonlinear differential operator and $w(x, y, t)$ is indicating the term occurring from source.

By operating with the well known LT on both sides of equation (10), we arrive at the following result

$$L[D_t^\alpha u] + L[R u] + L[N u] = L[w(x, y, t)]. \quad (11)$$

Making use of the differentiation property of the LT, we have

$$s^\alpha L[u] - \sum_{k=0}^{n-1} s^{\alpha-k-1} u^{(k)}(x, 0) + L[R u] + L[N u] = L[w(x, y, t)]. \quad (12)$$

Now simplifying Eq. (12), we get the following result

$$L[u] - \frac{1}{s^\alpha} \sum_{k=0}^{n-1} s^{\alpha-k-1} u^{(k)}(x, 0) + \frac{1}{s^\alpha} [L[R u] + L[N u] - L[w(x, y, t)]] = 0. \quad (13)$$

We define the nonlinear operator

$$\begin{aligned} N[\theta(x, y, t; q)] &= L[\theta(x, y, t; q)] \\ &- \frac{1}{s^\alpha} \sum_{k=0}^{n-1} s^{\alpha-k-1} \theta^{(k)}(x, y, t; q)(0^+) \\ &+ \frac{1}{s^\alpha} [L[R\theta(x, y, t; q)] + L[N\theta(x, y, t; q)] - L[w(x, y, t)]], \end{aligned} \quad (14)$$

here $q \in [0, 1/n]$ and $\theta(x, y, t; q)$ is indicating a real function of x, t and q . The homotopy is constructed as follows

$$\begin{aligned} (1 - nq) L[\theta(x, y, t; q) - u_0(x, t)] \\ = \hbar q H(x, y, t) N[u(x, y, t)], \end{aligned} \quad (15)$$

where L is denoting the LT operator, $n \geq 1$, $q \in [0, \frac{1}{n}]$ is the embedding parameter, $H(x, y, t)$ denotes a nonzero auxiliary function, $\hbar \neq 0$ is an auxiliary parameter, $u_0(x, y, t)$ is an initial guess of $u(x, y, t)$ and $\theta(x, y, t; q)$ is a unknown

function. Obviously, when the embedding parameter $q = 0$ and $q = \frac{1}{n}$, it holds

$$\theta(x, y, t; 0) = u_0(x, y, t), \quad \theta(x, y, t; \frac{1}{n}) = u(x, y, t), \quad (16)$$

respectively. Thus, as q increases from 0 to $\frac{1}{n}$, the solution $\theta(x, y, t; q)$ varies from the initial guess $u_0(x, y, t)$ to the solution $u(x, y, t)$. Expanding $\theta(x, y, t; q)$ in Taylor series with respect to q , we have

$$\theta(x, y, t; q) = u_0(x, y, t) + \sum_{m=1}^{\infty} u_m(x, y, t) q^m, \quad (17)$$

where

$$u_m(x, y, t) = \frac{1}{m!} \frac{\partial^m \theta(x, y, t; q)}{\partial q^m} \Big|_{q=0}. \quad (18)$$

If we select the auxiliary linear operator, the initial guess, the auxiliary parameter n , \hbar and the auxiliary function, the series (17) converges at $q = \frac{1}{n}$, then we have the following equation

$$u(x, y, t) = u_0(x, y, t) + \sum_{m=1}^{\infty} u_m(x, y, t) \left(\frac{1}{n}\right)^m, \quad (19)$$

which must be one of the solutions of the original nonlinear equations. According to the definition (19), the controlling equation can be obtained from the zero-order deformation equation (15).

