THE REACTION DIMERIZATION A Resourceful Slant Applied on the Fractional Partial Differential Equation

by

Najeeb ALAM KHAN [a*], ***Tooba HAMEED*** [a], ***Muhammad AYAZ*** [a], ***and Oyoon ABDUL RAZZAQ*** [b]

[b] Department of Mathematics, University of Karachi, Karachi, Pakistan
[b] Department of Humanities and Social Sciences, Bahria University, Karachi, Pakistan

Original scientific paper
https://doi.org/10.2298/TSCI190702399A

The paper presents an analysis to investigate the time-fractional coupled diffusion equation with non-linear reaction subject to piecewise initial conditions. The governance system is determined analytically, and numerically adopting an artificial neural network taking the Caputo fractional derivative. In this scheme, the differential equations are transformed into an optimization problem, and minimize the problem by using sophisticated computer simulation Nelder-Mead algorithm. Finally, an experiment has been executed in the application of o-phenylenedioxy-dimethylsilane reaction dimerization which is a trial solution of resources as coefficients. The obtained solution is analyzed by tabulation of numerical values and plotting time based graphs. The novelty of the solution will be provided by comparison with the previous work in the literature as a special case. The numerical outcomes demonstrate the momentous features, efficiency and reliability of the approach.

Key words: *reaction dimerization, neural network, fractional calculus*

Introduction

The reaction-diffusion equations and systems are of rigorous significance due to its widespread applications and model formations in various fields [1-5]. In this attempt, we examine a reversible chemical reaction between two species P and Q in a bounded region $\Omega \subset R$, the system of PDE forms the reaction-diffusion system [6]. The resulting reaction-diffusion system:

$$\mathrm{D}_t^{\alpha} u - a\Delta^{\beta} u + \psi_1 k\left[r_A(u) - r_B(v)\right] = 0 \quad \text{in } \Omega(0,T), \text{ for } 0 < \alpha \le 1,\ 1 < \beta \le 2 \tag{1}$$

$$\mathrm{D}_t^{\alpha} v - b\Delta^{\beta} v - \psi_2 k\left[r_A(u) - r_B(v)\right] = 0 \quad \text{in } \Omega(0,T) \text{ for } 0 < \alpha \le 1,\ 1 < \beta \le 2 \tag{2}$$

where D_t^{α}, Δ^{β}, are the fractional operator, $T > 0$ and Ω is a bounded set of R. The piecewise conditions are defined:

$$u_j(x,0) = \begin{cases} 0 & l \le x < m \\ u_j(x) & m \le x < o \end{cases} \tag{3}$$

* Corresponding author, e-mail: njbalam@yahoo.com

$$v_j(x,0) = \begin{cases} v_j(x) & l \le x < p \\ 0 & p \le x < o \end{cases} \tag{4}$$

For a reversible reaction:

$$2P \underset{c_2}{\overset{c_1}{\Leftrightarrow}} Q$$

the rate functions are of the form $r_P(u) = c_1u_2$ and $r_Q(v) = c_2(v)$ where k is the chemical kinetics factor, c_1 and c_2 are rate constants, a and b – the diffusion coefficients, for details see [6, 7]. It has captivated researcher's devotion which results in the prevailing amount of efforts to analyze such reaction-diffusion models which have the dependency on time and space co-ordinates and to develop various techniques to obtain the solution dealing with diverse linear and non-linear reaction terms and conditions. Al-Sawoor and Al-Amr [7] introduced a modification in variational iteration method using adomian polynomials for solving fast reversible reaction–diffusion system which added the precision the method for larger domains, Zhang *et al.* [8] provided the solution for non-linear reaction-diffusion systems in pattern formation by employing the direct discontinuous Galerkin method, the local integral equation method has been presented by Sladek *et al.* [9] for pattern creation simulations in reaction-diffusion systems, a preconditioned multigrid numerical technique for a reaction-diffusion system has been utilized by Bhowmik [10], Arraras *et al.* [11] exploited domain decomposition multigrid methods for analyzing non-linear reaction-diffusion problems. Zhao and Ge [12] examined the reaction-diffusion equation with distributed delay through Lie group theory and provided invariant solutions by general symmetry group theory.

In the last few decades, the utilization of fractional order derivative has gained substantial importance in various fields as it leads to a significant transformation of the system [13-15]. Copious non-linear phenomena have been demonstrated in diffusion and reaction-diffusion equations by persuading the fractional order derivative. Gafiychuk and Datsko [16] has provided the mathematical modelling of various instabilities in time fractional reaction-diffusion systems, Hristov [17, 18] employed the heat-balance integral method to solve the Dirac-like evolution, diffusion equation for fractional (half time) derivative and time fractional radial equation with anomalous diffusion from a central point source in a sphere, Haubold *et al.* [19] deliberate reaction-diffusion equation by utilizing the Laplace and Fourier transforms to achieve the solution in terms of the *H*-function and considering different definitions for time and space-derivative, Khan *et al.* [20] closed analytical solutions of fractional reaction-diffusion equations, an innovative iterative method for time fractional non-linear reaction-diffusion equation has been proposed by Baranwal *et al.* [21], Yang, *et al.* [22] obtained the solution of wave and diffusion equations by local fractional series expansion method on cantor sets, domain decomposition method has been extended for time fractional reaction-diffusion equation by Gong *et al.* [23], the solution for 2-D space-fractional reaction-diffusion equations has been proposed by Yang *et al.* [22] through a finite volume scheme with the preconditioned Lanczos method, and Qureshi *et al.* [24] has been investigated the blood ethanol concentration model with fractional derivative using Laplace transform and Yusuf *et al.* [25] considered Rosenou-Haynam and mKdV equations with the aid of effective technique the fractional homotopy perturbation transform method.

