CFD Letters

Journal homepage:
https://semarakilmu.com.my/journals/index.php/CFD_Letters/index
ISSN: 2180-1363

Semi-analytical Expressions of a Non-linear Reaction-Diffusion (R-D) Equations in a Mixed Quadratic-Cubic Autocatalytic Reactions

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ARTICLE INFO

Article history:
Received 3 May 2023
Received in revised form 8 June 2023
Accepted 9 July 2023
Available online 11 November 2023

Keywords:
Reaction–Diffusion(R-D) equations; Autocatalytic reactions; Non-linear boundary value problem; Homotopy analysis method; Numerical simulation

ABSTRACT

The semi-analytical expressions for the autocatalytic reactions with the mixed cubic and quadratic terms are derived. The kinetic model is associated with the diffusion, which is considered in a one-dimensional reactor. The semi-analytical solutions are derived for the concentrations of dimensionless reactant and dimensionless autocatalyst in the cubic autocatalytic reaction-diffusion equations for the steady-state and non-steady state by using the Homotopy analysis method (HAM). The derived approximate analytical solutions are compared with the numerical simulation and found to be very good fit for all values of the dimensionless parameters.

1. Introduction

Chemical reactions representing multiple steady-state solutions and oscillatory solutions have been of great enthusiasm to theorists and experimenters for over one hundred years. Some experimental models of oscillatory performance in chemical systems consisting of the Bray–Liebhafsky, Belousov–Zhabotinskyand Briggs–Rausher reactions, where periodic changes in concentration can be visualized as colour changes; Also, Corbel *et al.,* [1] reviewed these reactions and remaining oscillatory phenomena. The almost common reactor scenario in the literature, for chemical systems research is the continuous flow well-stirred tank reactor (CSTR). Typically, CSTRs are driven by system of Ordinary Differential Equations (ODE's) that can be analysed using standard methods. However, the reaction–diffusion cell is also an important reactor scenario, defined as a system of Partial Differential Equations (PDE's), and not easily analysed.

The theoretical model with both cubic and quadratic autocatalysis having linear decay of the catalyst is treated,

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https://doi.org/10.37934/cfdl.15.11.131150

$$\left.\begin{array}{l} A+2B\rightarrow 3B, \quad rate=(1-p)\beta a b^{2}, \\ A+B\rightarrow 2B, \quad rate=p\beta a b, \\ B\rightarrow C, \quad rate=\beta \gamma b, \end{array}\right\} \tag{1}$$

where a and b are the concentrations of the reactant and autocatalyst respectively. In Eq. (1), the first one is the reaction of cubic followed by the second is the reaction of quadratic and third is the linear catalyst of decay. The reaction ratio $p\in[0,1]$, calculate the stability for the reaction of the quadratic correlate with cubic reaction, where $p=0$ denotes cubic Gray–Scott model, also $p=1$ indicates the quadratic limit. The combined quadratic-cubic system is taken because, its dynamic stability and static shows a vast type of complex structures and phenomena which are much prosperous than the cubic and quadratic schemes alone.

The combined cubic-quadratic autocatalytic system in Eq. (1) is a system of the prototype, but Horváth *et al.,* [2] reports that the acid reaction namely the iodate–arsenous is one of the examples of combined cubic-quadratic autocatalytic system where the reaction of cubic influences the quadratic limit. This system has been broadly studied due to the presence of propagating wave fronts as the autocatalytically developed iodate spreads into regions with fresh reactant (arsenous acid). Horváth *et al.,* [2] found that instabilities developed when the ratio of reactant to autocatalyst diffusivities exceeds a critical value and found a good comparison between numerical solutions and experimental results. Merkin and Ševčíková [3] simulated the acid reaction namely iodate–arsenous by using the Dushman–Roebuck kinetic scheme and found suitable conditions to model it according to the cubic autocatalytic rate law. The form of travelling wave solution was shown to depend on the initial concentration ratio of reactant to autocatalyst.

Gray and Scott [4,5] studied cubic autocatalytic (Eq. (1) when $p=0$) in a CSTR. Three of steady-state bifurcation diagrams occurred, the unique, mushroom and isola patterns, and they also identified the Hopf bifurcation parameter region. Numerical simulations of the ODE model had shown the evolution of the system to both stable and unstable limit-cycles and also the oscillatory decay to a stable steady state. Kay *et al.,* [6] added an uncatalysed conversion step to the Eq. (1) which increased the number of bifurcation diagrams to five. The two new divergent patterns were the disruptive wave and isola disruptive wave patterns, both of which occurred in very small regions of the parameter space.

Scott [7] and Kay and Scott [8] studied the autocatalytic cubic system of reaction–diffusion cell represented in Eq. (1). The Partial Differential Equation model can be solved numerically by discretization, which permitted bifurcation diagrams of four steady-state to be identified. The disruptive-wave isola patterns cannot be found numerically, because the range of their parameters is too small. Furthermore, they treated the stability of the solution by calculating the eigenvalues for the discretized ODE form of the controlling PDE's.

Marchant [9] found a semi-analytical expression to the Gray and Scott model in a reaction–diffusion cell. The semi-analytical solutions established to be very accurate and this method proved an adequate substitute for the direct PDE discretization used by Scott [7]. Marchant [10] studied autocatalyst cubic in a One-Dimensional (1-D) reactor by replacing the linear decay for Gray and Scott model with the decomposition of the Michaelis–Menten catalyst decay being limited at high catalyst concentrations. The effect of changing Michaelis constant on the structure of parameter maps explaining the Hopf bifurcations and bifurcation patterns was reported. Thornton and Marchant [11] studied the effect of applying an electric field in the Gray and Scott model having reaction– diffusion–advection cell. The electric field, modelled as advection elements in the governing equations causes the migration of ions in the cell which alters the static and dynamic stability of the system. It used as a possible feedback mechanism. Also, it has been found that it can act as a switch between high-low conversion states and change the parameter map in which the Hopf bifurcation occurs. Wang *et al.,* [12] solved 2D and 3D convection–diffusion–reaction equations by using novel local knot method (LKM). Also, diffusion and convection-diffusion problem were solved by using localized space-time method of fundamental solutions (LSTMFS) proposed by Wang *et al.,* [13].

In this article, we investigate the considered mixed quadratic-cubic autocatalytic scheme defined in Eq. (1) on a One-Dimensional Reaction-Diffusion cell (1-D R-Dcell). Approximate analytical expressions are found by using the Homotopy analysis technique. A comparison is put together between the numerical simulation and approximate analytical expression of the governing PDE's determination and shows the accuracy of the semi-analytical expression.

The main aim of this study is to produce an approximate analytical solution for thenon-linear Reaction-Diffusion equations in a mixed quadratic-cubic autocatalytic reactions for both steady and non-steady state via HAM. The obtained approximate analytical solution and numerical simulation are compared and displayed graphically. Also, the effects of several parameters are depicted.