We take the vectors as

$$\vec{u}_m = \{u_0(x, y, t), u_1(x, y, t), \dots, u_m(x, y, t)\}. \quad (20)$$

The Differentiation on the zeroth-order deformation Equation (15) m -times with respect to q and then division by $m!$ and finally letting $q = 0$, it gives the m th-order deformation equation of the form:

$$L[u_m(x, y, t) - k_m u_{m-1}(x, y, t)] = \hbar H(x, y, t) \Re_m(\vec{u}_{m-1}). \quad (21)$$

Applying the inverse LT, we have

$$u_m(x, y, t) = k_m u_{m-1}(x, y, t) + \hbar L^{-1}[H(x, y, t) \Re_m(\vec{u}_{m-1})], \quad (22)$$

where $\Re_m(\vec{u}_{m-1})$ is presented as

$$\Re_m(\vec{u}_{m-1}) = \frac{1}{(m-1)!} \frac{\partial^{m-1} N[\theta(x, y, t; q)]}{\partial q^{m-1}} \Big|_{q=0}, \quad (23)$$

and k_m is given as

$$k_m = \begin{cases} 0, & m \leq 1, \\ n, & m > 1. \end{cases} \quad (24)$$

The convergence analysis of this type of series solution has already been done by Abbaoui and Cherruault [52].

5 Implementation of the method

Example 1. In this example, we analyze the following system of fractional reaction-diffusion Brusselator equations

$$\left. \begin{aligned} \frac{\partial^\alpha u}{\partial t^\alpha} &= u^2 v - (A+1)u + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + B, \\ \frac{\partial^\beta v}{\partial t^\beta} &= -u^2 v + Au + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \end{aligned} \right\} \quad (25)$$

subject to the initial conditions

$$\begin{aligned} u(x, y, 0) &= u_0 = \chi_1(x, y) = e^{-(x+y)}, \\ v(x, y, 0) &= v_0 = \chi_2(x, y) = e^{(x+y)}, \end{aligned} \quad (26)$$

where $0 < \alpha, \beta \leq 1$ are parameters describing the order of the time fractional derivatives, x is the space domain and t is time.

Using the q -HATM algorithm, we define the nonlinear operator as

$$\begin{aligned} N^1[\psi_1(x, y, t; q), \psi_2(x, y, t; q)] &= L[\psi_1(x, y, t; q)] \\ &- \left(1 - \frac{k_m}{n}\right) \frac{1}{s} \chi_1(x, y) - \frac{1}{s^\alpha} L[\psi_1^2(x, y, t; q) \psi_2(x, y, t; q) \\ &- (A+1)\psi_1(x, y, t; q) \\ &+ \mu \left(\frac{\partial^2 \psi_1(x, y, t; q)}{\partial x^2} + \frac{\partial^2 \psi_1(x, y, t; q)}{\partial y^2} \right) + \left(1 - \frac{k_m}{n}\right) B], \end{aligned} \quad (27)$$

$$\begin{aligned} N^2[\psi_1(x, y, t; q), \psi_2(x, y, t; q)] &= L[\psi_2(x, y, t; q)] \\ &- \left(1 - \frac{k_m}{n}\right) \frac{1}{s} \chi_2(x, y) \\ &- \frac{1}{s^\beta} L \left[-\psi_1^2(x, y, t; q) \psi_2(x, y, t; q) + A\psi_1(x, y, t; q) \right. \\ &\left. + \mu \left(\frac{\partial^2 \psi_2(x, y, t; q)}{\partial x^2} + \frac{\partial^2 \psi_2(x, y, t; q)}{\partial y^2} \right) \right], \end{aligned} \quad (28)$$

and the Laplace operator as

$$\left. \begin{aligned} L[u_m(x, t) - k_m u_{m-1}(x, t)] &= \hbar R_{1,m}[\vec{u}_{m-1}, \vec{v}_{m-1}], \\ L[v_m(x, t) - k_m v_{m-1}(x, t)] &= \hbar R_{2,m}[\vec{u}_{m-1}, \vec{v}_{m-1}], \end{aligned} \right\} \quad (29)$$