The non-linear aligning from the inputs to the outputs of the interrelated system of neurons can be produced by the artificial neural network (ANN). In the literature, it has been found out that ANN with a functional layer employing arbitrary continuous functions is adept with any anticipated degree of correctness. The ANN has successfully enforced with different

optimization technique on function approximation, system identification, digital communication, *etc.* There are some heuristic algorithms which are not insured, but which is nevertheless advantageous in certain workable directions, to find the optimal solution by (finitely terminating) algorithms of optimization problem. Some well-known heuristic algorithms are the memetic algorithm, stochastic tunneling, differential evolution, artificial bee colony, reactive search optimization, *etc.* Few gradient free algorithms also exist, to minimize a scalar-valued non-linear function of finite real variables. Since in 1965, the most extensively applied method for non-linear unconstrained optimization the Nelder-Mead algorithm (NMA) [26] has developed. Generally, about the NMA is that it converges conclusively to its minimizer without any derivative information.

In the present paper, an o-phenylenedioxy-dimethylsilane has been taken as an application which is a fast reversible reaction-diffusion system of eqs. (1)-(2) with the piecewise initial conditions of eqs. (3)-(4). The system has been examined by the efficient and reliable technique ANN in which continuous map functions taken as multilayers, and the hidden layer is expanded in term of a linear sum with corresponding weights. The constructed trial solution satisfied system, and initial conditions, hence the residual error function composed by mean of average. The NMA is enforced for the optimal solution of this residual error function with the values of corresponding weights. These weights are plugin to the trial solution, and behavior of time and space derivative are tabulated and plotted. Comparison with the numerical solution for $\alpha = 1$ and $\beta = 2$ has also been done.

Preliminarie

The essential definition and properties of the fractional calculus theory which is implemented in this article are illustrated in this section.

Caputo and Riemann-Liouville operators

Assume $\nu > 0$, $m = \lceil \nu \rceil$, and $f(x, t) \in C_m([0.1] \times [0.1])$ then the partial Caputo fractional derivative of $f(x, t)$ with respect to t is defined in [27]:

$$\mathrm{D}_t^{\nu} f(x,t) = \begin{cases} I_t^{m-\nu} \dfrac{\partial^m}{\partial t^m} f(x,t), & m-1 < \nu \le m \\ \dfrac{\partial^m}{\partial t^m} f(x,t), & \nu = m \in N \end{cases} \tag{5}$$

where D_t^{ν} is the Caputo fractional derivative and I_t^{ν} – the Riemann-Liouville fractional integral:

$$I_t^{\nu} f(t) = \begin{cases} \dfrac{1}{\Gamma(\nu)} \int_0^t (t-\psi)^{\nu-1} \int_0^t f(\psi)\, d\psi, & \nu \in \Re \\ f(t), & \nu = 0 \end{cases} \tag{6}$$

The notation D_t^{ν} is used, for the Caputo fractional derivative $\partial^{\nu}/\partial t^{\nu}$.

Caputo derivatives of sine and cosine functions

Let $\alpha > 0$, $m = \lceil \alpha \rceil$, and $0 \in \Re$. For any $t \in \Re$ the fractional derivatives of $\sin(\theta t)$ and $\cos(\theta t)$ are define in [28]:

$$\mathrm{D}_t^{\alpha} \sin(\theta\, t) = \theta^{\alpha} \sin\left(\theta\, t + \alpha \frac{\pi}{2}\right) \tag{7}$$

$$\mathrm{D}_t^{\alpha}\cos(\theta\, t)=\theta^{\alpha}\cos\left(\theta\, t+\alpha\frac{\pi}{2}\right) \tag{8}$$

The previous representation of $\mathrm{D}_t^{\alpha}\sin(\theta t)$ and $\mathrm{D}_t^{\alpha}\cos(\theta t)$ are given in details [28].

Implementation of neural network

The scheme here is designed to accumulate the dynamical behavior of the reaction dimerization system which is depend on two parts. Firstly, the construction of unsupervised error (fitness) function for eqs. (1)-(4) while in the second phase, minimization of fitness function with the help of NMA is executed.

Approximation of fractional order reaction diffusion equation

An ANN based model of PDE is designed by approximating the solution in term of continuous mappings of suitable continues function. The network is constructed on $u(x, t)$ and $v(x, t)$ for 1-D system at the different number of neurons N. The output network of an input layer, with a single hidden layer defined:

$$\hat{u}(x,t;\,\mathrm{A})=\sum_{j=1}^{N}\eta_j f\left(w_{1j}x+w_{2j}t+\gamma_j\right) \tag{9}$$

$$\hat{v}(x,t;\,\mathrm{B})=\sum_{j=1}^{N}\lambda_j g\left(v_{1j}x+v_{2j}t+l_j\right) \tag{10}$$