2. Mathematical Formulation of the Problem

The governing PDE's of a mixed quadratic-cubic autocatalytic reaction using the linear decay Eq. (1) in a One-Dimensional Reaction-Diffusion (1-D R–D) cell reported by Alharthi *et al.,* [14] are:

$$a_t = \delta a_{xx} - p\beta ab - (1-p)\beta ab^2 \tag{2}$$

$$b_t = b_{xx} + p\beta ab + (1-p)\beta ab^2 - \beta\gamma b \tag{3}$$

The respective boundary conditions of the Eq. (2) and Eq. (3) are given by

$$a_x = b_x = 0 \text{ at } x = 0 \tag{4}$$

$$a = 1, b = b_0 = k(say) \text{ at } x = 1 \text{ and } t = 0 \tag{5}$$

where the reactant and autocatalyst concentrations are given by a and b, respectively. The reactor boundary at $x=1$ is permeable and connected with constant concentrations of reactant and autocatalyst. At $x=0$ there is a zero-flow boundary condition. Alternatively, an identical reservoir could be located at $x=-1$; the solution is then symmetric about the centre of the cell $x=0$. The system has a dimensionless form and six parameters; b_0 is the autocatalyst reservoir concentration, $\beta(1-p)$ is the rate of cubic reaction, βp the rate of quadratic reaction, γ the rate of autocatalyst decay while δ is the diffusion coefficient for the reactant. The reaction ratio $p \in [0,1]$ measures the relative rates of quadratic and cubic reactions. Choosing $p=1$ will gives a purely quadratic system while $p=0$ gives the Gray and Scott cubic scheme. The parameters can be empirically tuned by changing the reservoir concentrations. Other options for changing the parameters are discussed by Scott [7], for example the diffusivity could be adjusted by adding inactive salts to the cell.

The non-linear differential Eq. (2) and Eq. (3) under non-steady state conditions are given by

$$\frac{\partial a}{\partial t}=\delta\frac{\partial^2 a}{\partial x^2}-p\beta ab-(1-p)\beta ab^2 \tag{6}$$

$$\frac{\partial b}{\partial t}=\frac{\partial^2 b}{\partial x^2}+p\beta ab+(1-p)\beta ab^2-\beta\gamma b \tag{7}$$

The corresponding initial and boundary conditions of the Eq. (6) and Eq. (7) are

At $t=0$, $a=1, b=b_0=k\,(say)$ (8)

At $x=0$, $\frac{\partial a}{\partial x}=\frac{\partial b}{\partial x}=0$ (9)

At $x=1$, $a=1, b=b_0=k(say)$ (10)

The non-linear differential Eq. (2) and Eq. (3) under steady-state conditions are given by

$$\delta\frac{d^2 a}{dx^2}-p\beta ab-(1-p)\beta ab^2=0 \tag{11}$$

$$\frac{d^2 b}{dx^2}+p\beta ab+(1-p)\beta ab^2-\beta\gamma b=0 \tag{12}$$

The corresponding initial and boundary conditions of the Eq. (6) to Eq. (9) are

At $x=0$, $\frac{da}{dx}=\frac{db}{dx}=0$ (13)

At $x=1$, $a=1, b=b_0=k\ (say)$ (14)

3. Approximate Analytical Solution of the One-Dimensional R-D Equation (Eq. (2) and Eq. (3)) by using Homotopy Analysis Method

Linear and non-linear differential equations can be modelled many phenomena are essentially important in different areas of science and technology. Many non-linear differential equations do not have analytical expressions. Semi-analytical methods such as the Homotopy perturbation method by Meena and Rajendran [15], Homotopy analysis method by Rasi *et al.,* [16], a new approach to Homotopy perturbation method by Mehala and Rajendran [17], Variational iteration method by Wazwaz [18], Adomian decomposition method by Adomian [19] and Akbari Ganji's method by Mary *et al.,* [20] can be utilized to attain specific solutions of non-linear differential equation.

The Homotopy analysis technique is a powerful semi-analytical method to solve non-linear Partial and Ordinary Differential equations by Liao [21,22]. The Homotopy analysis technique use homotopy concepts from the topology to generate the convergence series solution for non-linear systems. HAM was proposed by Shi-Jun Liao in 1992 and has been strongly utilized to solve many problems in

Physical and Chemical Science [23-28]. HAM does not need a small parameter to develop a perturbation solution and hence is applicable for both weakly and strongly non-linear problems. It provides an easy method to fine-tune and dominate the convergence region of solution series by assigning approximate values for auxiliary parameter h. Unlike other methods, it gives an analytical solution in terms of an infinite power series.

3.1 Approximate Analytical Solution for Steady State One-Dimensional R-D Equation

By using Homotopy analysis method, the approximate analytical solutions of concentration of reactant and autocatalyst in terms of distance x is given for the Eq. (11) and Eq. (12) is obtained as follows [23,24,29]:

$$a=1-\frac{h\,\beta k}{2\delta}\left[p+(1-p)\,k\right]x^2+\frac{h\,\beta k}{2\delta}\left[p+(1-p)\,k\right] \tag{15}$$

$$b=k+\frac{h\,\beta k}{2}\left[p+(1-p)\,k-\beta\gamma\right]x^2+\frac{h\,\beta k}{2}\left[p+(1-p)\,k-\beta\gamma\right] \tag{16}$$

3.2 Approximate Analytical Solution of the Eq. (6) and Eq. (7) for Non-Steady State by using the Homotopy Analysis Method

The non-steady state solution of Eq. (6) and Eq. (7) has been derived briefly by using the boundary conditions in Eq. (8) to Eq. (10).

We construct the homotopy for Eq. (6) and Eq. (7) as follows

$$(1-P)\left[\delta\frac{\partial^2 a}{\partial x^2}-\frac{\partial a}{\partial t}\right]=hP\left[\delta\frac{\partial^2 a}{\partial x^2}-p\beta ab-(1-p)\beta ab^2-\frac{\partial a}{\partial t}\right] \tag{17}$$

$$(1-P)\left[\frac{\partial^2 b}{\partial x^2}-\frac{\partial b}{\partial t}\right]=hP\left[\frac{\partial^2 b}{\partial x^2}+p\beta ab^2+(1-p)\beta ab^2-\beta\gamma b-\frac{\partial b}{\partial t}\right] \tag{18}$$

Consider the initial approximation solutions of the Eq. (17) and Eq. (18) as follows:

$$a=a_0+Pa_1+P^2a_2+\dots \tag{19}$$

$$b=b_0+Pb_1+P^2b_2+\dots \tag{20}$$

Substituting the Eq. (19) and Eq. (20) into the Eq. (17) and Eq. (18), we get

$$(1-P)\left[\delta\frac{\partial^2\left(a_0+Pa_1+P^2a_2+\ldots\right)}{\partial x^2}-\frac{\partial\left(a_0+Pa_1+P^2a_2+\ldots\right)}{\partial t}\right]$$
$$=hP\left[\begin{array}{l}\delta\dfrac{\partial^2\left(a_0+Pa_1+P^2a_2+\ldots\right)}{\partial x^2}-\\ -p\beta\left(a_0+Pa_1+P^2a_2+\ldots\right)\left(b_0+Pb_1+P^2b_2+\ldots\right)\\ -(1-p)\beta\left(a_0+Pa_1+P^2a_2+\ldots\right)\left(b_0+Pb_1+P^2b_2+\ldots\right)^2\\ -\dfrac{\partial\left(a_0+Pa_1+P^2a_2+\ldots\right)}{\partial t}\end{array}\right] \tag{21}$$

