

# Semi- Analytical Study on Non-Isothermal Steady R-D Equation in a Spherical Catalyst and Biocatalyst

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ARTICLE INFO	ABSTRACT
<b>Article history:</b> Received 3 May 2023 Received in revised form 5 June 2023 Accepted 8 July 2023 Available online 1 December 2023	The Lane-Emden Boundary Value Problem as it appears in chemical applications, science, and biochemical applications are employed. Two specific models are solved by applying the Ananthaswamy-Sivasankari method (ASM). The model in first problem is a reaction–diffusion equation of a spherical catalyst and the model in second problem is the reaction–diffusion process of a spherical biocatalyst. Obtain a reliable semi-analytical expression of the effectiveness factors and the concentrations. A graph is constructed for the obtained semi-analytical solutions. The effects of several parameters like dimensionless activation energy, Thiele modulus and dimensionless heat of reaction are shown in graphical representation. Our semi-analytical solution is compared with numerical simulation by using MATLAB and finds good fit in all parameters. The new analytical method ASM is helpful to solve many non-linear problems mainly Reaction-Diffusion equation.
<i>Keywords:</i> Lane–Emden equation; Spherical catalyst; Spherical biocatalyst; Ananthaswamy-Sivasankari method; Michaelis–Menten kinetics; Numerical simulation	

#### 1. Introduction

The Lane–Emden equation in Ref. [1-6] for shape factor  $\alpha$  has the form

$$y''(x) + \frac{\alpha}{x}y'(x) + f(y(x)) = 0, \alpha > 0$$
 (1)

The Lane–Emden equation is a basic equation in the theory of stellar structure of the shape factor for  $\alpha = 2$ , i.e., signifying spherical bodies. These equation also describes the changes in temperature or concentration in physics, chemistry, biology, biochemistry, and many others domains in Ref. [1-9]. The singular behaviour that occurs at x=0 gives the main difficulty for solving Eq. (1). Several numerical and analytical methods are utilized to solve Lane Emden equations with boundary conditions referred in Ref. [7, 10-20].

The Lane–Emden equation was first designed by astrophysicists Robert Emden and Jonathan Homer Lane and examined the behaviour of thermal in the spherical gas clouds dealing under the

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common attractiveness of molecules and obeying the classical laws of thermodynamics of Richardson *et al.*, [21]. The well–known Lane–Emden Equation is used to design more phenomena in astrophysics and mathematical physics, such as stellar structure theory, thermal behaviour of spherical gas clouds, isothermal gas spheres, and thermionic current theory. A significant amount of work has been done on these types of problems for various structures by previous studies [20-28]. A system of the Lane–Emden Equations emerge in the several model of phenomena in physical like the population evolution, pattern formation, chemical reactions, and others [29-32]. Lane-Emden Equations were solved numerically by Allayed *et al.*, [44] and analytically by Omaha [45].

In this article, we will first consider a single reaction that occurs non-isothermally on a spherical catalysts pellet. The concentration of chemical particles in a spherical catalyst is characterized by the Boundary Value Problem to the Lane–Emden Equation in Ref. [20, 33-35]. In addition, we will study reactions that proceed non-isothermally in spherical biocatalyst. Most chemical reactions take place inside the catalyst pellet, which are porous material by Saadatmandi [36]. We assume that the biochemical reaction follow Michaelis-Menten kinetics. Appropriate plots are used to illustrate the surprisingly high accuracy and fast convergence of our approximate solutions, while noting that an exact solution is almost always impossible to obtain. The recommended analysis indicates the reliability and is easily extended to more common in reaction-diffusion models in chemical reactor technology by Rach *et al.*, [4]. Also, Skrzypacz *et al.*, [50] and Golman *et al.*, [51] solved reaction-diffusion problems by using semi-analytical methods. The brief explanation of analytical and numerical simulation was explained by Crasta *et al.*, [52].

The major purpose of this study is to use ASM to obtain a semi- analytical solution of the nonisothermal steady Reaction-Diffusion (R-D) equation in a spherical catalyst and spherical biocatalyst. Now a days, researchers are solving this types of problems and provides solutions in implicit manner but our analytical findings offers solution in explicit form. As compared to several numerical methods and semi-analytical methods, this method requires a single iteration. The solution of semi-analytical and numerical simulation are then compared and showed in graphically. To interlined the effects of several parameters such as dimensionless activation energy, Thiele modulus and dimensionless heat of reaction. Also, the effectiveness factor is calculated by using ASM.

