Research Paper
Computational Methods for Differential Equations
http://cmde.tabrizu.ac.ir
Vol. 13, No. 2, 2025, pp. 432-449
DOI:10.22034/cmde.2024.60438.2586

A new approximate analytical method for solving some non-linear boundary value problems in Reaction-Diffusion model

Vembu Ananthaswamy*, Venkatasubban Vijayalaskhmi, and Jeya Kumar Anantha Jothi
Research Centre and PG Department of Mathematics, The Madura College (Affiliated to Madurai Kamaraj University), Madurai, Tamil Nadu, India.

Abstract

The applications of a Reaction-Diffusion boundary value problems are found in science, biochemical applications, and chemical applications. The Ananthaswamy-Sivasankari method (ASM) is employed to solve the considered specific models like non-linear reaction-diffusion model in porous catalysts, spherical catalysts pellet, and catalytic reaction-diffusion process in a catalyst slab. An accurate semi-analytical expression for the concentrations and effectiveness factors are given in the explicit form. Graphical representations are used to display the impacts of several parameters, including the Thiele modulus, characteristic reaction rate, concentration of half-saturation, reaction order and dimensionless constant in Langmuir-Hinshelwood kinetics. The impact of numerous parameters namely the Langmuir-Hinshelwood kinetics and Thiele modulus on effectiveness factors are displayed graphically. Our semi-analytical findings shows good match in all parameters when compared to numerical simulation using MATLAB. Many non-linear problems in chemical science especially, the Reaction-Diffusion equations, Michaelis-Menten kinetic equation, can be resolved with the aid of the new approximate analytical technique, ASM.

Keywords. Spherical Porous Catalyst, Steady-state Reaction-Diffusion equation, Non-linear boundary value problem, Ananthaswamy-Sivasankari method (ASM), Numerical Simulation.

2010 Mathematics Subject Classification. 34B15, 34E05, 34E15, 34E20.

1. Introduction

The prominent non-linear boundary value problem, the reaction-diffusion model involving porous catalysts with a Michaelis-Menten reaction term, has been re-examined by Shivanian [20]. In the case of diffusive along with advective transport based on the Michaelis-Menten reaction expression, Vosoughi [26] was examined the class for non-linear reactive transport models. Utilize the predictor homotopy analysis technique, which has been suggested as a way to forecast the multiplicity for non-linear BVP solutions. A broad model for reactive transport via multiple purposes in chemical as well as engineering for the environment has been solved analytically by Ellery et al. [8]. According to Steefel et al. [22], reactive transport modeling is a crucial tool for analyzing biological processes, chemical and coupled physical in earth systems. It also has the ability to more effectively integrate the findings of targeted basic investigations in earth materials. Regnier et al. [19] studied the area of contemporary geosciences which benefits greatly from reactive transport models. In order to resolve the one-dimensional steady-state for non-linear reactive transport model (RTM) intended for fluid along with solute transport models of soft tissues as well as microvessels, Ahmad et al. [3] introduced an artificial neural network approach. Abbasbandy [1] used the homotopy analysis approach, and this is a more successful approach for finding the approximate expression for the non-linear modelling of diffusion in addition to reaction within catalyst pellets for n^{th}-order reactions. In the study of non-linear boundary value issues involving chemical reaction kinetics, Abbasbandy et al. [2] examined two fundamental components of the homotopy analysis technique: (1) prediction and (2) efficient computation of many solutions. Rach et al. [18] investigate reactant diffusion in the presence of reaction heat inside the porous catalytic pellet.

Received: 06 February 2024 ; Accepted: 21 April 2024.
∗ Corresponding author. Email: ananthu9777@gmail.com .

The Lane-Emden boundary value problem in which the Arrhenius reaction rate is used to describe the reactant concentration. Systems for Volterra integral forms that correspond to Lane-Emden equations were introduced by Wazwaz et al. [29]. In order to manage such frameworks containing integral forms, the Adomian decomposition approach has been utilized. Lesnic [12] explained how a steady-state reaction-diffusion process that involves a power-law heat source which is non-linear and described by an ordinary differential equation having homogeneous dirichlet boundary conditions. Moitsheki et al. [15] highlighted the non-linear problem that arises from the catalyst's reaction and diffusion. In order to resolve this problem, the techniques of homotopy analysis, finite differences, and Adomian decomposition were used. According to the research of Valdes et al. [24] , integral equation formulations can yield precise numerical solutions for reaction-diffusion models. According to the study of Hadian-Rasanan et al. [11], a number of astrophysical phenomena can be expressed by the Lane-Emden equation for non-linear singular second-order differential equation. The research of Parand et al. [17], was to develop an approximate estimation towards a solution for non-linear Lane-Emden type equations of various orders by introducing a new orthogonal basis, namely the generalized fractional-order Chebyshev orthogonal functions (GFCFs). Numerous widely-known types of non-linear Lane-Emden type models were solved by Parand et al.[16] by comparing two effective computational strategies depending on Exponential as well as Rational Bessel (EB and RB) functions. A mathematical model for an immobilized enzyme system within porous spherical particles has been carried out by Ananthaswamy et al. [14] with the help of the homotopy perturbation technique. Subanya et al. [23] used two approaches based on the homotopy analysis approach to give a comparison of approximate analytical expressions for the immobilized enzyme within porous planar, cylindrical, and spherical particles.

The main objective of this research is utilizing ASM to achieve the semi-analytical solution for the Reaction-Diffusion (R-D) equations within a spherical porous catalyst. Currently, researchers solve these kinds of problems and provides solutions in an implicit manner, but our analytical results present solutions in an explicit form. In comparison to other numerical as well as semi-analytical methods, this method involves just a single steps. The semi-analytical findings and numerical simulations are subsequently compared and graphically displayed. In order to show the impacts of several parameters like Thiele modulus, characteristic reaction rate, concentration of half saturation and dimensionless constant in Langmuir-Hinshelwood kinetics, the graphical illustrations are presented. Additionally, effectiveness factor is calculated by employing ASM.

2. Mathematical formulation of the problem

2.1. **Non-linear Reaction-Diffusion (R-D) Model within the Porous Catalysts.** The following is the one-dimensional steady-state equation governed by Reactive Transport Model (RTM) (Ganie et al. [10])

$$\hat{D}\frac{d^2\theta}{dX^2} - V\frac{d\theta}{dX} - r(\theta) = 0, \;\; 0 \leq X \leq 1, \tag{2.1}$$

subject to the following boundary conditions:

$$\theta(L) = \theta_S \;\; and \;\; \frac{d\theta(0)}{dX} = 0, \tag{2.2}$$

the advective velocity is stand as V, $r(\theta)$ denotes the reaction process and $\hat{D}$ denotes as diffusivity parameter. Furthermore, Ellery et al. [8] and Shivanian et al. [20] discuss the great depth of the parameters.