where A and B are an unknown weight vectors define as A = [η, w, γ] and B = [λ, v, l] for approximate solution of $\hat{u}(x, t; \mathrm{A})$ and $\hat{v}(x, t; \mathrm{B})$. The vectors η, λ, w, v, γ, and l are specified in term of scaling parameters as $\eta = [\eta_1, \eta_2,...,\eta_N]$ and $\lambda = [\lambda_1, \lambda_2,...,\lambda_N]$, weighted input vectors $w = [w_1, w_2,..., w_{1N}, w_{21}, w_{22},...,w_{2N}]$, and $v = [v_{11}, v_{12},...,v_{1N}, v_{21}, v_{22},...,v_{2N}]$, and the bias vectors $\gamma = [\gamma_1, \gamma_2,..., \gamma_N]$ and $l = [l_1, l_2,..., l_N]$. Also f and g are defined as an activation function in which the argument (hidden layer) is the linear sum of the independent variables. The network has given in eqs. (9) and (10) is activated by using a suitable activation function. The α^{th}, and β^{th} order derivatives of $\hat{u}(x, t; \mathrm{A})$ and $\hat{v}(x, t; \mathrm{B})$ with respect to t and x:

$$\mathrm{D}_t^{\alpha}\hat{u}(x,t;\,\mathrm{A})=\sum_{j=1}^{N}\eta_j\mathrm{D}_t^{\alpha}f\left(w_{1j}x+w_{2j}t+\gamma_j\right) \tag{11}$$

$$\mathrm{D}_t^{\alpha}\hat{v}(x,t;\,\mathrm{B})=\sum_{j=1}^{N}\lambda_j\mathrm{D}_t^{\alpha}g\left(v_{1j}x+v_{2j}t+l_j\right) \tag{12}$$

$$\mathrm{D}_x^{\beta}\hat{u}(x,t;\,\mathrm{A})=\sum_{j=1}^{N}\eta_j\mathrm{D}_x^{\beta}f\left(w_{1j}x+w_{2j}t+\gamma_j\right) \tag{13}$$

$$\mathrm{D}_x^{\beta}\hat{v}(x,t;\,\mathrm{B})=\sum_{j=1}^{N}\lambda_j\mathrm{D}_x^{\beta}g\left(v_{1j}x+v_{2j}t+l_j\right) \tag{14}$$

The network of $\hat{u}(x, t; \mathrm{A})$ and $\hat{v}(x, t; \mathrm{B})$ have two important aspects: First, it must satisfy the piecewise conditions are defined in eqs. (3) and (4) second construction of error function of the network. In the problem eqs. (1)-(2) if the trial solutions $\hat{u}(x, t; \mathrm{A})$ and $\hat{v}(x, t; \mathrm{B})$ satisfies the conditions (3)-(4), then the minimization problem will be simplified:

$$E(\mathrm{A};\mathrm{B})=\min\left\{\frac{1}{n\times n}\sum_{i=1}^{n}\sum_{j=1}^{n}E_{DE}\left(x_j,t_i:\mathrm{A};\mathrm{B}\right)+\frac{1}{2n}\sum_{j=1}^{n}\left[E_1\left(x_j:\mathrm{A}\right)+E_2\left(x_j:\mathrm{B}\right)\right]\right\} \tag{15}$$

where $t_j = (t_1, t2,...,t_n)$, $x_i = (x_1, x_2,...,x_n)$ belong to $[t_0, T]$ and $[x_0, X]$, respectively. Also, the function $E_{DE}(x, t : \mathrm{A}; \mathrm{B})$ is constructed:

$$E_{DE}(x,t,\mathrm{A},\mathrm{B}) = \left(\mathrm{D}_t^{\alpha}\hat{u}(x,t;\ \mathrm{A}) - a\Delta^{\beta}\hat{u}(x,t;\ \mathrm{A}) + \gamma_1\left\{r_A\left[\hat{u}(x,t;\ \mathrm{A})\right] - r_B\left[\hat{v}(x,t;\ \mathrm{B})\right]\right\}\right)^2 +$$
$$+\left(\mathrm{D}_t^{\alpha}\hat{v}(x,t;\ \mathrm{B}) - b\Delta^{\beta}\hat{v}(x,t;\ \mathrm{B}) - \gamma_2\left\{r_A\left[\hat{u}(x,t;\ \mathrm{A})\right] - r_B\left[\hat{v}(x,t;\ \mathrm{B})\right]\right\}\right)^2 \tag{16}$$

and, $E_1(x; \mathrm{A})$, and $E_2(x; \mathrm{B})$ are expanded by using the initial and boundary conditions of eqs. (3)-(4):

$$E_1(x;\mathrm{A}) = \left[\hat{u}(x;\mathrm{A}) - u(x,0)\right]^2, \quad E_2(x;\mathrm{B}) = \left[\hat{v}(x;\mathrm{B}) - v(x,0)\right]^2 \tag{17}$$

Learning procedure NMA

As an alternative of solving the system (1)-(2), we solve the system (15). For the required minimum error problem, put on the function $E(\mathrm{A}; \mathrm{B})$ in NMA which is a popular approximate gradient free algorithm for the optimal solution. Suppose that P =[A; B], in which A and B are the optimal solution vector of the optimization problem (15). The procedural implementation of NMA can be follow:

Step 1: Construct an initial 24N simplex P, with 24N + 1 vertices and estimate the value of E(P) at the vertices.

Step 2: Rearrange the vertices in order that, $E(\mathrm{P}_1) \le E(\mathrm{P}_2) \le ... \le E(\mathrm{P}_{N+}1)$ at $\mathrm{P}_1, \mathrm{P}_2,...,\mathrm{P}_{N+1}$, respectively. Here, P_{N+1} is the worse value, and P_1 – the best value. Analogous position influences of E(P) are carried out, at each iteration.