$$(1-P)\left[\frac{\partial^2\left(b_0+Pb_1+P^2b_2+\ldots\right)}{\partial x^2}-\frac{\partial\left(b_0+Pb_1+P^2b_2+\ldots\right)}{\partial t}\right]$$
$$=hP\left[\begin{array}{l}\dfrac{\partial^2\left(b_0+Pb_1+P^2b_2+\ldots\right)}{\partial x^2}+p\beta\left(a_0+Pa_1+P^2a_2+\ldots\right)\left(b_0+Pb_1+P^2b_2+\ldots\right)\\ +(1-p)\beta\left(a_0+Pa_1+P^2a_2+\ldots\right)\left(b_0+Pb_1+P^2b_2+\ldots\right)^2\\ -\beta\gamma\left(b_0+Pb_1+P^2b_2+\ldots\right)-\dfrac{\partial\left(b_0+Pb_1+P^2b_2+\ldots\right)}{\partial t}\end{array}\right] \tag{22}$$

Now equating the coefficients of P^0 and P^1 in the Eq. (21) and Eq. (22), we get

$$P^0:\ \frac{\partial^2 a_0}{\partial x^2}-\frac{\partial a_0}{\partial t}=0 \tag{23}$$

$$\frac{\partial^2 b_0}{\partial x^2}-\frac{\partial b_0}{\partial t}=0 \tag{24}$$

$$P^1:\ \delta\frac{\partial^2 a_1}{\partial x^2}-\frac{\partial a_1}{\partial t}-\left(\delta\frac{\partial^2 a_0}{\partial x^2}-\frac{\partial a_0}{\partial t}\right)=h\left[\delta\frac{\partial^2 a_0}{\partial x^2}-p\beta\,a_0b_0-(1-p)\beta\,a_0b_0^2-\frac{\partial a_0}{\partial t}\right] \tag{25}$$

$$\frac{\partial^2 b_1}{\partial x^2}-\frac{\partial b_1}{\partial t}-\left(\frac{\partial^2 b_0}{\partial x^2}-\frac{\partial b_0}{\partial t}\right)=h\left[\frac{\partial^2 b_0}{\partial x^2}+p\beta\,a_0b_0^2+(1-p)\beta\,a_0b_0^2-\beta\gamma\,b_0-\frac{\partial b_0}{\partial t}\right] \tag{26}$$

The initial and boundary conditions of the Eq. (17) and Eq. (18) becomes

At $x=0,\quad \dfrac{\partial a_i}{\partial x}=0,\ i=0,1,2,3\ldots$ (27)

$$\frac{\partial b_i}{\partial x}=0,\ i=0,1,2,3\ldots \tag{28}$$

At $x=1,\quad a_0=1,;\ a_i=0,\ i=2,3,4,\ldots$ (29)

$$b_0 = k,;\, b_i = 0,\, i = 2,3,4,\ldots \tag{30}$$

At $t = 1,\quad a_0 = 1,;\, a_i = 0,\, i = 2,3,4,\ldots$ (31)

$$b_0 = k,;\, b_i = 0,\, i = 2,3,4,\ldots \tag{32}$$

Applying the Laplace transform to the Eq. (23) to Eq. (26) with respect to $t,$ we have

$$\delta\frac{\partial^2 \overline{a_0}}{\partial x^2} - \left[s\overline{a_0} - a_0(t=0)\right] = 0 \tag{33}$$

$$\frac{\partial^2 \overline{b_0}}{\partial x^2} - \left[s\overline{b_0} - b_0(t=0)\right] = 0 \tag{34}$$

$$\delta\frac{\partial^2 \overline{a_1}}{\partial x^2} - \left[s\overline{a_1} - a_1(t=0)\right] = \frac{h}{s}\left[p\,\beta\, a_0\, b_0 - (1-p)\beta\, a_0 b_0^2\right] \tag{35}$$

$$\frac{\partial^2 \overline{b_1}}{\partial x^2} - \left[s\overline{b_1} - b_1(t=0)\right] = \frac{h}{s}\left[p\beta\, a_0 b_0 + (1-p)\beta\, a_0 b_0^2 - \beta\,\gamma\, b_0\right] \tag{36}$$

The corresponding boundary conditions becomes

At $x = 0,\quad \frac{\partial \overline{a_i}}{\partial x} = 0,\, i = 0,1,2,3,\ldots$ (37)

$$\frac{\partial \overline{b_i}}{\partial x} = 0,\, i = 0,1,2,3,\ldots \tag{38}$$

At $x = 1,\quad \overline{a_0} = \frac{1}{s};\, \overline{a_i} = 0,\ i = 2,3,4,\ldots$ (39)

$$\overline{b_0} = \frac{k}{s};\, \overline{b_i} = 0,\ i = 2,3,4,\ldots \tag{40}$$

At $t = 1,\quad \overline{a_0} = \frac{1}{s};\, \overline{a_i} = 0,\ i = 2,3,4,\ldots$ (41)

$$\overline{b_0} = \frac{k}{s};\, \overline{b_i} = 0,\ i = 2,3,4,\ldots \tag{42}$$

Solving an Eq. (33) by using the boundary conditions in Eq. (39) to Eq. (42), we get

$$\overline{a_0} = \frac{1}{s} \tag{43}$$

Taking the inverse Laplace transform for both sides of Eq. (43), we get

$$a_0 = 1 \tag{44}$$

Solving an Eq. (34) by using the boundary conditions in Eq. (39) to Eq. (42), we get

$$\overline{b_0} = \frac{k}{s} \tag{45}$$

Taking the inverse Laplace transform for both sides of Eq. (45), we get

$$b_0 = k \tag{46}$$

Solving an Eq. (35) by using the boundary conditions in Eq. (39) to Eq. (42), we get

$$\overline{a_1} = -\frac{h}{s^2}\left[p\beta k + (1-p)\beta k^2\right]\frac{\cosh\sqrt{\frac{s}{\delta}}x}{\cosh\sqrt{\frac{s}{\delta}}} + \frac{h}{s^2}\left[p\beta k + (1-p)\beta k^2\right] \tag{47}$$

Now, let us invert Eq. (47) using the complex inversion formula.