By introducing the non-dimensional variables mentioned below:

$$\theta(\chi) = \frac{\theta(X)}{\theta_S}, \;\; \chi = \frac{X}{L},$$

Now substituting the above non-dimensional parameters into Eq. (2.1) yield:

$$\frac{d^2\theta}{d\chi^2} - P\frac{d\theta}{d\chi} - r(\chi) = 0, \;\; 0 \leq \chi \leq 1, \tag{2.3}$$

where $P = \frac{LV}{\hat{D}}$ is so-called Peclet number. The model was used to porous catalyst pellets to represent a diffusion and reaction model in the absence of advection of transport, $P = 0$. Since Michaelis-Menten [8] assumes that $r(\chi)$ is a

non-dimensional response, Eq. (2.3) is changed as follows:

$$\frac{d^2\theta}{d\chi^2} - \frac{\beta\theta(\chi)}{\alpha+\theta(\chi)} = 0, \quad 0 \le \chi \le 1, \tag{2.4}$$

the boundary conditions as:

$$\frac{d\theta(0)}{d\chi} = 0, \quad \theta(1) = 1, \tag{2.5}$$

where α represents the concentration for half saturation which is non-negative as well as β indicates characteristic reaction rate. While $\beta < 0$ then instead during product reactions we have seems at the reactives.

2.2. **Non-linear Reaction-Diffusion (R-D) Model inside Spherical Catalysts Pellet.** Consider the steady-state differential equation associated with the reaction-diffusion process within the spherical geometric pellet at isothermal conditions (Magyari [13]) .

$$D_e\left(\frac{d^2c}{dr^2} + \frac{2}{r}\frac{dc}{dr}\right) = k_v c^n, \tag{2.6}$$

where c indicates the reactant concentration at pore for catalyst pellet, D_e is the Effective Diffusion Coefficient for reactant, the distance from the pellet core represents r and k_v is the reaction rate constant. In the given equation, where n is the reaction order, the range $[0, \infty]$ is admitted. The boundary conditions at surface of catalyst along with the center of catalyst are considered, respectively as follows:

$$c\,|_{r=r_0} = c_s \ \ (Surface\ \ of\ \ catalyst), \tag{2.7}$$

$$\frac{dc}{dr}\,|_{r=0} = 0 \ \ (Center\ \ of\ \ catalyst). \tag{2.8}$$

The non-dimensional variables are as follows:

$$R = \frac{r}{r_0}, \quad C(R) = \frac{c(r)}{c_s}, \tag{2.9}$$

where r indicates the radial coordinate, the radius of the pellet is represented by r_0, R denotes the non-dimensional radial coordinate, the surface concentration is c_s and c is the concentration.

By utilizing Eq. (2.9), Eqs. (2.6)-(2.8) turns to

$$\frac{d^2C}{dR^2} + \frac{2}{R}\frac{dC}{dR} - \phi^2 C^n = 0, \tag{2.10}$$

with boundary conditions are given as follows:

$$C\,|_{R=1} = 1, \quad \frac{dC}{dR}\,|_{R=0} = 0, \tag{2.11}$$

where $\phi = \left(\frac{k_v r_0^2 c_s^{n-1}}{D_e}\right)^{\frac{1}{2}}$ represents the Thiele modulus.

The concentration around the center for the catalyst is the quantity of physical interest $C(0) = C_0$, where C stands of the non-dimensional concentration, C_0 is the non-dimensional concentration within the center for the pellet, as well as the concentration gradient at the surface of catalyst $\frac{dC}{dR}\,|_{R=1}$. The above equation is likewise about the Lane-Emden kind [9, 11, 16, 17]. To implement the procedure, first we have to change the controlling Eqs. (2.10)-(2.11) from a physical region into a region by using the mapping. (Mohammadia et al. [14])

$$R = \frac{x+1}{2}, \quad -1 \le x \le 1, \tag{2.12}$$

where R represents the non-dimensional radial coordinate, x denotes the transformed independent variable. Using $u(x) = C(2R-1)$ in Eq. (2.10), the differential equation with boundary conditions into the interval $[-1, 1]$ is converted into:

$$\frac{d^2u}{dx^2} + \frac{2}{x+1}\frac{du}{dx} - \frac{\phi^2}{4}u^n = 0. \tag{2.13}$$

The corresponding boundary conditions are as follows:

$$u\,|_{x=1}=1,\quad \frac{du}{dx}\,|_{x=-1}=0. \tag{2.14}$$

2.3. **Catalytic Reaction-Diffusion process in a Catalyst Slab.** Considered a specific uni-molecular reaction takes place within the catalyst based on the corresponding stoichiometry for the current study as stated in Danish et al. [7]:

$$A \rightarrow products,$$

Material balance across species A produces the generic continuity equation shown below:

$$\frac{\partial C_A}{\partial t} = \nabla.D_e.\nabla C_A - (-r_A)\,, \tag{2.15}$$

where D_e indicates the effective diffusion coefficient for A and is considered to stay constant throughout the length of the pore L. For a steady-state catalyst slab, Eq. (2.15) simplifies to

$$D_e\frac{d^2C_A}{dX^2} = (-r_A)\,. \tag{2.16}$$

The associated boundary conditions are:

$$C_A = C_{AS}\ \ at\ \ X=L\ \ \ (pore\ \ mouth)\,, \tag{2.17}$$

$$\frac{dC_A}{dX} = 0\ \ at\ \ X=0\ \ \ (pore\ \ center)\,. \tag{2.18}$$

The Eq. (2.16) along with the corresponding boundary conditions have to be simplified using the non-dimensional variables listed below:

$$X=\frac{x}{L},\ \ Y=\frac{C_A}{C_{AS}},\ \ \phi = L\sqrt{\frac{(-r_{AS})}{D_eC_{AS}}},\ \ (-r_y)=\frac{(-r_A)}{(-r_{AS})}, \tag{2.19}$$

$$\frac{d^2Y}{dX^2} - \phi^2\,(-r_y) = 0. \tag{2.20}$$

The respective boundary conditions are:

$$Y=1\ \ at\ \ X=1, \tag{2.21}$$

$$\frac{dY}{dX}=0\ \ at\ \ X=0. \tag{2.22}$$

The reaction rate is given by $(-r_A)=k_nC_A^n$ and $(-r_A)=\frac{K_1C_A}{1+K_2C_A}$ in power law and Langmuir-Hinshelwood kinetics, correspondingly. Then Eq. (2.20) takes on the non-dimensional form seen below. However, the boundary conditions remain unchanged.

$$\frac{d^2Y}{dX^2} - \phi^2y^n = 0, \tag{2.23}$$

$$\frac{d^2Y}{dX^2} - \phi^2\frac{Y}{1+KY} = 0. \tag{2.24}$$

Aside from Y, there is a further variable known as the effectiveness factor (η), which is characterized by the ratio for a overall reaction rate via diffusion to reaction rate when it had been tested within the pore mouth. This represents an important quantity because it is primarily related to the design of the catalytic reactor. It is given mathematically by the subsequent expression over the catalyst slab:

$$Effectiveness\ \ factor\,(\eta) = \frac{1}{\phi^2}\frac{dY}{dX}\,|_{X=1}\,. \tag{2.25}$$

3. Approximate analytical expressions for the Porous catalyst by utilizing Ananthaswamy-Sivasankari Method (ASM)

The Ananthaswamy-Sivasankari method (ASM) [5, 6, 21, 25] is a novel approach for solving the non-linear ordinary differential equations in second-order. Also, it is applicable to the solve differential equations, both linear and non-linear. This approach can also be simply extended to address a variety of further non-linear problems that arise in chemical, biological, and physical sciences. However, the new technique provided here is relevant to boundary value problems. It is possible to create new boundary conditions of the differential equation along with its derivatives.