where

$$\begin{aligned} R_{1,m}[\vec{u}_{m-1}, \vec{v}_{m-1}] &= L\{u_{m-1}(x, t)\} - \left(1 - \frac{k_m}{n}\right) \frac{1}{s} e^{-(x+y)} \\ &- \frac{1}{s^\alpha} L \left\{ \sum_{k=0}^{m-1} u_{m-k-1} \sum_{i=0}^k u_{k-i} v_i - (A+1)u_{m-1} \right. \\ &\left. + \mu \left(\frac{\partial^2 u_{m-1}}{\partial x^2} + \frac{\partial^2 u_{m-1}}{\partial y^2} \right) + B \left(1 - \frac{k_m}{n}\right) \right\}. \end{aligned} \quad (30)$$

$$\begin{aligned} R_{2,m}[\vec{u}_{m-1}, \vec{v}_{m-1}] &= L\{v_{m-1}(x, t)\} - \left(1 - \frac{k_m}{n}\right) \frac{1}{s} \sin x \\ &- \frac{1}{s^\beta} L \left\{ -\sum_{k=0}^{m-1} u_{m-k-1} \sum_{i=0}^k u_{k-i} v_i + Au_{m-1} \right. \\ &\left. + \mu \left(\frac{\partial^2 v_{m-1}}{\partial x^2} + \frac{\partial^2 v_{m-1}}{\partial y^2} \right) \right\}. \end{aligned} \quad (31)$$

It is obvious, that the solution of the m th-order deformation equations (29) for $m \geq 1$ becomes

$$\left. \begin{aligned} u_m(x, t) &= k_m u_{m-1}(x, t) + \hbar L^{-1}\{R_{1,m}[\vec{u}_{m-1}, \vec{v}_{m-1}]\} \\ v_m(x, t) &= k_m v_{m-1}(x, t) + \hbar L^{-1}\{R_{2,m}[\vec{u}_{m-1}, \vec{v}_{m-1}]\}, \end{aligned} \right\} \quad (32)$$

On solving the above equations, it gives

$$\begin{aligned} u_0 &= e^{-(x+y)}, \quad v_0 = e^{(x+y)}, \\ u_1 &= -\hbar(-A+2\mu+Be^{(x+y)})e^{-(x+y)} \frac{t^\alpha}{\Gamma(\alpha+1)}, \\ v_1 &= -\hbar(-1+A+2\mu e^{2(x+y)})e^{-(x+y)} \frac{t^\beta}{\Gamma(\beta+1)}, \\ u_2 &= (n+\hbar)u_1 + \hbar^2((A^2+2\mu(1+2\mu)-A(1+4\mu) \\ &+ B(1-A)e^{(x+y)})e^{-(x+y)} \frac{t^{2\alpha}}{\Gamma(2\alpha+1)} \\ &+ (-1+A+2\mu e^{2(x+y)})e^{-3(x+y)} \frac{t^{\alpha+\beta}}{\Gamma(\alpha+\beta+1)}), \\ v_2 &= (n+\hbar)v_1 - \hbar^2((-2+A)(A-2\mu)e^{-(x+y)} \\ &- B(2-A)) \frac{t^{\alpha+\beta}}{\Gamma(\alpha+\beta+1)} \\ &+ \hbar^2(-1+2\mu e^{2(x+y)})(-1+A+2\mu e^{2(x+y)}) \frac{t^{2\beta}}{\Gamma(2\beta+1)}, \\ &\vdots \end{aligned} \quad (33)$$

and so on, in this manner the rest of the iterative components can be derived. Therefore, the family of q -HATM series solutions of the system (25) is given as pair of equations in the following form

$$\left. \begin{aligned} u(x, y, t) &= u_0(x, y, t) + \sum_{m=1}^{\infty} u_m(x, y, t) \left(\frac{1}{n}\right)^m, \\ v(x, y, t) &= v_0(x, y, t) + \sum_{m=1}^{\infty} v_m(x, y, t) \left(\frac{1}{n}\right)^m. \end{aligned} \right\} \quad (34)$$