If $\overline{y(s)}$ represents the Laplace transform of a function $y(\tau)$, then according to the complex inversion formula $y(\tau) = \frac{1}{2\pi i}\oint_c \exp(s\tau)\overline{y(s)}ds$, where the integration has to be performed along a line $s = c$ in the complex plane and $s = x + iy$. The real number c is chosen in such a way that $s = c$ which lies to the right of all singularities, otherwise it is assumed to be arbitrary. In practice, the integral is evaluated by considering the contour integral presented on the right-hand side of the equation, which is then evaluated using the so-called Bromwich contour. In analytic functions $F(z)$, the contour integrals are computed by using the residue theorem.

$$\oint_c F(z)dz = 2\pi i\sum_n \mathrm{Re}\,s[F(z)]_{z=z_0} \tag{48}$$

where the residues are computed at the poles of the function $F(z)$. Hence from Eq. (48), we note that

$$y(\tau) = \sum_n \mathrm{Re}\,s[\exp[s\tau]\overline{y}(s)]_{s=s_0} \tag{49}$$

From the theory of complex variables, we can show that the residue of a function $F(z)$ at a simple pole $z = a$ and is given by

$$\mathrm{Re}\,s[F(z)]_{s=a} = \lim_{z\to a}\{(z-a)F(z)\} \tag{50}$$

By means of complex inversion formula, we have

$u_0(x,\tau)=\dfrac{1}{2\pi i}\displaystyle\int_{\gamma-i\infty}^{\gamma+i\infty} e^{s\tau}\,\overline{u_0}(x,s)ds =$ sum of the contributions from all the poles of the integrand.

In order to invert an Eq. (47), we need to evaluate

$$\operatorname{Re}s\left(-\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\frac{\cosh\sqrt{\frac{s}{\delta}}x}{\cosh\sqrt{\frac{s}{\delta}}}+\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\right)$$

Now, finding the poles of $\overline{a_1}$, we see that there is a pole at $s=0$ and there are infinitely many poles given by the solution of the equation $\cosh\sqrt{\frac{s}{\delta}}=0$, i.e. there are infinite number of poles at $s_n=-(2n+1)^2\dfrac{\delta\pi^2}{4}$, where $n=1,2,3,\ldots$

Hence, we note that

$$\begin{aligned}L^{-1}\left(\overline{a_1}\right)=\operatorname{Re}s&\left[-\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\frac{\cosh\sqrt{\frac{s}{\delta}}x}{\cosh\sqrt{\frac{s}{\delta}}}+\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\right]_{s=0}\\&+\operatorname{Re}s\left[e^{st}\left(-\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\frac{\cosh\sqrt{\frac{s}{\delta}}x}{\cosh\sqrt{\frac{s}{\delta}}}\right)\right]_{s=s_n}\end{aligned}\tag{51}$$

The first residue in Eq. (51) is given by

$$\begin{aligned}&\operatorname{Re}s\left[-\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\frac{\cosh\sqrt{\frac{s}{\delta}}x}{\cosh\sqrt{\frac{s}{\delta}}}+\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\right]_{s=0}\\&=\lim_{s\to0}\frac{d}{ds}e^{st}\left(-\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\left[\frac{\cosh\sqrt{\frac{s}{\delta}}x}{\cosh\sqrt{\frac{s}{\delta}}}\right]\right)+h\left[p\beta k+(1-p)\beta k^2\right]t\\&=-\frac{h\left(p\beta k+(1-p)\beta k^2\right)x^2}{2}+\frac{h\left(p\beta k+(1-p)\beta k^2\right)}{2}\end{aligned}\tag{52}$$

The second residue in Eq. (51) is presented by

$$\begin{aligned}
&\operatorname{Re}s\left[e^{st}\left(\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\frac{\cosh\sqrt{s}x}{\cosh\sqrt{s}}\right)\right]_{s=s_n}\\
&\qquad=\lim_{s\to s_n}e^{st}\left[\frac{h}{s^2}\left[p\beta k+(1-p)\beta k^2\right]\right]\frac{\cosh\sqrt{s}x}{\frac{d}{ds}\left(\cosh\sqrt{s}\right)}\\
&\qquad=16h\left(p\beta k+(1-p)\beta k^2\right)\sum_{n=0}^{\infty}\frac{(-1)^{n+1}e^{-\frac{\delta(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{\delta(2n+1)^3\pi^3}
\end{aligned} \tag{53}$$

Adding the Eq. (52) and Eq. (53), we get

$$\begin{aligned}
a_1=&-\frac{h\left(p\beta k+(1-p)\beta k^2\right)x^2}{2}+\frac{h\left(p\beta k+(1-p)\beta k^2\right)}{2}\\
&+16h\left(p\beta k+(1-p)\beta k^2\right)\sum_{n=0}^{\infty}\frac{(-1)^{n+1}e^{-\frac{\delta(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{\delta(2n+1)^3\pi^3}
\end{aligned} \tag{54}$$

Solving an Eq. (36) by using the boundary conditions in Eq. (39) to Eq. (42), we get

$$\overline{b_1}=\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\frac{\cosh\sqrt{s}x}{\cosh\sqrt{s}}-\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right) \tag{55}$$

The above equations are also inverted by using the residue inversion approach.

Now, finding the poles of $\overline{b_1}$ we see that there is a pole at $s=0$ and there are infinitely many poles given by the solution of the equation $\cosh\left(\sqrt{s}\right)=0$, i.e. there are infinite number of poles at $s_n=-(2n+1)^2\frac{\pi^2}{4}$ where $n=1,2,3,\ldots$

Hence, we note that

$$\begin{aligned}
L^{-1}\left(\overline{b_1}\right)=&\operatorname{Re}s\begin{bmatrix}\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\frac{\cosh\sqrt{s}\,x}{\cosh\sqrt{s}}\\ -\frac{h\beta k}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\end{bmatrix}_{s=0}\\
&+\operatorname{Re}s\left[e^{st}\left(\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\frac{\cosh\sqrt{s}\,x}{\cosh\sqrt{s}}\right)\right]_{s=s_n}
\end{aligned} \tag{56}$$

The first residue in an Eq. (56) is given by

$$
\begin{aligned}
&\operatorname{Re} s\left[\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\frac{\cosh\sqrt{s}x}{\cosh\sqrt{s}}-\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\right]_{s=0}\\
&\quad=\lim_{s\to 0}\frac{d}{ds}e^{st}\left(\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\frac{\cosh\sqrt{s}x}{\cosh\sqrt{s}}\right)-h\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)t\\
&\quad=\frac{h}{2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)x^2-\frac{h}{2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)
\end{aligned}
\tag{57}
$$

The second residue in Eq. (56) is given by

$$
\begin{aligned}
&\operatorname{Re} s\left[e^{st}\left(\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\frac{\cosh\sqrt{s}x}{\cosh\sqrt{s}}\right)\right]_{s=s_n}\\
&\qquad=\lim_{s\to s_n}e^{st}\left[\frac{h}{s^2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\right]\frac{\cosh\sqrt{s}x}{\frac{d}{ds}\left(\cosh\sqrt{s}\right)}\\
&\qquad=16h\left(pk\beta+(1-p)\,\beta k^2-\beta\gamma k\right)\sum_{n=0}^{\infty}\frac{(-1)^{n+1}e^{-\frac{(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{(2n+1)^3\pi^3}
\end{aligned}
\tag{58}
$$

Adding the Eq. (57) and Eq. (58), we get

$$
\begin{aligned}
b_1=&\frac{h}{2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)x^2-\frac{h}{2}\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\\
&+16h\left(pk\beta+(1-p)\beta k^2-\beta\gamma k\right)\sum_{n=0}^{\infty}\frac{(-1)^{n+1}e^{-\frac{(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{(2n+1)^3\pi^3}
\end{aligned}
\tag{59}
$$