## 2. Mathematical Formulation of the Problems

## 2.1 Mathematical Model of Spherical Catalyst Equation

Several industrial reactors incorporate the heterogeneous reaction kinetics of packed catalyst pellets. A single catalytic pellet of radius R can be treated as a porous medium through which reactants occur simultaneously.

The species and energy balances for diffusive transport inside the pellet can be written as follows (Rach *et al.,* [46]):

$$D\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}C_A\right) + r_A = 0$$

$$= 0$$

$$= 1 \frac{1}{d}\left(r^2\frac{d}{dr}C_A\right) + r_A = 0$$
(2)

$$K\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}T\right) + r_A\Delta H = 0 \tag{3}$$

where the Arrhenius reaction rate of the temperature internal to the catalytic pellet is

$$r_A = k_{ref} C_A \exp\left[\frac{-E}{R_g} \left(\frac{1}{T} - \frac{1}{T_S}\right)\right]$$
(4)

The boundary conditions are:

$$C_A|_{r=R} = C_{AS} \tag{5}$$

i.e., physically the steady-state values at the surface are known and there is zero flux at the origin.

We assume that a first-order irreversible reaction takes place within the catalytic particle, the Heat of reaction  $\Delta H$ , effective diffusivity D and effective thermal conductivity K are constants, no external resistance to mass and heat transfer exists and the reaction is exothermic.

From Eq. (2) and (3):

$$K\frac{d}{dr}\left(r^{2}\frac{d}{dr}T\right) = \Delta HD\frac{d}{dr}\left(r^{2}\frac{d}{dr}C_{A}\right)$$
(8)

Applying the integral operator  $\int_{R}^{r} \int_{0}^{r} (.) dr dr$  to both sides of Eq. (8) and using the boundary conditions in Eq. (5)-(7) provides:

$$T - T_S = \frac{(-\Delta H)D}{K} (C_{AS} - C_A)$$
(9)

Substituting Eq. (9) into Eq. (4), we obtain the Arrhenius reaction rate in terms of the reactant concentration internal to the catalytic pellet.

$$r_{A} = -k_{ref}C_{A} \exp\left[\frac{E}{R_{g}T_{S}} \frac{\frac{(-\Delta H)DC_{AS}}{KT_{S}} \left(1 - \frac{C_{A}}{C_{AS}}\right)}{1 + \frac{(-\Delta H)DC_{AS}}{KT_{S}} \left(1 - \frac{C_{A}}{C_{AS}}\right)}\right]$$
(10)

Substituting Eq. (10) into Eq. (2) and introducing the following dimensionless variables and parameters [3, 36, 38-41, 47].

$$x = \frac{r}{R}, u = \frac{C_A}{C_{AS}}, \gamma = \frac{E}{R_g T_a}, \beta = \frac{(-\Delta H)DC_{AS}}{KT_S}, \varphi^2 = \frac{k_{ref}R^2}{D},$$
(11)

where x represents the dimensionless concentration along radial direction of catalytic pellet, rdenotes the distance along radial direction of catalytic pellet, R indicates the Radius of the spherical catalytic pellet, u represents the dimensionless concentration along radial direction of catalytic pellet,  $C_A$  is the concentration of reactant Ainside the catalytic pellet,  $C_{AS}$  is the concentration of reactant A at the surface of catalytic pellet,  $\gamma$  is the dimensionless activation energy, E represents the activation energy,  $R_g$  indicates the universal gas constant,  $T_a$  is the temperature inside the catalytic pellet,  $T_S$  is the temperature at the surface of catalytic pellet,  $\beta$  is the dimensionless heat of reaction,  $\Delta H$  is the heat of reaction, D is the effective diffusivity inside the catalytic pellet, K is the effective thermal conductivity inside the catalytic pellet,  $\varphi$  is the Thiele modulus,  $k_{ref}$  is the reference reaction constant.

. . .

Rach *et al.*, [3], and in some of the references therein, we obtained the Lane-Emden BVP for the normalized concentration u(x) as (Rancher Singh [37]). Which models the dimensionless concentration of chemical species within a spherical catalyst. In Eq. (12),  $\gamma$  indicates the Dimensionless activation energy,  $\beta$  denotes the Dimensionless heat of reaction, and  $\varphi$  represents the Thiele modulus as calculated at the surface of the spherical catalytic pellet by Rich *et al.*, [3]

$$u''(x) + \frac{2}{x}u'(x) - \varphi^2 u(x) \exp\left[\frac{\gamma\beta(1 - u(x))}{1 + \beta(1 - u(x))}\right] = 0$$
(12)

$$u'(0) = 0, u(1) = 1 \tag{13}$$

The effectiveness factor  $\eta$  for a spherical pellet [20, 33-35] is defined as:

$$\eta = \frac{3}{\varphi^2} \frac{du}{dx} \Big|_{x=1}$$
(14)