3.1. Approximate analytical expression for non-linear Reaction-Diffusion model in Porous Catalysts.

The approximate analytical expression to Eq. (2.4) which satisfies the boundary condition is shown below:

$$\theta(\chi) = le^{a\chi} + me^{-a\chi}, \tag{3.1}$$

$$\frac{d\theta}{d\chi} = ale^{a\chi} - ame^{-a\chi}. \tag{3.2}$$

We obtain the value of the parameters l and m by employing the boundary condition Eq. (2.5) in Eqs. (3.1) and (3.2).

$$l = m, \quad m = \frac{1}{e^{a} + e^{-a}}. \tag{3.3}$$

As a result, Eq. (3.1), becomes

$$\theta(\chi) = \frac{e^{a\chi} + e^{-a\chi}}{e^{a} + e^{-a}}. \tag{3.4}$$

Now, employing Eq. (3.4) in Eq. (2.4) and simplifying, we get

$$a^2\left(\frac{e^{a\chi} + e^{-a\chi}}{e^{a} + e^{-a}}\right) - \frac{\beta\left(\frac{e^{a\chi}+e^{-a\chi}}{e^{a}+e^{-a}}\right)}{\alpha + \left(\frac{e^{a\chi}+e^{-a\chi}}{e^{a}+e^{-a}}\right)} = 0. \tag{3.5}$$

If $\chi = 1$, Eq. (3.5) becomes

$$a^2 - \frac{\beta}{\alpha + 1} = 0. \tag{3.6}$$

After solving Eq. (3.6), we obtain the value for the parameter α as follows:

$$a = \sqrt{\frac{\beta}{\alpha + 1}}. \tag{3.7}$$

As a result, an approximate analytical expression for Eq. (2.4) is derived as follows:

$$\theta(\chi) = \frac{e^{a\chi} + e^{-a\chi}}{e^{a} + e^{-a}}, \tag{3.8}$$

where a is obtained from the Eq. (3.7).

3.2. Approximate analytical expressions for non-linear Reaction-Diffusion Model in Spherical Catalysts Pellet.

3.2.1. *For dimensionless concentration $C(R)$ Eq.* (2.10). The approximate analytical expression to Eq. (2.10) which satisfies the boundary condition is shown below:

$$C(R) = le^{aR} + me^{-aR}, \tag{3.9}$$

$$\frac{dC}{dR} = ale^{aR} - ame^{-aR}. \tag{3.10}$$

We obtain the value of the parameters l and m by employing the boundary condition Eq. (2.11) in Eqs. (3.9) and (3.10).

$$l = m, \quad m = \frac{1}{e^a + e^{-a}}. \tag{3.11}$$

As a result, Eq. (3.9), becomes

$$C(R) = \frac{e^{aR} + e^{-aR}}{e^a + e^{-a}}. \tag{3.12}$$

Now, employing Eq. (3.12) in Eq. (2.10) and simplifying, we get

$$a^2\left(\frac{e^{aR} + e^{-aR}}{e^a + e^{-a}}\right) + \frac{2}{R}a\left(\frac{e^{aR} - e^{-aR}}{e^a + e^{-a}}\right) - \phi^2\left(\frac{e^{aR} - e^{-aR}}{e^a + e^{-a}}\right)^n = 0. \tag{3.13}$$

If $R = 1$, Eq. (3.13) becomes

$$a^2 + 2a - \phi^2 = 0. \tag{3.14}$$

After solving Eq. (3.14), we obtain the value for the parameter a as follows:

$$a = -1 + \sqrt{1 + \phi^2}. \tag{3.15}$$

As a result, an approximate analytical expression for Eq. (2.10) is derived as follows:

$$C(R) = \frac{e^{aR} + e^{-aR}}{e^a + e^{-a}}, \tag{3.16}$$

where a is obtained from the Eq. (3.15).

3.2.2. *For dimensionless concentration $U(X)$ Eq.* (2.13). The approximate analytical expression to Eq. (2.13) which satisfies the boundary condition is given below:

$$u(X) = le^{aX} + me^{-aX}, \tag{3.17}$$

$$\frac{du}{dX} = ale^{aX} - ame^{-aX}. \tag{3.18}$$

We obtain the value of the parameters l and m by employing the boundary condition Eq. (2.14) in Eqs. (3.17) and (3.18).

$$l = m, \quad m = \frac{1}{e^a + e^{-a}}. \tag{3.19}$$

As a result, Eq. (3.17), becomes

$$u(X) = \frac{e^{aX} + e^{-aX}}{e^a + e^{-a}}. \tag{3.20}$$

Now, employing Eq. (3.20) in Eq. (2.13) and simplifying, we get

$$a^2\left(\frac{e^{2aX} + e^{-2aX}}{e^{2a} + e^{-2a}}\right) + \frac{2}{X+1}a\left(\frac{e^{2aX} - e^{-2aX}}{e^{2a} + e^{-2a}}\right) - \frac{\phi^2}{4}\left(\frac{e^{2aX} - e^{-2aX}}{e^{2a} + e^{-2a}}\right)^n = 0. \tag{3.21}$$

If $R = 1$, Eq. (3.21) becomes

$$a^2 + a\left(\frac{e^{2a} - e^{-2a}}{e^{2a} + e^{-2a}}\right) - \frac{\phi^2}{4} = 0. \tag{3.22}$$

After solving Eq. (3.22), we obtain the value for the parameter a as follows:

$$a = 0.1457. \tag{3.23}$$

As a result, the semi-analytical results for Eq. (2.13) are derived as follows:

$$u(X) = \frac{e^{aX} + e^{-aX}}{e^{a} + e^{-a}}, \tag{3.24}$$

where a is obtained from the Eq. (3.23).

3.3. **Approximate analytical expressions for Catalytic Reaction-Diffusion process in a Catalyst Slab.**

3.3.1. *For Dimensionless concentration $Y(X)$ Eq.* (2.23). The approximate analytical expression to Eq. (2.23) which satisfies the boundary condition is given below:

$$Y(X) = le^{aX} + me^{-aX}, \tag{3.25}$$

$$\frac{dY}{dX} = ale^{aX} - ame^{-aX}. \tag{3.26}$$

We obtain the value of the parameters l and m by employing the boundary condition Eq. (2.22) in Eqs. (3.25) and (3.26).

$$l = m, \quad m = \frac{1}{e^{a} + e^{-a}}. \tag{3.27}$$

As a result, Eq. (3.25) becomes

$$Y(X) = \frac{e^{aX} + e^{-aX}}{e^{a} + e^{-a}}. \tag{3.28}$$

Now, employing Eq. (3.28) in Eq. (2.23) and simplifying, we get

$$a^2 \left(\frac{e^{aX} + e^{-aX}}{e^{a} + e^{-a}} \right) - \phi^2 \left(\frac{e^{aX} + e^{-aX}}{e^{a} + e^{-a}} \right)^n = 0. \tag{3.29}$$

If $X = 1$, Eq. (3.29) becomes

$$a^2 - \phi^2 = 0. \tag{3.30}$$

After solving Eq. (3.30), we obtain the value for the parameter a as follows:

$$a = \phi. \tag{3.31}$$

As a result, an approximate analytical expression for Eq. (2.23) is derived as follows:

$$Y(X) = \frac{e^{aX} + e^{-aX}}{e^{a} + e^{-a}}, \tag{3.32}$$

where a is obtained from the Eq. (3.31).