From Eq. (19) and Eq. (20), we get the following result

$a\approx a_0+a_1$ and $b\approx b_0+b_1$

Adding the Eq. (44) and Eq. (54), we get

$$
\begin{aligned}
a=&1-\frac{h\beta k\left(p+(1-p)k\right)x^2}{2}+\frac{h\beta k\left(p+(1-p)k\right)}{2}\\
&+16h\beta k\left(p+(1-p)k\right)\sum_{n=0}^{\infty}\frac{(-1)^{n+1}e^{-\frac{\delta(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{\delta(2n+1)^3\pi^3}
\end{aligned}
\tag{60}
$$

Adding the Eq. (46) and Eq. (59), we get

$$b = k + \frac{hk\beta}{2}\left(p + (1-p)k - \gamma\right)x^2 - \frac{hk\beta}{2}\left(p + (1-p)k - \gamma\right) + 16hk\beta\left(p + (1-p)k - \gamma\right)\sum_{n=0}^{\infty}\frac{(-1)^{n+1} e^{-\frac{(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{(2n+1)^3\pi^3} \tag{61}$$

3.3 Approximate Analytical Solution for Non-Steady State One-Dimensional R-D Equation

By using Homotopy analysis method and Laplace transform technique, the approximate analytical expressions of concentration of reactant and autocatalyst in terms of time t given in Sub-section 3.2 of the Eq. (6) and Eq. (7) is obtained as follows [29-34]:

$$a = 1 - \frac{h\beta k}{2\delta}\left[p + (1-p)k\right]x^2 + \frac{h\beta k}{2\delta}\left[p + (1-p)k\right] + 16h\beta k\left[p + (1-p)k\right]\sum_{n=0}^{\infty}\frac{(-1)^{n+1} e^{-\frac{\delta(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{\delta(2n+1)^3\pi^3} \tag{62}$$

$$b = k + \frac{h\beta k}{2}\left[p + (1-p)k - \beta\gamma\right]x^2 + \frac{h\beta k}{2}\left[p + (1-p)k - \beta\gamma\right] + 16h\beta k\left[p + (1-p)k - \gamma\right]\sum_{n=0}^{\infty}\frac{(-1)^{n+1} e^{-\frac{(2n+1)^2\pi^2 t}{4}}\cos\left(\frac{2n+1}{2}\pi x\right)}{(2n+1)^3\pi^3} \tag{63}$$

Moreover, Omar *et al.,* [34] briefly explained how to apply the Laplace transform for non-linear PDEs.

4. Numerical Simulation

The semi-analytical solutions for the dimensionless concentration of the reactant and autocatalyst for non-steady state and steady state have been obtained using Homotopy analysis method. The solutions derived using HAM for non-steady state is explained in Sub-section 3.2 respectively. The achieved approximate analytical expressions along with the numerical simulation by using MATLAB have been plotted in Figure 1 to Figure 4. The MATLAB programming for the considered model is given in Sub-section 4.1. The specific application of numerical simulation was described in depth by Ghouizi *et al.,* [35].

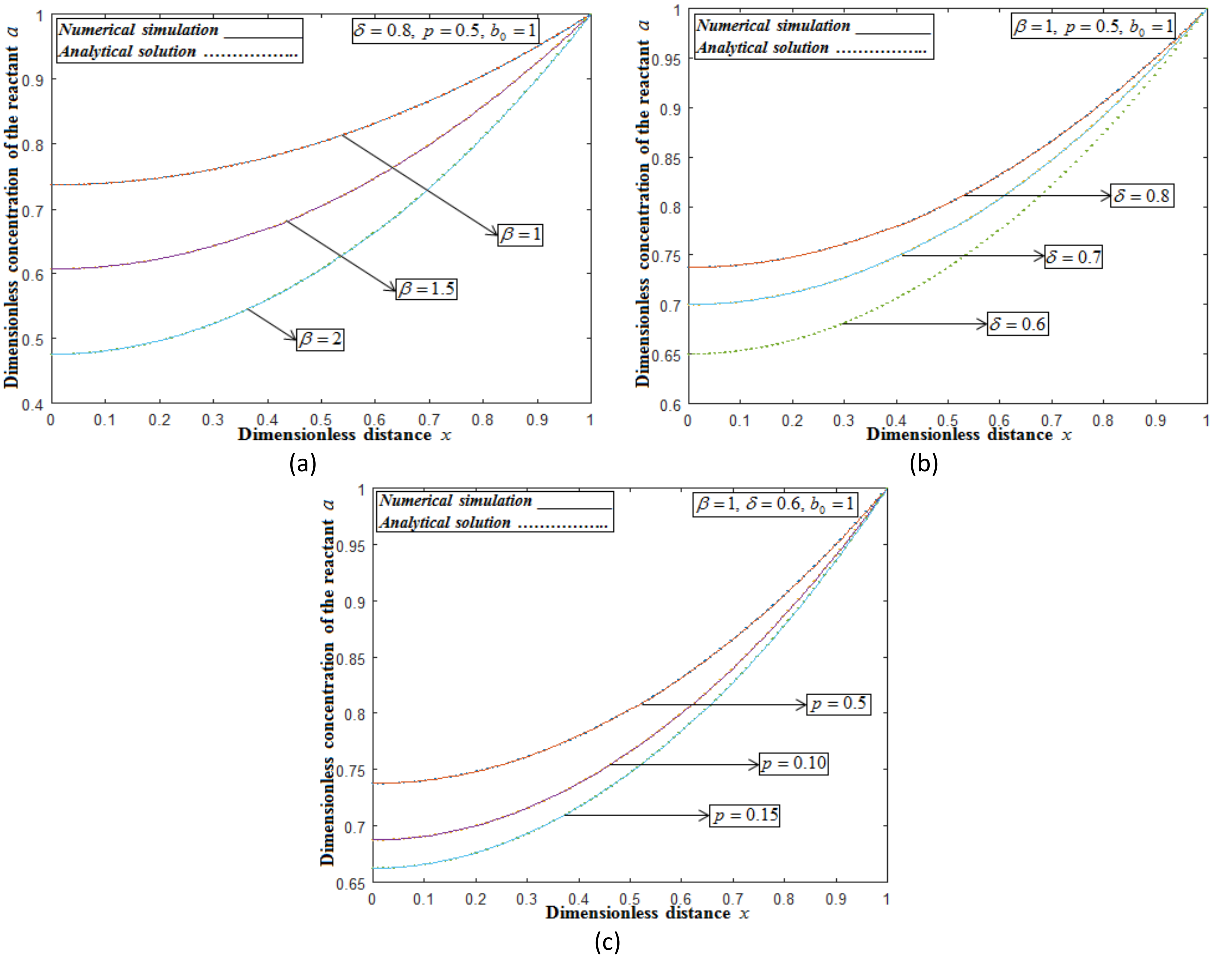
4.1 MATLAB Program for The Non-Steady One-Dimensional R-D Equation (Eq. (1) to Eq. (4))

```
function pdex4
m = 0;
x = linspace(0,1);
t = linspace(0,0.5);
```

```
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,2)')
%———————————————————————
figure
plot(x,u2(end,:))
title('u2(x,t)')
xlabel('Distance x')
ylabel('u2(x,2)')
% ——————————————————————–
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1];
f = [1; 1] .* DuDx;
g=0.5;
b=1;
r=0.5;
d=0.8;
F=(-r*b*u(1)*u(2)-(1-r)*b*u(1)*u(2)*u(2))/(d);
F1=(r*b*u(1)*u(2)+(1-r)*b*u(1)*u(2)*u(2)-b*g*u(2))
s=[F; F1];
% ——————————————————————–
function u0 = pdex4ic(x);
u0 = [1; 1];
% ——————————————————————–
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = [0;0];
ql = [1;1];
pr = [ur(1)-1;ur(2)-0.5];
qr = [0;0];
```