If we set $\alpha = \beta = 1$ and $\hbar = -1$, $n = 1$ then clearly, we can observed that the solution $\sum_{m=0}^N u_m(x, y, t) \left(\frac{1}{n}\right)^m$ and $\sum_{m=0}^N v_m(x, y, t) \left(\frac{1}{n}\right)^m$ when $N \rightarrow \infty$ it converges to the exact solution of standard reaction-diffusion Brusselator system. The values of \hbar is selected corresponding to arbitrary selected $n(n \geq 1)$, from \hbar -curve, we compare some values of \hbar and $n(n \geq 1)$ with exact and HAM solution, showing the validity of these parameters.

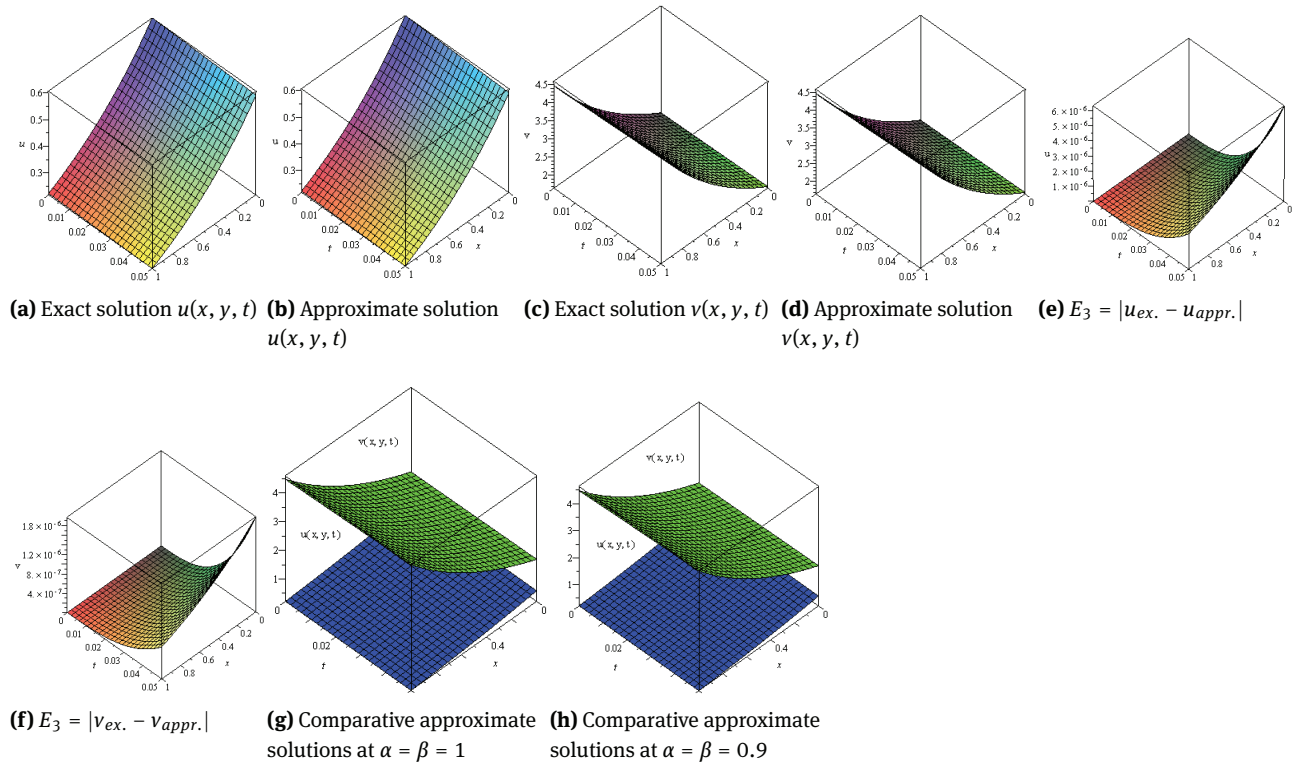


Fig. 1: Shape of 3rd order classical HAM (q-HATM, $n = 1$) approximate solutions $u(x, y, t)$ and $v(x, y, t)$ of system (25) at $y = 0.5$, $\hbar = -1$, $\alpha = \beta = 1$; v/s x and time t : 1(e)–1(f) show the efficiency of proposed method is noticed through the absolute error; 1(g)–1(h) comparisons are made, show the efficiency of fractional order shape solution.