Step 3: Calculate $\tilde{\mathrm{P}}$ (centroid), excluding P_{N+1}:

$$\mathrm{P} = \text{—}\sum \mathrm{P} \tag{18}$$

Step 4: Find the reflection of P_{N+1}:

$$\mathrm{P}_{\rho} = \tilde{\mathrm{P}} + \wp_1\left(\tilde{\mathrm{P}} - \mathrm{P}_{N+1}\right), \quad \wp_1 > 0 \tag{19}$$

though the typical value of $\wp_1 = 1$ is often used.

Step 5: update the new vertex P_{ρ}:

If $E(\mathrm{P}_1) \le E(\mathrm{P}_{\rho}) < E(\mathrm{P}_N)$ then, P_{N+1}.

If $E(\mathrm{P}_{\rho}) < E(\mathrm{P}_1)$ then seek a more bold move by expanding the vertex:

$$\mathrm{P}_{\varsigma} = \mathrm{P}_{\rho} + \wp_2\left(\mathrm{P}_{\rho} - \tilde{\mathrm{P}}\right) \ \text{ with } \wp_2 = 2$$
$$\text{If } E\left(\mathrm{P}_{\zeta}\right) < E\left(\mathrm{P}_{\rho}\right), \text{ then } \mathrm{P}_{\zeta} \to \mathrm{P}_{N+1} \text{ else } \mathrm{P}_{N+1} \to \mathrm{P}_{\rho} \tag{20}$$

If $E(\mathrm{P}_N) < E(\mathrm{P}_{\rho})$, then by contraction:

$$\mathrm{P}_{\sigma} = \mathrm{P}_{N+1} + \wp_3\left(\tilde{\mathrm{P}} - \mathrm{P}_{N+1}\right) \ \text{ with } \ \wp_3 = \frac{1}{2}$$
$$\text{If } E\left(\mathrm{P}_{\sigma}\right) < E\left(\mathrm{P}_{N+1}\right), \text{ then, update } \mathrm{P}_{N+1} \to \mathrm{P}_{\sigma} \tag{21}$$

If all the previous steps fail, then:

$$\mathrm{P}_i = \mathrm{P}_1 + \wp_4(\mathrm{P}_i - \mathrm{P}_1), \quad \text{for } \ i = 2,3,...,N+1 \tag{22}$$

Then, go to the *Step 1*, and start over again until the optimal solution is achieve. Finally, replacing it into eqs. (9) and (10), for the approximate numerical solution of eqs. (1) and (2).

Numerical simulation and result discussion

A reversible chemical reaction of o-phenylenedioxy-dimethylsilan [15] between two species P and Q in a bounded region $\Omega \subset R$ have been considered, the system of PDE forms the reaction diffusion system [16]. Here, the reaction is of the type:

$$2P \underset{c_2}{\overset{c_1}{\Leftrightarrow}} Q$$

hence the reaction terms take the form $r_P(u) = c_1u^2$, $r_Q(v) = c_2v$, $\psi_1 = 2$, and $\psi_2 = 1$. The resulting reaction-diffusion system depends on x-co-ordinate of spatial co-ordinates and time:

$$\mathrm{D}_t^{\alpha} u(x,t) = a\ \Delta_x^{\beta} u(x,t) - 2k\left[c_1 u^2(x,t) - c_2 v(x,t)\right], \quad \text{in} \quad [0,0.1]\times(0,T) \tag{23}$$

$$\mathrm{D}_t^{\alpha} v(x,t) = a\ \Delta_x^{\beta} v(x,t) + k\left[c_1 u^2(x,t) - c_2 v(x,t)\right], \quad \text{in} \quad [0,0.1]\times(0,T) \tag{24}$$

And the piecewise initial conditions:

$$u(x,0) = \begin{cases} 0 & x \in [0,0.03] \\ \dfrac{1}{2}\sin\left(\dfrac{50\pi}{7}(x-0.03)\right) & x \in [0.03,0.07] \\ \dfrac{1}{2}\sin\left(\dfrac{50\pi}{7}(x-0.03)\right) & x \in [0.07,0.1] \end{cases} \tag{25}$$

$$v(x,0) = \begin{cases} \dfrac{1}{4}\cos\left(\dfrac{50\pi}{7}x\right) & x \in [0,0.03] \\ \dfrac{1}{4}\cos\left(\dfrac{50\pi}{7}x\right) & x \in [0.03,0.07] \\ 0 & x \in [0.07,0.1] \end{cases} \tag{26}$$

To illustrate the methodology of the ANN technique by a suitable number of neurons ($N = 1$), consider a numerical example of a system of eqs. (23) and (24), to activate the designednetwork here we take $f(\bullet) = \sin(\bullet)$ and $g(\bullet) = \cos(\bullet)$ as an activation function. The trial solution of eqs. (9) and (10) is constructed:

$$\hat{u}(x,t;\mathrm{A}) = \begin{cases} \displaystyle\sum_{j=1}^{N} \eta_{1j} \sin\left(w_{1,1j}x + w_{2,1j}t + \gamma_{1j}\right) & x \in [0,0.03] \\ \displaystyle\sum_{j=1}^{N} \eta_{2j} \sin\left(w_{1,2j}x + w_{2,2j}t + \gamma_{1j}\right) & x \in [0.03,0.07] \\ \displaystyle\sum_{j=1}^{N} \eta_{3j} \sin\left(w_{1,3j}x + w_{2,3j}t + \gamma_{1j}\right) & x \in [0.07,0.1] \end{cases} \tag{27}$$