5. Results and Discussion

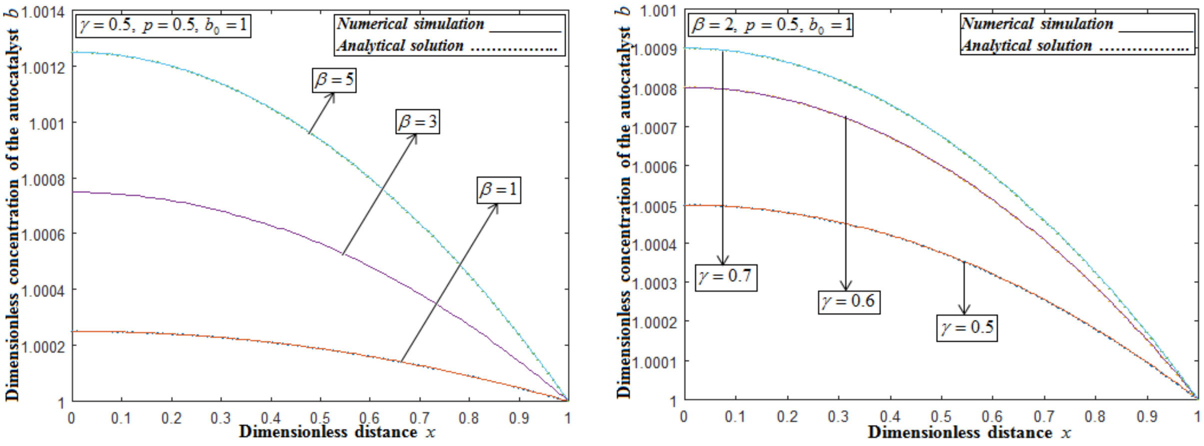
The approximate analytical solution of the concentrations for the reactant and the autocatalyst for non-steady is given in Sub-section 3.2. Figure 1 shows that dimensionless concentration of the reactant a versus the dimensionless distance x by using Eq. (15). From the Figure 1(a), Figure 1(b) and Figure 1(c) it is clear that, when the values β,δ and p increases, the corresponding dimensionless concentration decreases for specified values of the further dimensionless parameters. Figure 2 depicts that dimensionless concentration of the autocatalyst b versus the dimensionless distance x by using Eq. (16). Figure 2(a), Figure 2(b) and Figure 2(c) displays that, when β, γ and p increases, the corresponding dimensionless concentration increases for fixed values of the remaining dimensionless parameters.



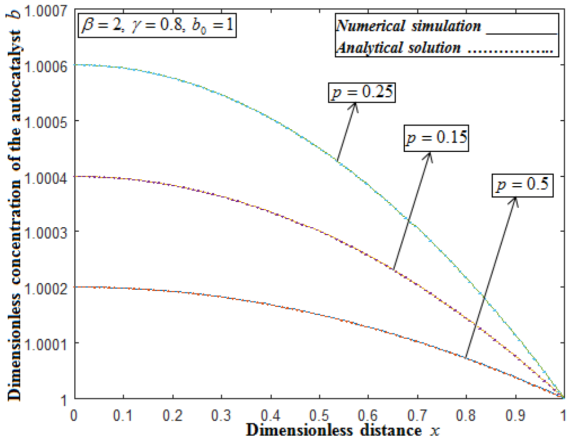
(a) (b)

(c)

Fig. 1. Dimensionless concentration of the reactant a versus dimensionless distance x. The curves are marked by using Eq. (15) for different values of (a) β, (b) δ, and (c) p and specified values of the remaining dimensionless parameters



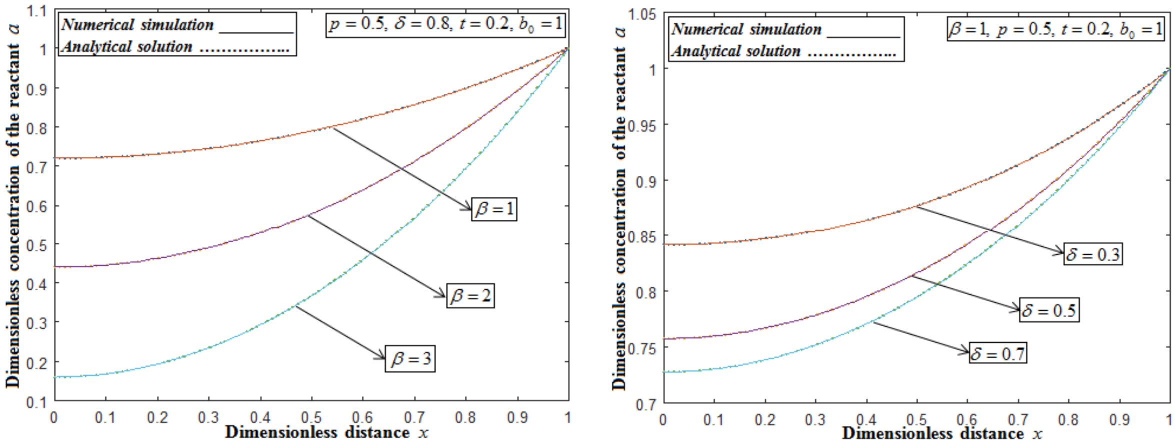
(a) (b)



(c)

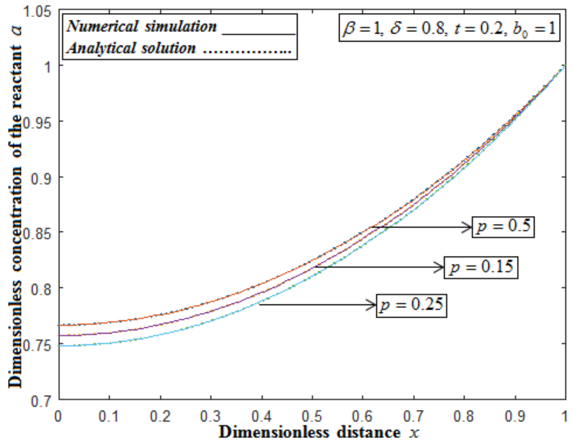
Fig. 2. Dimensionless concentration of the autocatalyst b versus dimensionless distance x. The curves are drawn by using Eq. (16) for different values of (a) β, (b) γ, and (c) p and specified values of the remaining dimensionless parameters

Figure 3 demonstrates that dimensionless concentration of the reactant a versus the dimensionless distance x by using Eq. (62). From these Figure 3(a), Figure 3(b) and Figure 3(c) it is noted that, when β, δ and p increases, the corresponding dimensionless concentration decreases for certain values of the further dimensionless parameters. Figure 4 shows that dimensionless concentration of the autocatalyst b versus the dimensionless distance x by using Eq. (63). As in Figure 4(a) and Figure 4(c), it portrays that when β and p increases, the corresponding dimensionless concentration also increases for specified values of the remaining dimensionless parameters. From the Figure 4(b) it is evident that, when γ increases, the corresponding dimensionless concentration decreases for specified values of the further dimensionless parameters.