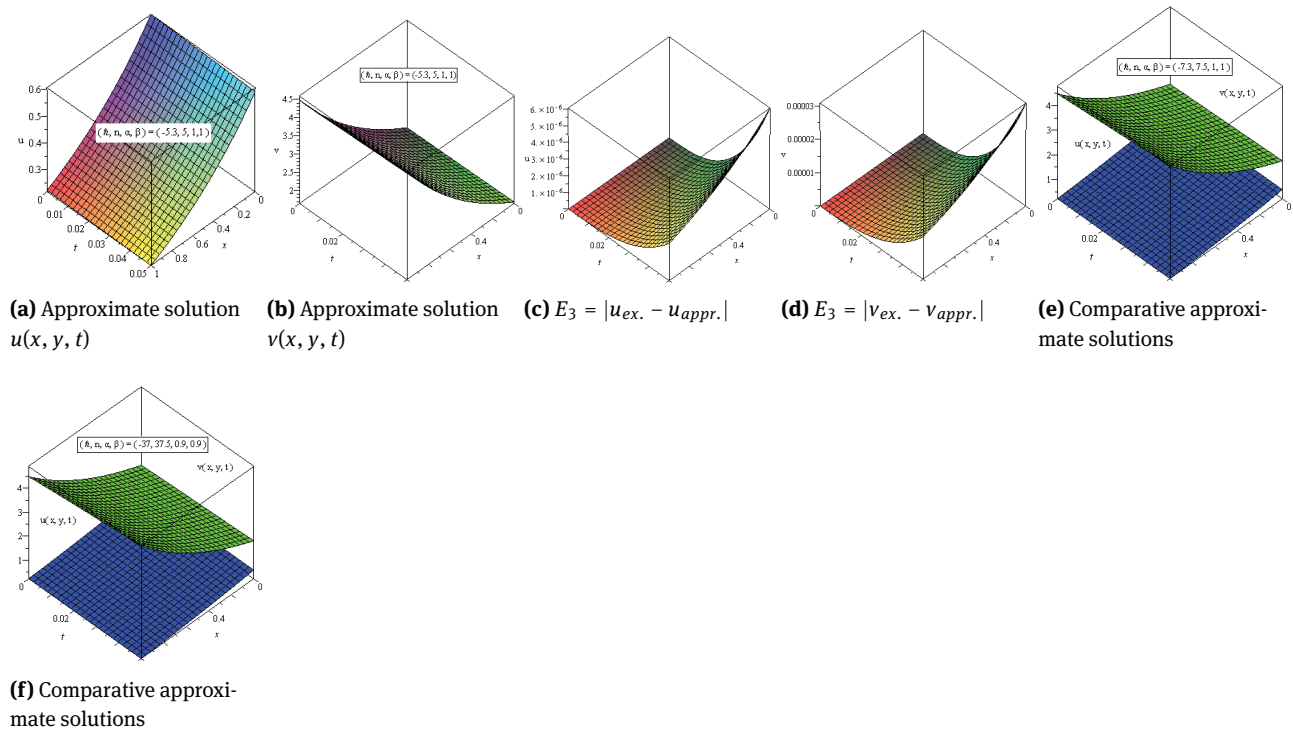


Fig. 2: Shape of family of 3rd order q -HATM approximate solutions $u(x, y, t)$ and $v(x, y, t)$ of system (25) with different values of $(\hbar, n, \alpha, \beta)$ at $y = 0.5$ v/s x and time t show the efficiency of auxiliary parameters \hbar and n ($n \geq 1$): 2(c)–2(d) represented the absolute error at $(\hbar, n, \alpha, \beta) = (-5.3, 5, 1, 1)$ with their exact solution; 2(e)–2(f) comparisons are made, show the efficiency of fractional order shape solution.