3.3.2. *Basic concepts of the Variational Iteration Method (VIM).* conisder the diferential equation:

$$L[u(x)] + N[u(x)] = g(x), \tag{3.33}$$

where L denotes the linear operator, N represents a non-linear operator and $g(x)$ indicates the given continuous function [27, 28]. We can develop an accurate functional in the following way using the variational iteration method:

Following is a non-linear differential equation is used to help explain the fundamental ideas of the variational iteration technique:

$$u_{n+1}(x) = u_n(x) + \int_0^x \lambda \left[L[u_n \tau] + N\left[u_n^{-}(\tau)\right] - g(\tau) \right] dt, \tag{3.34}$$

where general Lagrange multiplier is represented by λ [27, 28] thereby variational theory allows to be identified best, u_n represents the n^{th} approximate solution along with u_n^- indicates a restricted variation, i.e., $u_n^- = 0$. The Eq. (2.23) can be expressed as follows with the aid of the variation iteration technique mentioned above.

$$y_{m+1}(x) = y_m(x) + \int_0^x \lambda \left((y_m)^{"}(t) - \phi^2 y_0^n(t) \right) dt. \tag{3.35}$$

After considering the previous explanation, we determine that $\lambda = t - x$ and we can set

$$y_0(x) = 3x^3 - 2x^2. \tag{3.36}$$

Consequently, the Eq. (3.35) becomes

$$y_{m+1}(x) = y_m(x) + \int_0^x (t-x) \left((y_m)^{"}(t) - \phi^2 (y_0)^n(t) \right) dt. \tag{3.37}$$

Now, take $m = 0$, Eq. (3.37) becomes,

$$\begin{aligned} y_1(x) &= y_0(x) + \int_0^x (t-x) \left((y_0)^{"}(t) - \phi^2 (y_m)^n(t) \right) \\ &= (3x^3 - 2x^2) + \int_0^x (t-x) \left[(18t - 4) - \phi^2 \left(3t^{3n} - 2t^{2n} \right) \right] dt \\ &= (3x^3 - 2x^2) + \int_0^x \left(18t^2 - 4t - \phi^2 3t^{3n+1} - \phi^2 2t^{2n+1} - 18tx + 4x \right) dt + \int_0^x \left(\phi^2 3t^{3n} + \phi^2 2t^{2n} \right) dt, \\ y_1(x) &= (3x^3 - 2x^2) + \left[\frac{18x^3}{3} - \frac{4x^2}{2} - \phi^2 \frac{3x^{3n+2}}{3n+2} - \phi^2 \frac{2x^{2n+2}}{2n+2} - \frac{18x^3}{2} + 4x^2 \right] + \phi^2 \frac{3x^{3n+2}}{3n+1} + \phi^2 \frac{2x^{2n+2}}{2n+1}. \end{aligned}$$

By using Eqs. (3.36) and (3.38), we get

$$y(x) = (3x^3 - 2x^2) + \left[\frac{18x^3}{3} - \frac{4x^2}{2} - \phi^2 \frac{3x^{3n+2}}{3n+2} - \phi^2 \frac{2x^{2n+2}}{2n+2} - \frac{18x^3}{2} + 4x^2 \right] + \phi^2 \frac{3x^{3n+2}}{3n+1} + \phi^2 \frac{2x^{2n+2}}{2n+1}. \tag{3.38}$$

3.3.3. *For Dimensionless concentration $Y(X)$ Eq.* (2.24). The approximate analytical expression to Eq. (2.24) which satisfies the boundary condition is shown below:

$$Y(X) = Le^{AX} + Me^{-AX}, \tag{3.39}$$

$$\frac{dY}{dX} = ALe^{AX} - AMe^{-AX}. \tag{3.40}$$

We obtain the value of the parameters L and M by employing the boundary condition Eq. (2.22) in Eqs. (3.39) and (3.40).

$$L = M, \quad M = \frac{1}{e^A + e^{-A}}. \tag{3.41}$$

As a result, Eq. (3.39), becomes

$$Y(X) = \frac{e^{AX} + e^{-AX}}{e^A + e^{-A}}. \tag{3.42}$$

Now, employing Eq. (3.42) in Eq. (2.24) and simplifying, we get

$$A^2 \left(\frac{e^{AX} + e^{-AX}}{e^A + e^{-A}} \right) - \frac{\phi^2 \left(\frac{e^{AX} + e^{-AX}}{e^A + e^{-A}} \right)}{1 + K \left(\frac{e^{AX} + e^{-AX}}{e^A + e^{-A}} \right)} = 0. \tag{3.43}$$

If $X = 1$, Eq. (3.43) becomes

$$A^2 - \frac{\phi^2}{1+K} = 0. \tag{3.44}$$

After solving Eq. (3.44), we obtain the value for the parameter A as follows:

$$A = \frac{\phi}{\sqrt{1+K}}. \tag{3.45}$$

As a result, an approximate analytical expression for Eq. (2.24) is derived as follows:

$$Y(X) = \frac{e^{AX} + e^{-AX}}{e^{A} + e^{-A}}, \tag{3.46}$$

where A is obtained form the Eq. (3.45).

Effectivenss factor for Eq. (2.25) as follows:

$$\eta = \frac{\phi\left(e^{\frac{2\phi}{\sqrt{1+K}}} - 1\right)}{\sqrt{1+K}\left(e^{\frac{2\phi}{\sqrt{1+K}}} + 1\right)}. \tag{3.47}$$

4. Numerical simulation

The Ananthaswamy-Sivasankari method (ASM) was used to provide approximate analytical results for the non-dimensional concentration of a spherical porous catalyst in steady-state. Figures 1-18 depict the outcomes of the semi-analytical results as well as the numerical simulation obtained with MATLAB. Appendix A has the MATLAB programming for Eq. (2.4), Appendix B contains the programming for Eq. (2.10), Appendix C gives the programming for Eq. (2.13), and Appendix D provides the programming for Eq. (2.24).

5. Results and Discussions

The semi-analytical outcomes corresponding to the non-dimensional concentration for the spherical porous catalyst in steady-state are provided in subsections 3.1, 3.2, and 3.3 employing the Ananthaswamy-Sivasankari technique. Moreover, the variational iteration technique is used to solve Eq. (2.23) as given in subsubsection 3.3.2.

For Reaction-Diffusion model in Porous Catalysts: Figures 1 to 6 plots the non-dimensional concentration $\theta(\chi)$ versus the non-dimensional distance χ by employing Eq. (3.8). Figures 1, 3, and 5 indicate that as the amount of the characteristic reaction rate β grows, so does the non-dimensional concentration. Figures 2, 4, and 6 show that as the concentration of half-saturation α increases, so does the non-dimensional concentration.