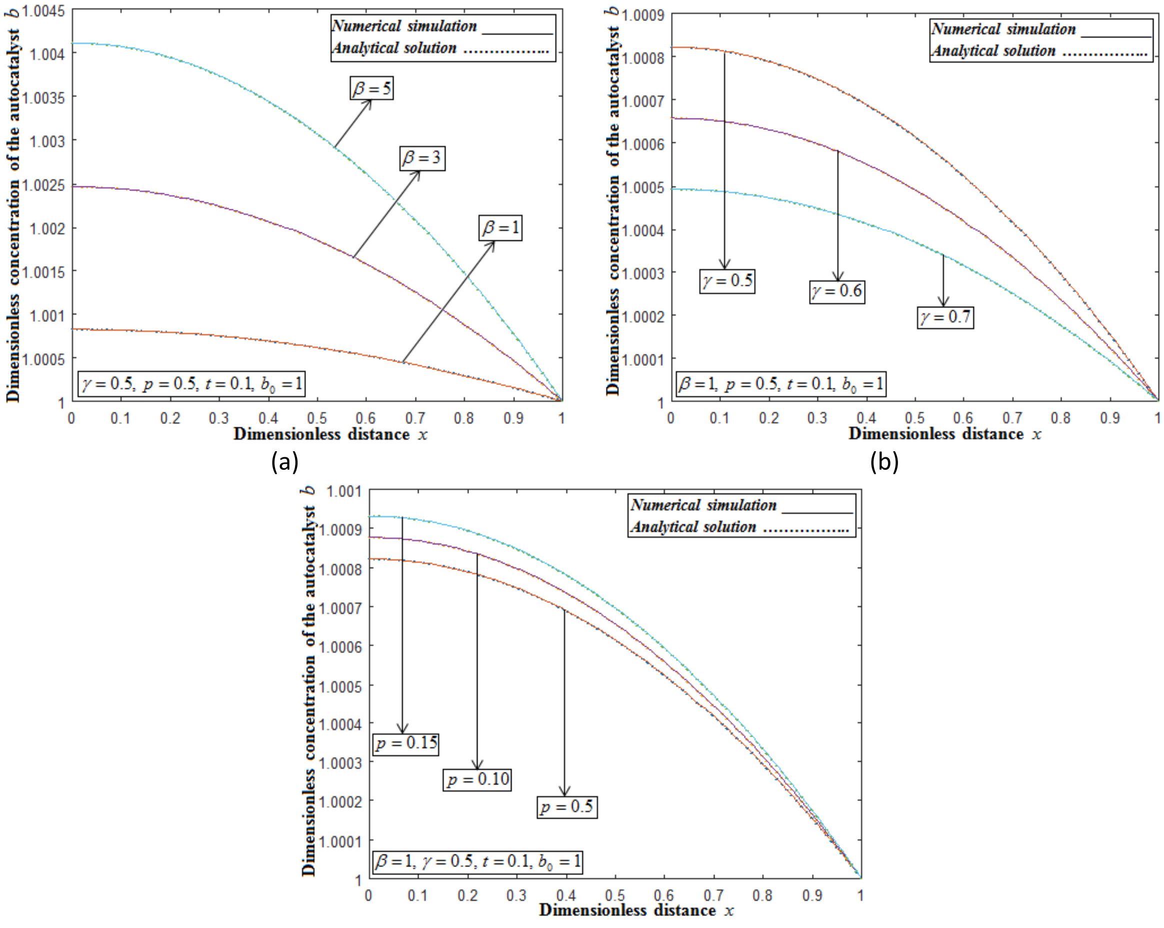
(a)

(b)



(c)

Fig. 3. Dimensionless concentration of the reactant a versus dimensionless distance x. The curves are marked by using Eq. (62) for different values of (a) β, (b) δ, and (c) p and specified values of the remaining dimensionless parameters

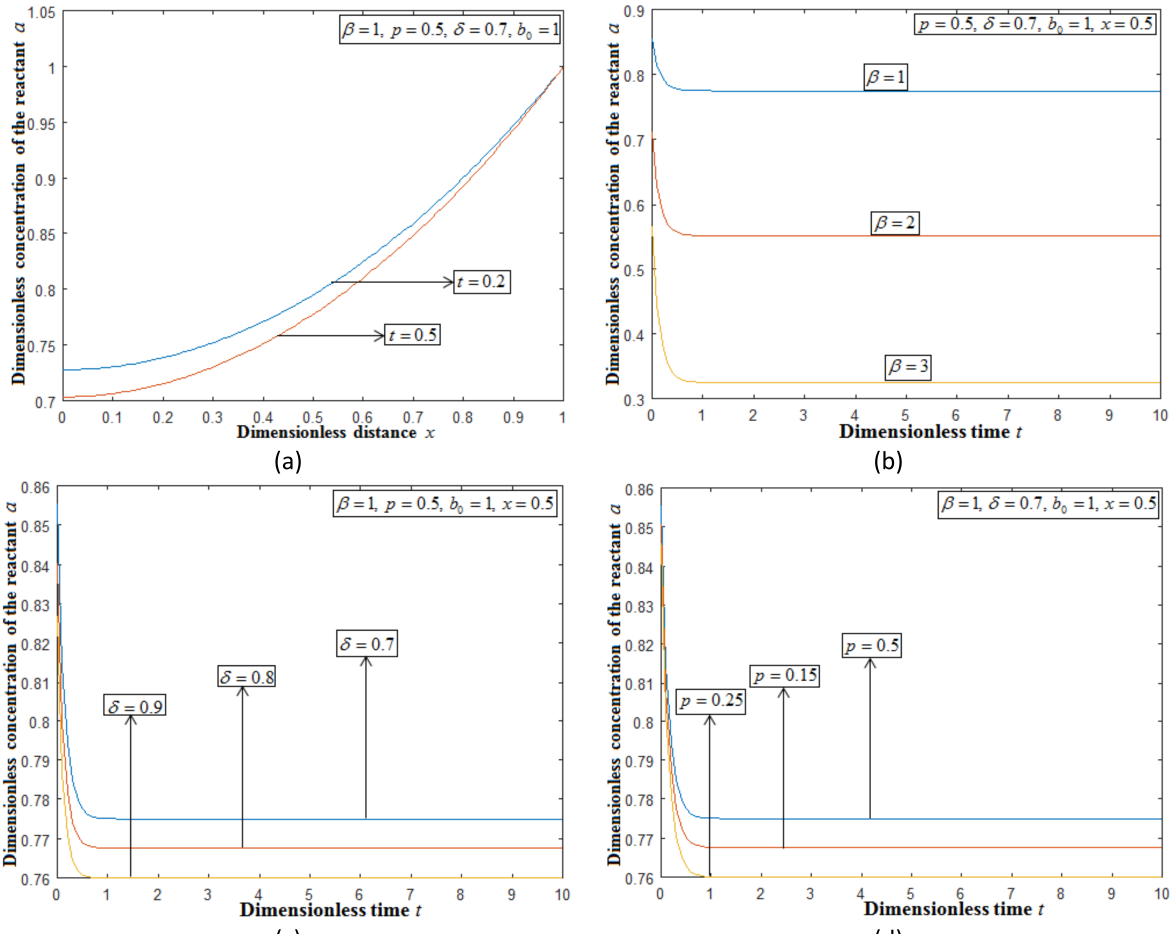


(a) (b)