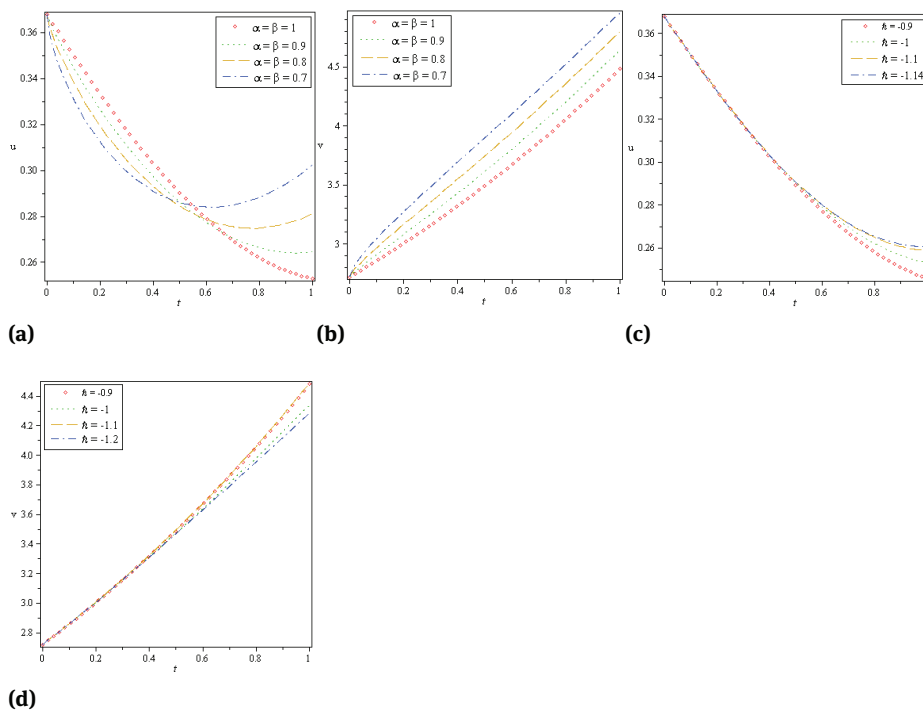


Fig. 3: Show the 3rd order HAM (q -HATM, $n = 1$) approximate solutions of system (25) at $x = y = 0.5$ versus time t 3(a)–3(b) comparative graphical representation between different values of α . It is clear to see that the solution of fractional order is not only a function of time but also continuous function for fractional order; 3(c)–3(d) existing the validity of absolute convergence range described in \hbar -curve.