For Reaction-Diffusion Model in Spherical Catalysts pellet: Figures 7 and 8 depict the non-dimensional concentration $C(R)$ with the non-dimensional distance R utilizing Eq. (3.16). Figures 7 and 8 illustrates that when the values of the Thiele modulus ϕ^2 grow, the non-dimensional concentration drops. Figures 9 and 10 depicts the non-dimensional concentration $u(x)$ against the non-dimensional distance x with Eq. (3.24). Figures 9 and 10 portays that by raising the amount of Thiele modulus ϕ, the non-dimensional concentration falls.

For Catalytic Reaction-Diffusion process in a catalyst slab: Figures 11 - 14 illustrate that the non-dimensional concentration $Y(X)$ against the non-dimensional distance X by using Eqs. (3.34) and (3.38). As seen in Figures 11 - 13, as the amounts of the Thiele modulus ϕ grow, the non-dimensional concentration drops. Figure 14 illustrates that as the Thiele modulus ϕ grows, so does the non-dimensional concentration. Figures 15 and 16 represents the non-dimensional concentration versus the non-dimensional distance using Eq. (3.46). Figure 15 demonstrates that by raising the parameters value of Thiele modulus ϕ, the non-dimensional concentration diminishes. Figure 16 depicts that when the parameters of Langmuir-Hinshelwood kinetics K grow, so does the non-dimensional concentration.

For Effectiveness factor: Figure 17 exhibits that Effectiveness factor η with the Langmuir Hinshelwood kinetics K using Eq. (3.47). It demonstrates that as the values of the Thiele modulus ϕ rise, so does the effectiveness factor. Figure 18 indicates that Effectiveness factor η against the Thiele modulus ϕ utilizing Eq. (3.47). It is obvious that when the amount of Hinshelwood kinetics K grows, the effectiveness factor falls.

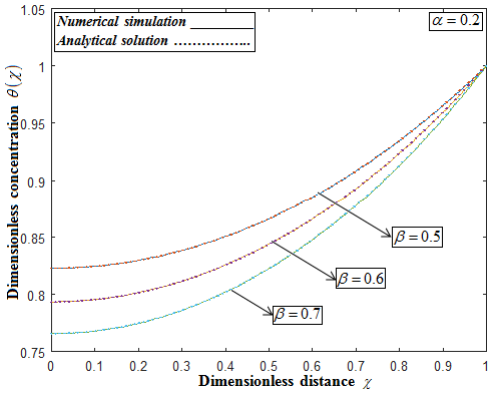

FIGURE 1. Effect of characteristic reaction rate β in non-dimensional concentration $\theta(\chi)$ by utilizing Eq. (3.8).

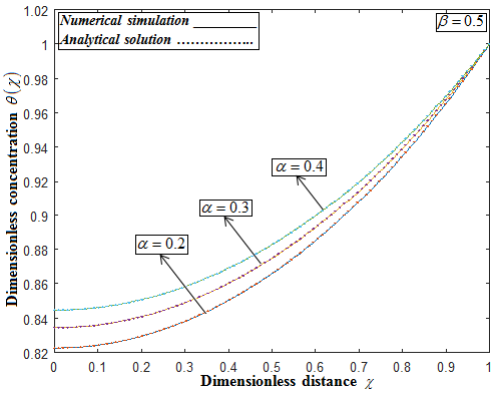

FIGURE 2. Impact of concentration of half saturation α in non-dimensional concentration $\theta(\chi)$ by using Eq. (3.8).

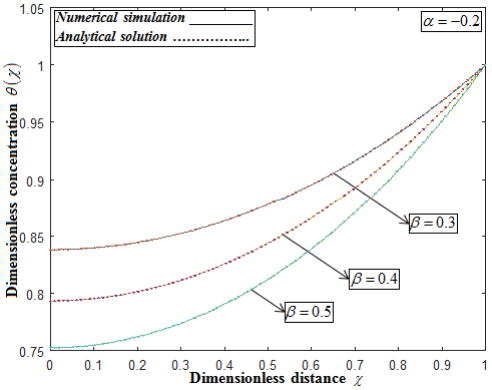

FIGURE 3. Variation of characteristic reaction rate β in non-dimensional concentration $\theta(\chi)$ by employing eqn. Eq. (3.8).

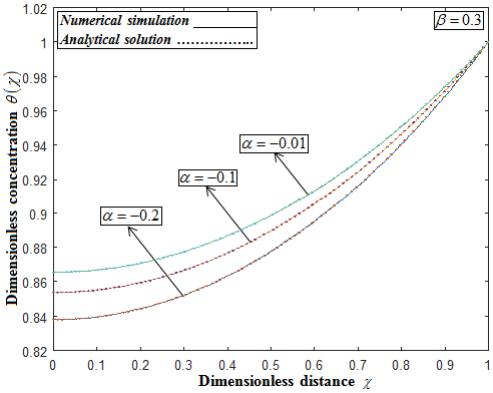

FIGURE 4. Influence of concentration of half saturation α in non-dimensional concentration $\theta(\chi)$ by utilizing Eq. (3.8).

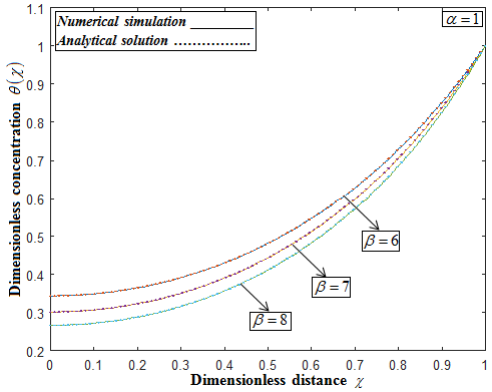

FIGURE 5. Effect of characteristic reaction rate β in non-dimensional concentration $\theta(\chi)$ by using Eq. (3.8).

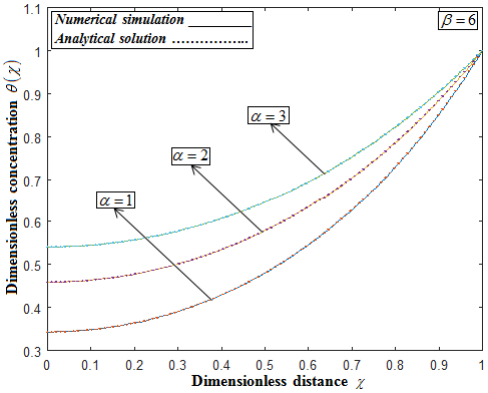

FIGURE 6. Impact of concentration for half saturation α in non-dimensional concentration $\theta(\chi)$ by employing Eq. (3.8).

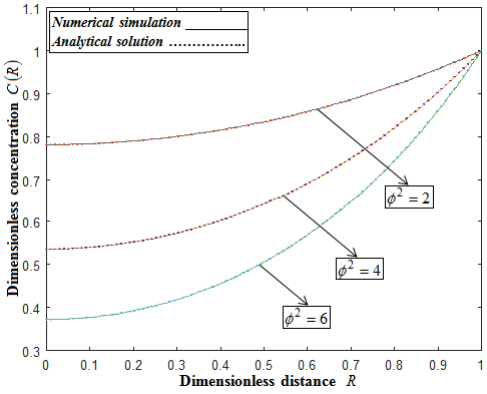

FIGURE 7. Variation of Thiele modulus ϕ^2in non-dimensional concentration $C(R)$ by utilizing Eq. (3.16).