(c)

Fig. 4. Dimensionless concentration of the autocatalyst b versus dimensionless distance x. The curves are marked by using Eq. (63) for different values of (a) β, (b) γ, and (c) p and specified values of the remaining dimensionless parameters

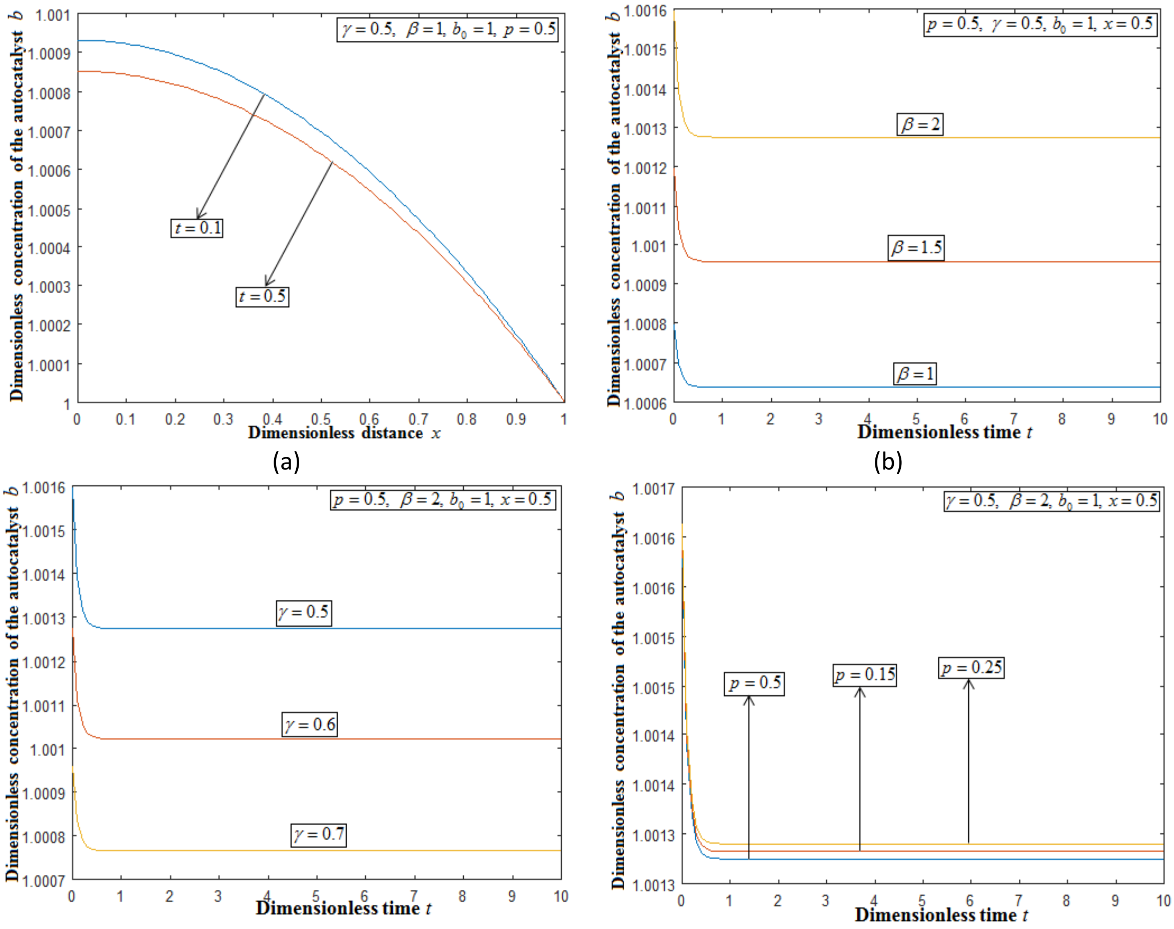
Figure 5(a) shows that dimensionless concentration of the reactant a versus the dimensionless distance x by using Eq. (62). From the Figure 5(b) to Figure 5(d) illustrates that dimensionless concentration of the reactant a versus the dimensionless time t by using Eq. (62). Figure 5(a) it describes that, when t increases, the corresponding dimensionless concentration decreases for certain values of the further dimensionless parameters. From these Figure 5(b) to Figure 5(d) it is observed that, when increases β, δ and p, the corresponding dimensionless concentration decreases for fixed values of the remaining dimensionless parameters. Figure 6(a) shows that dimensionless concentration of the autocatalyst b versus the dimensionless distance x by using Eq. (63). As in Figure 6(b) to Figure 6(d) it is cleared that dimensionless concentration of the autocatalyst x versus the dimensionless time t by using Eq. (63). According to the Figure 6(a) depicts that, when t increases, the corresponding dimensionless concentration decreases for specified values of the further dimensionless parameters. Figure 6(b) and Figure 6(d) it displays that, when increases β and p, the corresponding dimensionless concentration increases for specified values of the further dimensionless parameters. Figure 6(c) depicts that, when increases γ, the corresponding dimensionless concentration decreases for specified values of the other dimensionless parameters.



(a) (b)

(c) (d)

Fig. 5. Dimensionless concentration of the reactant a versus dimensionless distance x. The curves are plotted by using Eq. (62) for different values of (a) t, (b) β, (c) δ, and (d) p and specified values of the remaining dimensionless parameters



(a) (b)

(c) (d)

Fig. 6. Dimensionless concentration of the autocatalyst b versus dimensionless distance x. The curves are marked by using Eq. (63) for different values of (a) t, (b) β, (c) γ, and (d) p and specified values of the remaining dimensionless parameters

6. Conclusions

In this paper, the approximate analytical solutions for the concentrations of reactant and autocatalyst in cubic autocatalysis were derived for both time dependent and independent. With the help of Homotopy analysis technique, the semi-analytical solution was reached. For small parameter values, the results are in perfect fit with the numerical results. The approximate analytical results obtained under non-steady state will help the researchers to visualize the effects of various parameters on concentration. The graphs were displayed to show the impacts of several parameters by varying the values including rate of cubic reaction, rate of quadratic reaction, rate of autocatalyst, and diffusion coefficient. These impacts of chemical parameters can be useful for many researchers and chemical engineers to control the model at any state (steady and non-steady) with the help of the derived semi-analytical expressions.

Acknowledgement

This research was not funded by any grant.

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