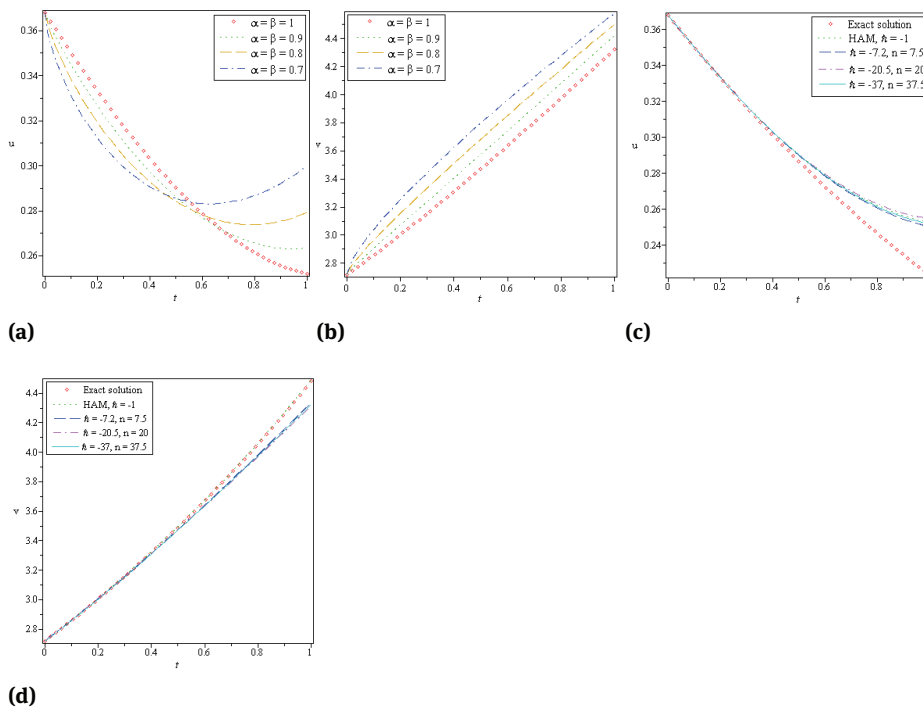


Fig. 4: Show the 3rd order q -HATM approximate solutions of system (25) at $x = y = 0.5$ versus time t : 4(a)–4(b) comparative graphical representation between different values of $\alpha = \beta$ at $(\hbar, n) = (-37, 37.5)$, existing the validity of fractional order with auxiliary parameters \hbar and fractional value of n ; 4(c)–4(d) existing the validity of family of proposed method solutions by using different values of \hbar and n at $\alpha = 1$.