$$\hat{v}(x,t;\ \mathrm{B}) = \begin{cases} \sum_{j=1}^{N} \lambda_{1j}\, g\left(v_{1,1j}x + v_{2,1j}t + l_{1j}\right) & x \in [0, 0.03] \\ \sum_{j=1}^{N} \lambda_{2j}\, g\left(v_{1,2j}x + v_{2,2j}t + l_{2j}\right) & x \in [0.03, 0.07] \\ \sum_{j=1}^{N} \lambda_{3j}\, g\left(v_{1,3j}x + v_{2,3j}t + l_{3j}\right) & x \in [0.07, 0.1] \end{cases} \tag{28}$$

As per the procedure given in the last section, however, the fitness function $E(x, t, \mathrm{A}, \mathrm{B})$ developed for this problem constructed using eq. (15):

$$E(\mathrm{A},\mathrm{B}) = \begin{cases} E_{11}(\mathrm{A},\mathrm{B}) & x \in [0, 0.03] \\ E_{22}(\mathrm{A},\mathrm{B}) & x \in [0.03, 0.07] \\ E_{33}(\mathrm{A},\mathrm{B}) & x \in [0.07, 0.1] \end{cases} \tag{29}$$

On discretizing $t \in [0, 1]$ and x is in respective intervals for n equal segments, the fitness function of (29) takes the following form:

$$E(\mathrm{A},\mathrm{B}) = \min \frac{1}{3\times n\times n} \sum_{i=1}^{n}\sum_{j=1}^{n} E_{DE,1}\left(x_j, t_i, \mathrm{A}, \mathrm{B}\right) + E_{DE,2}\left(x_j, t_i, \mathrm{A}, \mathrm{B}\right) + E_{DE,3}\left(x_j, t_i, \mathrm{A}, \mathrm{B}\right) +$$
$$+ \frac{1}{6\times n} \sum_{j=1}^{n} \left[E_{11}\left(x_j, \mathrm{A}\right) + E_{12}\left(x_j, \mathrm{B}\right) + E_{13}\left(x_j, \mathrm{A}\right) + E_{21}\left(x_j, \mathrm{B}\right) + E_{22}\left(x_j, \mathrm{A}\right) + E_{23}\left(x_j, \mathrm{B}\right) \right] \tag{30}$$

The values of the rate constants, diffusion coefficients and chemical kinetic factor are considered as $c_1 \approx 1.072\mathrm{e}^{-4}$ L^2/mol^2, $c_2 \approx 2.363\mathrm{e}^{-6}$ L^2/mol^2, $a \approx 1.579\mathrm{e}^{-9}$ m^2/s^2, $b \approx 1.042\mathrm{e}^{-9}$ m^2/s^2, and $k = 1$. The learning (optimization) of weights for eq. (30) has been made with NMA using computational software MATHEMATICA 10. The optimized values of neurons (weight) of the network are plotted in figs. 1(a)-1(d) that are used in eq. (30), to evaluate the values of $E(\mathrm{A}, \mathrm{B})$, which are around 10^{-15} to 10^{-11} and tabulated in tab. 1. The smaller the value of the fitness function, the better is the performance of the algorithm. The 3-D view of function $E(x, T)$ can be seen in fig. 2. To obtain the derived solution of eqs. (23) and (24) set of optimum weights is utilizing in eqs. (27) and (28):

$$\hat{u}(x,t) = \begin{cases} 1.51224\times 10^{-6} \sin\left(0.03956x + 0.81391t + 0.008057\right) & x \in [0, 0.03] \\ 0.49999 \sin\left(-22.44000x + 0.00002t + 3.81479\right) & x \in [0.03, 0.07] \\ 0.500017 \sin\left(-22.42860x + 0.00020t + 3.81398\right) & x \in [0.07, 0.1] \end{cases} \tag{31}$$

$$\hat{v}(x,t) = \begin{cases} 0.24994 \cos\left(-22.5038x + -4.72332\times 10^{-6} t + 0.00190\right) & x \in [0, 0.03] \\ -0.25013 \cos\left(22.42380x - 0.00002t + 3.14269\right) & x \in [0.03, 0.07] \\ -2.22096\times 10^{-7} \cos\left(1.13908x + 0.475521t + 0.34305\right) & x \in [0.07, 0.1] \end{cases} \tag{32}$$