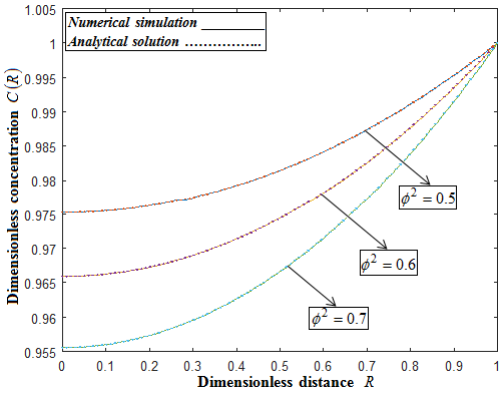

FIGURE 8. Influence of Thiele modulus ϕ^2 in non-dimensional concentration $C(R)$ by using Eq. (3.16).

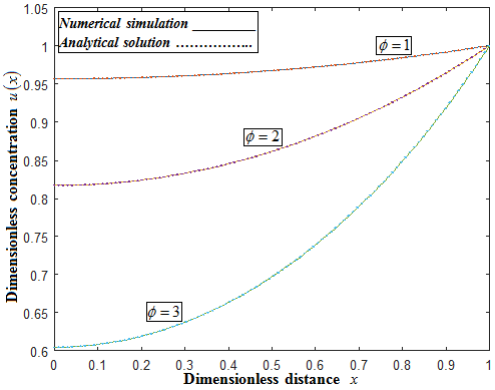

FIGURE 9. Effect of Thiele modulus ϕ in non-dimensional concentration $u(x)$ by employing Eq. (3.24).

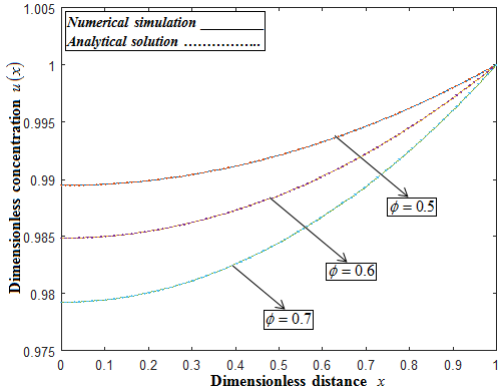

FIGURE 10. Impact of Thiele modulus ϕ in non-dimensional concentration $u(x)$ by utilizing Eq. (3.24).

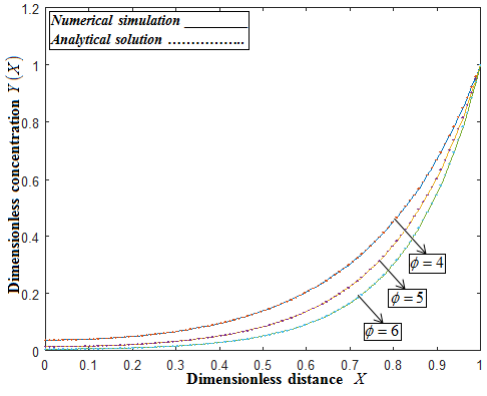

FIGURE 11. Variation of Thiele modulus ϕ in non-dimensional concentration $Y(X)$ by employing Eq. (3.32).

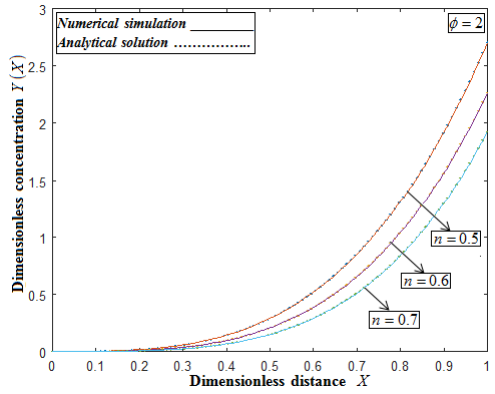

FIGURE 12. Impact of reaction order n in non-dimensional concentration $Y(X)$ by using Eq. (3.38).

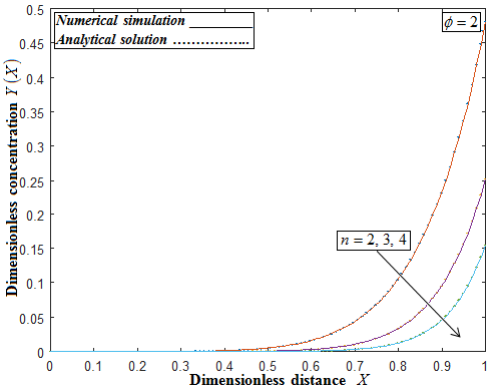

FIGURE 13. Influence of reaction order n in non-dimensional concentration $Y(X)$ by utilizing Eq. (3.38).

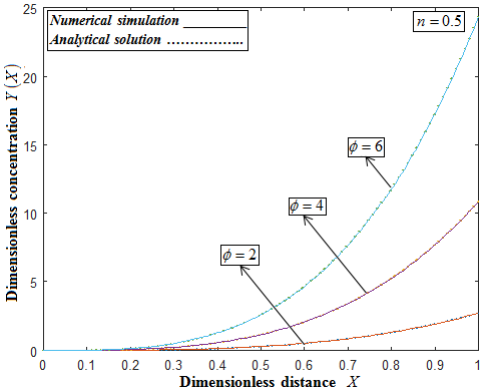

FIGURE 14. Effect of Thiele modulus ϕ in non-dimensional concentration $Y(X)$ by using Eq. (3.38).

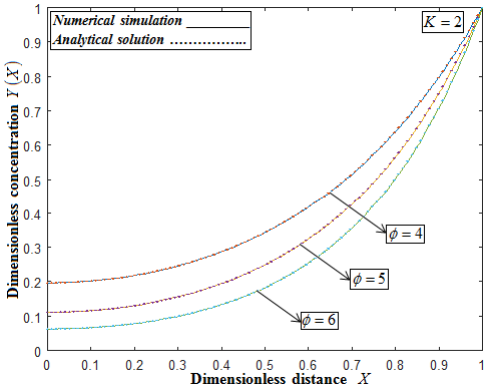

FIGURE 15. Influence of Thiele modulus ϕ in non-dimensional concentration $Y(X)$ by employing Eq. (3.46).

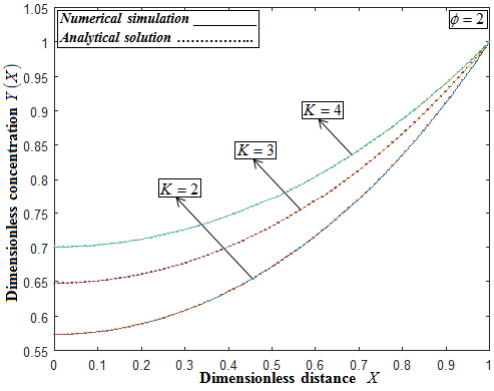

FIGURE 16. Effect of Langmuir-Hinshelwood kinetics K in non-dimensional concentration $Y(X)$ by utilizing Eq. (3.46).