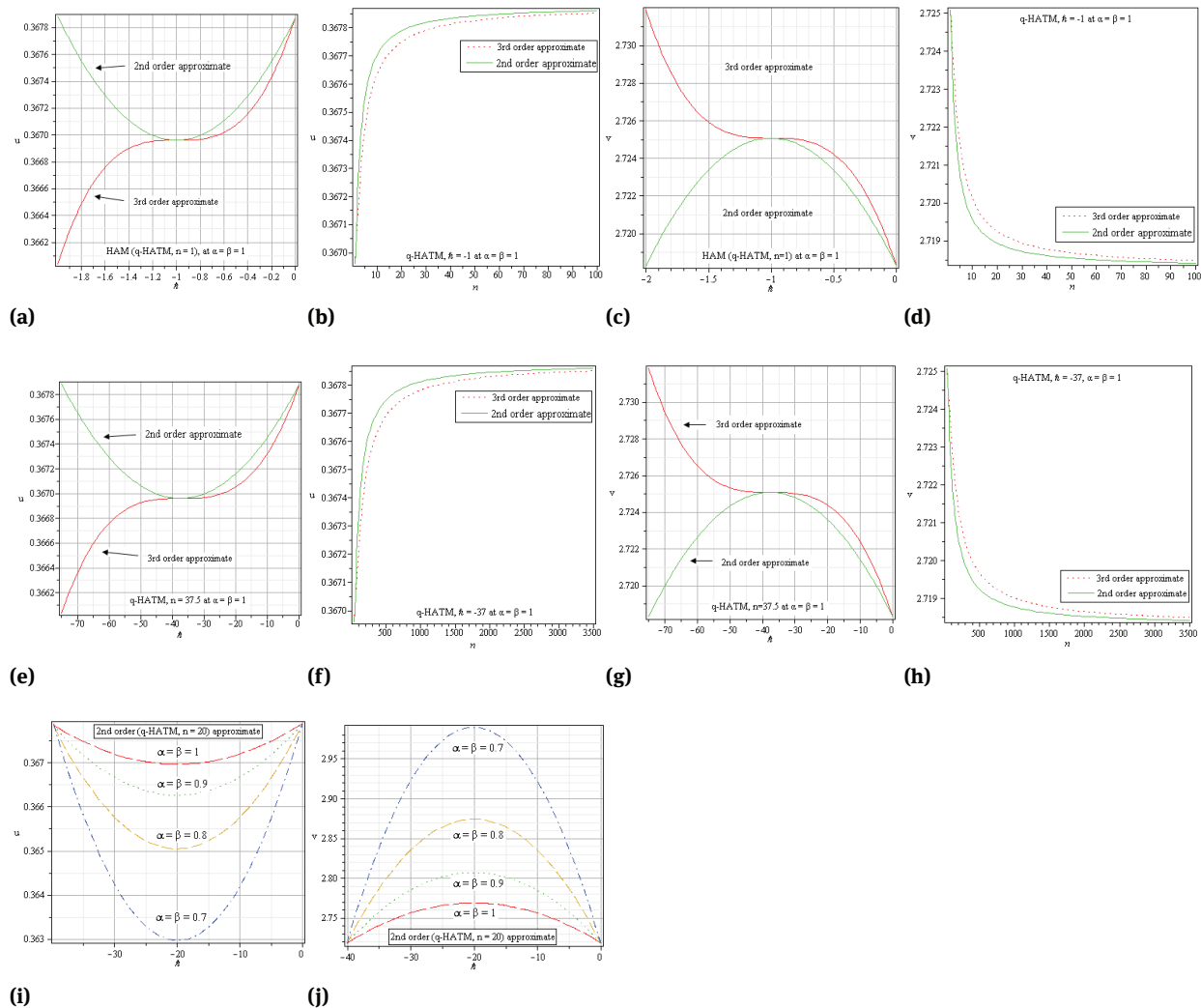


Fig. 5: 3rd and 2nd order \hbar and n -curves, \hbar -curve show the valid range of \hbar , 2nd order approximate decided the valid range of \hbar at $x = 0.5$, $t = 0.005$ for different n of $u(x, y, t)$ and $v(x, y, t)$ of system (25): for 5(a) $-1.999 \leq \hbar < 0$; 5(c) $-2.003 \leq \hbar < 0$; 5(e) $-75.01 \leq \hbar < 0$; 5(g) $-75.03 \leq \hbar < 0$; 5(i) $-39.65 \leq \hbar < 0$; 5(j) $-40.4 \leq \hbar < 0$ and the nearly horizontal line segments which guaranteed the convergence of related series; 5(i)–5(j) show the validity of Brownian motion i.e. $\alpha = 0.9, 0.8, 0.7$, \hbar -curves. It is depicted that all the \hbar -curves, seem to the same values of $u(x, y, t)$ and $v(x, y, t)$ for same order and different arbitrary selected n ($n \geq 1$), proved the validity of auxiliary parameters \hbar and n which provided the multiple approximate trustworthy solutions. The asymptotic n -curves, show the validity of valid range of \hbar , it seem to the same values of $u(x, y, t)$ and $v(x, y, t)$ correspondingly 2nd order approximate \hbar -curve. It is observed that the valid range of \hbar directly proportion to n ($n \geq 1$).

6 Conclusions

In this work, q -HATM is used to examine fractional dynamical Brusselator reaction-diffusion system with initial conditions. The main power of proposed algorithm is the \hbar and asymptotic n -curves, that provide the valid large convergence range. We can observed that the solution series $\sum_{m=0}^N u_m(x, y, t)(\frac{1}{n})^m$ and $\sum_{m=0}^N v_m(x, y, t)(\frac{1}{n})^m$ when $N \rightarrow \infty$, converge to the exact solution. Notably significant inves-

tigations of solutions of the Brusselator model have been done earlier with various schemes [16–25] which have their local point effects. The present article involves a more generalized effective approach, proposed for the Brusselator system say q -HATM, providing the family of series solutions with nonlocal generalized effects. The outcomes show that the proposed computational algorithm is very efficient and user friendly to handle nonlinear fractional differential equations.

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