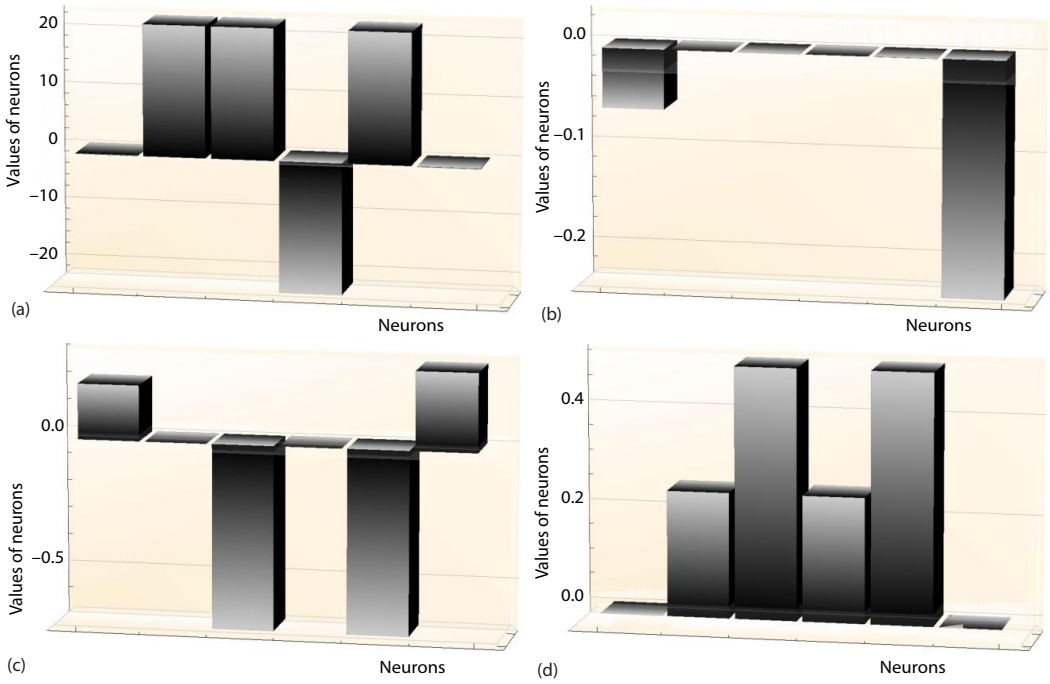

Figure 1. (a)-(d) Set of weights vectors, at $\alpha = 1$ and $\beta = 2$; (a) η and λ, (b) w_1 and w_2, (c) v_1 and v_2, and (d) k and l

The numerical solution presented in eqs. (31) and (32) is plotted in figs. 3(a) and 3(b). Comparison among ANN and HAM [15] results for $\alpha = 1.0$ and $\beta = 2.0$ has been shown in tab. 2. To prove the existence of the solution of the system (1) and (2), the topological degree theory in finite dimensional spaces was used in [6] and define the expression:

$$\hat{w}(x,t) = \frac{1}{\psi_2}\hat{u}(x,t) + \frac{1}{\psi_1}\hat{v}(x,t) \tag{33}$$

In fig. 3(c) the function $w(x, t)$ is plotted with the help of eqs. (31) and (32).

Table 1. Minimum values of the fitness function E(A, B) at $\alpha = 1.0$ and $\beta = 2.0$

$k = 1$	Best	$4.65820 \cdot 10^{-11}$
	Worst	$1.77108 \cdot 10^{22}$
$k = 10$	Best	$3.80618 \cdot 10^{-9}$
	Worst	$5.50484 \cdot 10^{26}$
$k = 50$	Best	$9.32117 \cdot 10^{-9}$
	Worst	$2.13262 \cdot 10^{31}$
$k = 100$	Best	$2.29713 \cdot 10^{-7}$
	Worst	$1.38578 \cdot 10^{18}$
$k = 1000$	Best	$1.14943 \cdot 10^{-5}$
	Worst	$2.37731 \cdot 10^{24}$