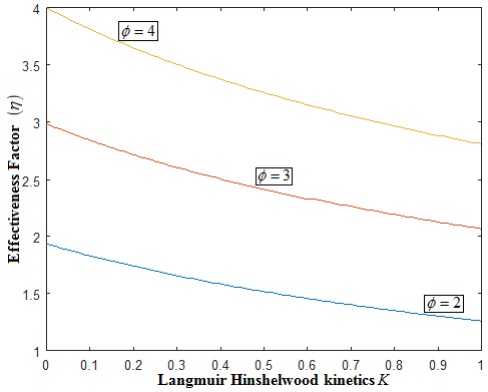

FIGURE 17. Impact of Thiele modulus ϕ in Effectiveness factor (η) by using Eq. (3.47).

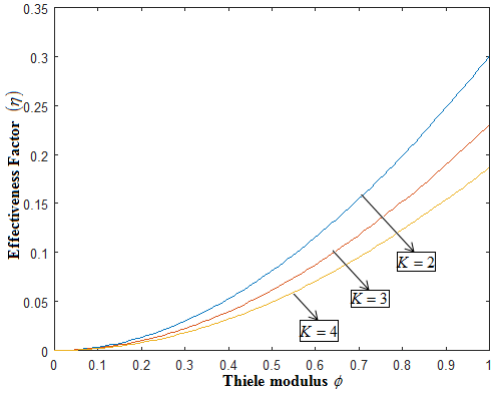

FIGURE 18. Variation of Langmuir-Hinshelwood K kinetics in Effectiveness factor (η) by employing Eq. (3.47).

6. Conclusion

The non-linear boundary value issue describing reaction-diffusion in an idealized spherical porous catalyst was investigated. The Ananthaswamy- Sivasankari method (ASM) was used for all models, which considerably improved the efficiency of computation with overcoming the pellets difficulty. The findings were in excellent agreement together with the numerical simulation for all parameter values. The results obtained by the Ananthaswamy-Sivasankari technique were more accurate and closely resembled the results of the numerical simulation. The subsequent conclusions were arrived:

- Effectiveness factor (η) rises by raising the Thiele modulus.
- Effectiveness factor (η) drops by raising the Langmuir-Hinshelwood kinetics K.

Appendix A: MATLAB programming for non-linear Reaction-diffusion model within the Porous catalysts Eq. (2.4)

$functionpdex4$
$m = 0;$
$x = linspace(0, 1);$
$t = linspace(0, 10000);$
$sol = pdepe(m, @pdex4pde, @pdex4ic, @pdex4bc, x, t);$
$u1 = sol(:, :, 1);$
$figure$
$plot(x, u1(end, :))$
$title('u1(x, t)')$
$xlabel('Distancex')$
$ylabel('u1(x, 2)')$
$function[c, f, s] = pdex4pde(x, t, u, DuDx)$
$c = 1;$
$f = DuDx;$
$b = 0.5;$
$a = 0.2$
$F = -b * u(1)/(a + u(1));$
$s = F;$
$functionu0 = pdex4ic(x);$
$u0 = 1;$
$function[pl, ql, pr, qr] = pdex4bc(xl, ul, xr, ur, t)$
$pl = 0;$
$ql = 1;$
$pr = ur - 1;$
$qr = 0;$

Appendix B: MATLAB programming for non-linear Reaction-Diffusion (R-D) model inside Spherical Catalysts Pellet Eq. (2.10)

$functionpdex4$
$m = 2;$
$x = linspace(0, 1);$
$t = linspace(0, 1);$
$sol = pdepe(m, @pdex4pde, @pdex4ic, @pdex4bc, x, t);$
$u1 = sol(:, :, 1);$
$figure$
$plot(x, u1(end, :))$
$title('u1(x, t)')$
$xlabel('distancex')$

```
ylabel('u1(x,1)')
function[c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = 1.*DuDx;
p = sqrt(2);
F = -p^2*u(1);
s = F;
functionu0 = pdex4ic(x);
u0 = 0;
function[pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = ur(1) - 1;
qr = 0;
```

Appendix C: MATLAB programming for non-linear Reaction-Diffusion (R-D) model inside Spherical Catalysts Pellet Eq. (2.13)

```
functionpdex4
m = 2;
x = linspace(0,1);
t = linspace(0,1);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('distancex')
ylabel('u1(x,1)')
function[c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = 1.*DuDx;
p = 3.63;
F1 = -((p^2)/4)*u(1);
s = F1;
functionu0 = pdex4ic(x);
u0 = 0;
function[pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = ur(1) - 1;
qr = 0;
```

Appendix D: MATLAB programming for non-linear Reaction-Diffusion process in Catalyst Slab Eq. (2.24)

```
functionpdex4
m = 0;
x = linspace(0,1);
t = linspace(0,100);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
```

$u1 = sol(:,:,1);$
$figure$
$plot(x, u1(end,:))$
$title('Solutionatt = 2')$
$xlabel('Distancex')$
$ylabel('u1(x,2)')$
$function[c, f, s] = pdex4pde(x, t, u, DuDx)$
$c = 1;$
$phi = 2;$
$K = 3;$
$f = 1. * DuDx;$
$F = -(phi)^2 * u(1)/(1 + (K * u(1)));$
$s = F;$
$functionu0 = pdex4ic(x)$
$u0 = 1;$
$function[pl, ql, pr, qr] = pdex4bc(xl, ul, xr, ur, t)$
$pl = 0;$
$ql = 1;$
$pr = ur(1) - 1;$
$qr = 0;$

Symbol	Meaning
V	Advective velocity
$r(\theta)$	Reaction process
$\hat{D}$	Diffusivity parameter
P	Peclet number
α	Concentration of half saturation
β	Characteristic reaction rate
θ	Dimensionless concentration
χ	Dimensionless distance
c	Reactant concentration
c_s	Surface concentration
C	Dimensionless concentration
C_0	Dimensionless concentration in the center of the pellet
D_e	Effective diffusion coefficient
r	Radial coordinate
r_0	Radius of the pellet
k_v	Reaction rate constant
n	Reaction order
R	Dimensionless radial coordinate
ϕ	Thiele modulus
u	Dimensionless concentration
x	Dimensionless distance
Y	Dimensionless concentration
X	Dimensionless distance
L	Constant along the pore length
C_A	Concentration of reactant A
C_{AS}	Concentration of reactant A at the pore mouth
r_A	Reaction rate of species A
r_{AS}	Reaction rate of species A at catalyst surface
D_e	Diffusion constant of reactant inside the pore
r_y	Dimensionless reaction rate
K	Dimensionless constant in Langmuir-Hinshelwood kinetics
K_1, K_2	Constants in Langmuir-Hinshelwood kinetics
k_n	n^{th}order reaction rate constant
η	Effectiveness factor

Appendix E: Nomenclature.

Conflict of interests

The authors declare that there is no conflict of interests.