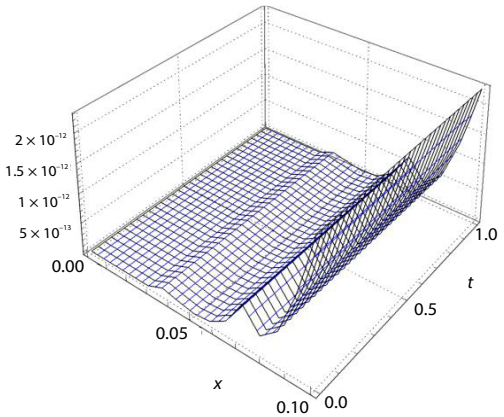

Figure 2. The fitness function $E(x, t)$, at $\alpha = 1$ and $\beta = 2$

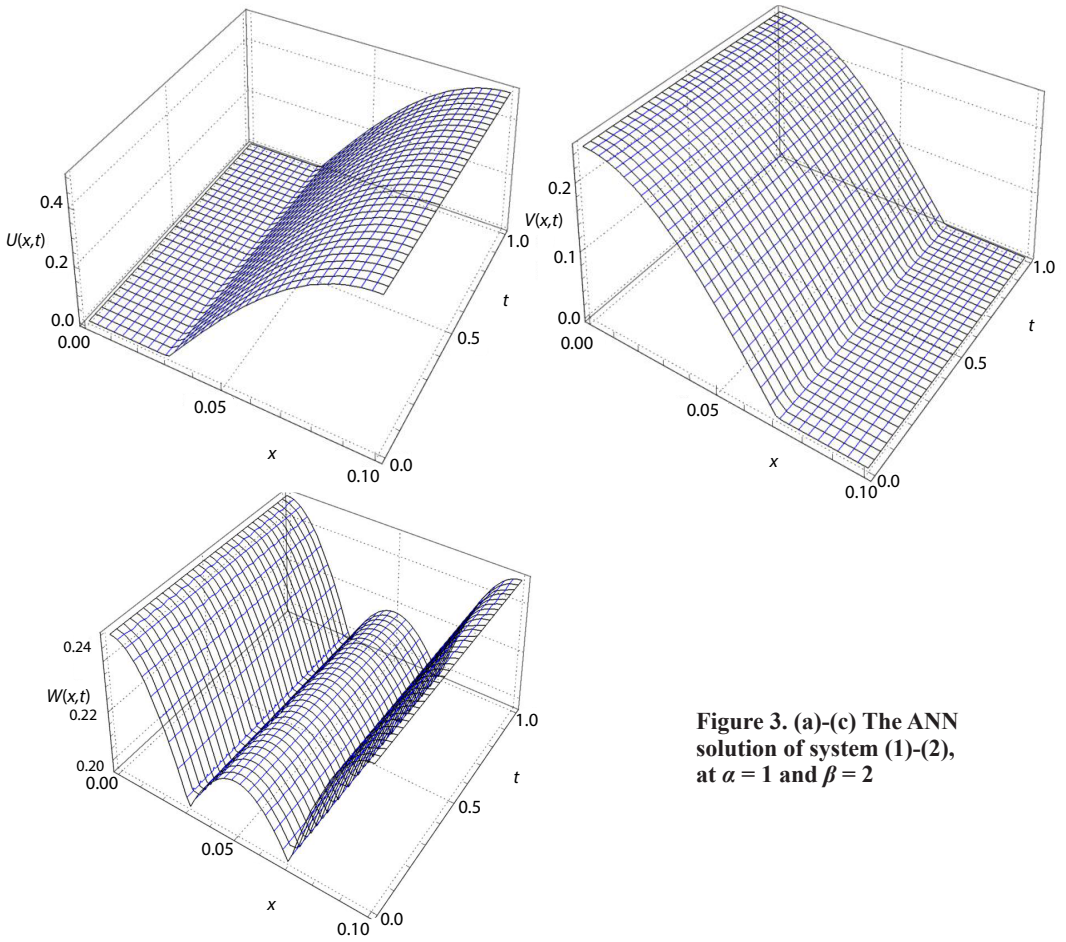

Figure 3. (a)-(c) The ANN solution of system (1)-(2), at $\alpha = 1$ and $\beta = 2$

Table 2. Comparison of ANN with HAM [15], VIM [7] (as a special case of $\alpha = 1.0$ and $\beta = 2.0$) at $t = 1$

x	$u(x, t)$			$v(x, t)$		
	ANN	*HAM*	*VIM*	*ANN*	*HAM*	*VIM*
0.00	$1.181497 \cdot 10^{-6}$	$1.181497 \cdot 10^{-6}$	$1.181497 \cdot 10^{-6}$	0.249999	0.249999	0.249999
0.02	$1.064492 \cdot 10^{-6}$	$1.064492 \cdot 10^{-6}$	$1.064492 \cdot 10^{-6}$	0.225241	0.225241	0.225241
0.04	0.111248	0.111258	0.111258	0.155877	0.155873	0.155873
0.06	0.311734	0.311724	0.311724	0.055637	0.055640	0.055640
0.08	0.450439	0.450440	0.450440	$1.684136 \cdot 10^{-5}$	$2.175344 \cdot 10^{-5}$	$2.175261 \cdot 10^{-5}$
0.10	0.499999	0.499945	0.499946	$1.684331 \cdot 10^{-5}$	$2.679816 \cdot 10^{-5}$	$2.679706 \cdot 10^{-5}$

Conclusions

A novel approach for the time fractional fast reaction diffusion system with piecewise initial conditions has been obtained through the reliable analytical approximation scheme. The values of the rate constants, diffusion coefficients and chemical kinetic factor are considered in

numerical values. It will let us solve the fractional order partial differential equation for those sets when the exact solution are difficult to obtained. The main features, findings and future research of the present study are summarized:

- It is possible to use other novel function as an activation function, say tangent hyperbolic, Mexican hat wavelet, Chebyshev polynomials, Legendre polynomials, and, *etc.*
- Graphical results of fig. 3(a)-3(c), capture the essential behavior of the diffusion system at $\alpha = 1.0$ and $\beta = 2.0$.
- The obtained approximate solution is continuous and differentiable in closed analytical form so that the value of the solution can be obtained at any arbitrary point.
- The precision of the scheme can be grown up by increasing the number of perceptron or using any optimization method such as heuristic algorithms.

Nomenclature

A, B – optimal weights vectors
a, b – diffusion coefficients, [m^2s^{-1}]
c_i – rate constants, [L^2mol^{-2}]
E(A, B) – residual error function
f, g – activation function
k – chemical kinetics factor
l, m, o – real numbers
P, Q – reaction species

Greek symbols

λ_i, η_i, w_i, v_i, γ_i, l_i – weights of ANN

References

[1] Zhang, L., Spatiotemporal Patterns in a Ratio-Dependent Food Chain Model with Reaction-Diffusion, *Abstract and Applied Analysis*, *2014* (2014), ID 130851
[2] Alford, J. G., A Reaction-Diffusion Model of the Darien Gap Sterile Insect Release Method, *Communications in Non-Linear Science and Numerical Simulation*, *22* (2015), 1, pp. 175-185
[3] Bani-Yaghoub, M., *et al*., Understanding the Interplay between Density Dependent Birth Function and Maturation Time Delay Using a Reaction-Diffusion Population Model, *Ecological Complexity*, *21* (2015), Mar., pp. 14-26
[4] Guin, L. N., Spatial Patterns through Turing Instability in a Reaction-Diffusion Predator-Prey Model, *Mathematics and Computers in Simulation, 109* (2015), Mar., pp. 174-185
[5] Xiao, Y., Sun, C., Higher-Order Asymptotic Attraction of Pullback Attractors for a Reaction-Diffusion Equation in Non-Cylindrical Domains, Non-Linear Analysis: *Theory, Methods and Applications*, *113* (2015), Jan., pp. 309-322
[6] Eymard, R., *et al*., Numerical Approximation of a Reaction-Diffusion System with Fast Reversible Reaction, *Chinese Annals of Mathematics Series B*, *31* (2010), 5, pp. 631-654
[7] Al-Sawoor, A. J., Al-Amr, M. O., A New Modification of Variational Iteration Method for Solving Reaction-Diffusion System with Fast Reversible Reaction, *Journal of the Egyptian Mathematical Society*, *22* (2014), 3, pp. 396-401
[8] Zhang, R., *et al.*, Direct Discontinuous Galerkin Method for Non-Linear Reaction-Diffusion Systems in Pattern Formation, *Applied Mathematical Modelling*, *38* (2014), 5 pp. 1612-1621
[9] Sladek, V., *et al*., Shirzadi, A., The Local Integral Equation Method for Pattern Formation Simulations in Reaction-Diffusion Systems, *Engineering Analysis with Boundary Elements*, *50* (2015), Jan., pp. 329-340
[10] Bhowmik, S. K., A Multigrid Preconditioned Numerical Scheme for a Reaction-Diffusion System, *Applied Mathematics and Computation*, *254* (2015), Mar., pp. 266-276
[11] Arrarás, A., *et al*., Domain Decomposition Multigrid Methods for Non-Linear Reaction-Diffusion Problems, *Communications in Non-linear Science and Numerical Simulation*, *20* (2015), 3, pp. 699-710
[12] Zhao, Z., Ge, W., Symmetry Analysis of Reaction Diffusion Equation with Distributed Delay, *Communications in Non-linear Science and Numerical Simulation, 24* (2015), 1, pp. 11-20
[13] Qureshi, S., Yusuf, A., Mathematical Modelling for the Impacts of Deforestation on Wildlife Species Using Caputo Differential Operator Chaos, *Solitons and Fractals*, *126* (2019), Sept., pp. 32-40
[14] Khan, N. A., Hameed, T., An Implementation of Haar Wavelet Based Method for Numerical Treatment of Time-Fractional Schrodinger and Coupled Schrodinger Systems, *IEEE/CAA Journal of Automatica Sinica*, *6* (2019), 1, pp. 177-187

[15] Khan, N. A., *et al.*, Approximate Solutions to Time-Fractional Schrödinger Equation Via Homotopy Analysis Method, *ISRN Mathematical Physics*, *2012* (2012), ID 197068
[16] Gafiychuk, V., Datsko, B., Mathematical Modelling of Different Types of Instabilities in Time Fractional Reaction-Diffusion Systems, *Computers and Mathematics with Applications*, *59* (2010), 3, pp. 1101-1107
[17] Hristov, J., Heat-Balance Integral to Fractional (Half-Time) Heat Diffusion Sub-Model, *Thermal Science, 14* (2010) 2, pp. 291-316
[18] Hristov, J. Y., Starting Radial Subdiffusion from a Central Point through a Diverging Medium (a Sphere): Heat-Balance Integral Method, *Thermal Science*, *15* (2011) Suppl. 1, pp. S5-S20
[19] Haubold, H. J., *et al*., Further Solutions of Fractional Reaction-Diffusion Equations in Terms of the H-Function, *Journal of Computational and Applied Mathematics*, *235* (2011), 5, pp. 1311-1316
[20] Khan, N. A., *et al.*, A Heuristic Optimization Method of Fractional Convection Reaction: An Application Diffusion Process, *Thermal Science*, *22* (2018), Suppl. 1, pp. S243-S252
[21] Baranwal, V. K., *et al*., An Analytic Algorithm for Time Fractional Non-Linear Reaction-Diffusion Equation Based on a New Iterative Method, *Communications in Non-linear Science and Numerical Simulation*, *17* (2012) 10, pp. 3906-3921
[22] Yang, A.-M., *et al*., Local Fractional Series Expansion Method for Solving Wave and Diffusion Equations on Cantor Sets, *Abstract and Applied Analysis*, *2013* (2013), ID 351057
[23] Gong, C., *et al*., A Domain Decomposition Method for Time Fractional Reaction-Diffusion Equation, *The Scientific World Journal*, *2014* (2014), ID 681707
[24] Qureshi, S., *et al*., Fractional Modelling of Blood Ethanol Concentration System with Real Data Application, *Chaos, An Interdisciplinary Journal of Non-linear Science*, *29* (2019), 1, 013143
[25] Yusuf, A., *et al*., Efficiency of the New Fractional Derivative with Non-Singular Mittag-Leffler Kernel to Some Non-Linear Partial Differential Equations, *Chaos, Solitons and Fractals*, *116* (2018), Nov., pp. 220-226
[26] Nelder, J. A., Mead, r., A Simplex Method for Function Minimization, *The Computer Journal*, *7* (1965), 4, pp. 308-313
[27] Podlubny, I., *Fractional Differential Equations,* Elsevier, Irvine, Cal., USA, 1998
[28] Garrappa, R*., et al.*, Evaluation of Fractional Integrals and Derivatives of Elementary Functions: *Overview and Tutorial, Mathematics*, *7* (2019), 5, 407

Paper submitted: July 2, 2019
Paper revised: October 04, 2019
Paper accepted: October 11, 2019