Acknowledgement

The authors are very grateful to the reviewers for carefully reading the paper and for their comments and suggestions which have improved the paper. Also, the authors are thankful to Sri. S. Natanagopal, Secretary, The Madura College Board, Dr. J. Suresh, The Principal, The Madura College and Dr. S. Muthukumar, Head of the Department, The Madura College, Madurai, Tamil Nadu, India for their constant support to our research work.

References

[1] S. Abbasbandy, *Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by means of the homotopy analysis method*, Chemical Engineering Journal., *136*(2-3) (2008), 144-150.

[2] S. Abbasbandy, E. Magyari, and E. Shivanian, *The homotopy analysis method for multiple solutions of nonlinear boundary value problems*, Communications in Nonlinear Science and Numerical Simulation., *14*(9-10) (2009), 3530-3536.

[3] I. Ahmad, H. Ilyas, and A. Urooj, *Novel applications of intelligent computing paradigms for the analysis of nonlinear reactive transport model of the fluid in soft tissues and microvessels*, Neural Computing and Applications., *31*(2) (2019), 9041-9059.

[4] V. Ananthaswamy and L. Rajendran, *Approximate analytical solution of non-linear kinetic equation in a porous pellet*, International Journal of Modern Global Journal of pure and applied mathematics., *8*(2) (2012), 101-111.

[5] V. Ananthaswamy, V. Vijayalakshmi, J. Anantha Jothi, and S. Sivasundaram, *A mathematical analysis of transport and kinetics in electrocatalytic thin film biosensors with non-Michaelis-Menten kinetics*, Mathematics in Engineering, Science and Aerospace (MESA)., *14*(2) (2022), 633-648.

[6] J. Chitra, V. Ananthaswamy, S. Sivasankari, and S. Sivasundaram, *A new approximate analytical method (ASM) for solving non-linear boundary value problem in heat transfer through porous fin*, Mathematics in Engineering, Science and Aerospace (MESA)., *14*(1) (2023), 841-859.

[7] M.Danish, S. Kumar, and S. Kumar, *Revisiting reaction-diffusion process in a porous catalyst: improving the Adomian solution*, Chemical Product and Process Modeling., *5*(1) (2010).

[8] A. J. Ellery and M. J. Simpson, *An analytical method to solve a general class of nonlinear reactive transport models*, Chemical engineering journal., *169*(1-3) (2011), 313-318.

[9] D. Flockerzi and K. Sundmacher, *On coupled Lane-Emden equations arising in dusty fluid models*, In Journal of physics: conference series., *268*(1) (2011), 01200.

[10] A. H. Ganie, I. U. Rahman, M. Sulaiman, and K. Nonlaopon, *Solution of nonlinear reaction-diffusion model in porous catalysts arising in micro-vessel and soft tissue using a metaheuristic*, IEEE Access., *10* (2022), 41813-41827.

[11] A. H. Hadian-Rasanan, D. Rahmati, S. Gorgin, and K. Parand *A single layer fractional orthogonal neural network for solving various types of LaneEmden equation*, New Astronomy., *75* (2020), 101307.

[12] D. Lesnic, *A nonlinear reactiondiffusion process using the Adomian decomposition method*, International Communications in Heat and Mass Transfer., *34*(2) (20079), 129-135.

[13] E. Magyari, *Exact analytical solutions of diffusion reaction in spherical porous catalyst*, Chemical Engineering Journal., *17*(2) (2010), 266-270.

[14] E. Mohammadia and E. Shivaniana, *A hybrid method of successive linearization method (SLM) and collocation method to steady regime of the reaction-diffusion equation*, Computational Mathematics and Computer Modeling with Application., *1*(2) (2022), 1-7.

[15] R. J. Moitsheki, T. Hayat, M. Y. Malik, and F. M. Mahomed, *Symmetry analysis for the nonlinear model of diffusion and reaction in porous catalysts*, Nonlinear Analysis: Real World Applications., *11*(4) (2010), 3031-3036.

[16] K. Parand, A. Ghaderi-Kangavari, and M. Delkosh, *Two efficient computational algorithms to solve the nonlinear singular Lane-Emden equations*, T. Astrophysics., *63* (2020), 133-150.

[17] K. Paranda and M. Delkhosha, *An effective numerical method for solving the nonlinear singular Lane-Emden type equations of various orders*, Currents., *5*(6) (2017).

[18] R. Rach, J. S. Duan, and A. M. Wazwaz, *On the solution of non-isothermal reaction-diffusion model equations in a spherical catalyst by the modified Adomian method*, Chemical Engineering Communications., *202*(8) (2015), 1081-1088.

[19] P. Regnier, P. Jourabchi, and C. P. Slomp, *Reactive-transport modeling as a technique for understanding coupled biogeochemical processes in surface and subsurface environments*, Netherlands Journal of Geosciences., *82*(1) (2003).

[20] E. Shivanian, *On the multiplicity of solutions of the nonlinear reactive transport model*, Ain Shams Engineering Journal., *5*(2) (2014), 637-645.

[21] S. Sivasankari, V. Ananthaswamy, and S. Sivasundaram, *A new approximate analytical method for solving some non-linear initial value problems in physical sciences*, Mathematics in Engineering Science and Aerospace (MESA).,

14(1) (2023).

[22] C. I. Steefel, D. J. DePaolo, and P. C. Lichtner, *Reactive transport modeling: An essential tool and a new research approach for the Earth sciences*, Earth and Planetary Science Letters., *240*(3-4) (2005), 539-558.

[23] R. R. Subanya, V. Ananthaswamy, and S. Sivasundarama, *Semi analytical expressions of a non-linear boundary value problem for immobilized enzyme in porous planar, cylindrical and spherical*, Nonlinear Studies., *30*(1) (2023).

[24] F. J. Valdes-Parada, M. Sales-Cruz, J. A. Ochoa-Tapia, and J. Alvarez-Ramirez, *On Greens function methods to solve nonlinear reactiondiffusion systems*, Computers and Chemical Engineering., *32*(3) (2008), 503-511.

[25] V. Vijayalakshmi, V. Ananthaswamy, and J. Anantha Jothi, *Semi-Analytical Study on Non-Isothermal Steady RD Equation in a Spherical Catalyst and Biocatalyst*, CFD Letters., *15*(12) (2023), 60-76.

[26] H. Vosoughi, E. Shivanian, and S. Abbasbandy, *Unique and multiple PHAM series solutions of a class of nonlinear reactive transport model*, Numerical Algorithms., *61* (2012), 515-52.

[27] A. M. Wazwaz, *The variational iteration method for analytic treatment for linear and nonlinear ODEs*, Applied Mathematics and Computation.., *212*(1) (2009), 120-134.

[28] A. M. Wazwaz, *The variational iteration method for solving linear and nonlinear ODEs and scientific models with variable coefficients*, Central European Journal of Engineering., *4* (2014), 64-7.

[29] A. M. Wazwaz, R. Rach, and J. S. Duan, *A study on the systems of the Volterra integral forms of the LaneEmden equations by the Adomian decomposition method*, Mathematical Methods in the Applied Sciences., *37*(1) (2014), 10–19.