# 2.2 Mathematical Model Spherical Biocatalyst Equation

We consider an inert permeable spherical solid particle. Bacterial immobilization has been made inside the permeable particle by usual methods and this permeable particle with bacteria immobilized inside it is termed as biocatalyst. This biocatalyst is immersed in a pool of liquid containing the substrate. It is further assumed that the resistance due to film surrounding the biocatalyst is negligibly small under the operating conditions in the bioreactor. Thus, the substrate (A) diffuses inside biocatalyst and the biochemical reaction occurs therein simultaneously. The application of mass balance for the substrate (A) over a thin spherical shell inside the biocatalyst yields the following model equation along with the coupled BCs (boundary conditions) (Danish *et al.*, [48]):

$$D_e\left(\frac{d^2C_A}{dr^2} + \frac{2}{r}\frac{dC_A}{dr}\right) = \frac{r_mC_A}{K_m + C_A}$$
(15)

The respective boundary conditions are given as:

$$C_A = C_{AS} \text{ at } r = R \text{ (catalyst surface)}$$
(16)  

$$\frac{dC_A}{dr} = 0 \text{ at } r = 0 \text{ (centre of the catalyst)}$$
(17)

While deriving this model equation it is assumed that the biochemical reaction follows Michaelis-Menten kinetics. The details of derivation of Eq. (15) to Eq. (17) may be found in an excellent text book by Fouler [49]. Introducing the following dimensionless variables [3, 38-41].

$$x = \frac{r}{R}, u = \frac{C_A}{C_{AS}}, \beta = \frac{C_{AS}}{K_m}, \varphi^2 = \frac{-r_{AS}R^2}{D_e C_{AS}} = \frac{R^2 r_m}{D_e K_m (1+\beta)},$$
(18)

Where  $\varphi$  denotes the Thiele modulus and  $\varphi^2$  signifies the ratio of the intrinsic chemical reaction rate in the absence of mass transfer limitation to the rate of diffusion through the catalyst, i.e

$$\varphi^{2} = \frac{reaction rate at the catalyst surface}{diffusion rate through the catalyst pores}$$
(19)

Saadatmandi [36] was demonstrated that the spherical biocatalyst equation was organized by the Lane- Emden Boundary Value Problem for the normalized concentration u(x) as (Randhir Singh [37]). Eq. (15) to Eq. (17) becomes:

$$u''(x) + \frac{2}{x}u'(x) - \varphi^2 \frac{(1+\beta)u(x)}{1+\beta u(x)} = 0,$$
(20)

u'(0) = 0, (Center of the catalyst) (21) (22)

u(1) = 1, (Catalyst surface)

which models the dimensionless concentration of chemical species in the spherical biocatalyst.

In Eq. (20),  $\beta$  defines the dimensionless heat of reaction, and  $\varphi$  notes the Thiele modulus as estimated at the surface of the spherical catalytic pellet in Ref. [3, 38-41].

The effectiveness factor  $\eta$  for a spherical pellet in Ref. [20, 33-36, 38-41] is defined as:

$$\eta = \frac{3}{\varphi^2} \frac{du}{dx} \Big|_{x=1}$$
(23)

As mentioned above, we use the new approximate analytical method called Ananthaswamy-Sivasankari method (ASM) is utilized to solve the two models of Eqs. (12) and (20).

# 3. Approximate Analytical Expression for Eqs. (12) and (20) by using ASM

A new approach called Ananthaswamy-Sivasankari method (ASM) is demonstrated for the calculation of the second order non-linear ordinary differential equations. It also used to the solve differential equations for both linear and non-linear. This technique is also easily elongated to address several additional non-linear problems in the chemical, biological sciences and physical. However, the presented new technique is applicable to boundary value issues. Additional boundary conditions for the differential equation and its derivatives can be constructed. Section (a) explains the basic concept of ASM.

(a) Basic concept of Ananthaswamy-Sivasankari Method (ASM) (Chitra et al., [42]; Sivasankari et al., [43])

Consider first the non-linear boundary value problem

$$q: f(y, y', y'') = 0$$
(24)

Where q represents the second order non-linear differential equation such that y = y(x, c, d, ...) in which c, d are given parameters and at  $x = x_0$  can be finite with the following boundary conditions:

$$Atx = x_0 y(x) = y_\alpha(or)y'(x) = y_\beta$$
<sup>(25)</sup>

Assume that the approximate analytical solution for the non-linear equation is an exponential function of the form:

$$y(x) = le^{ax} + me^{-ax}$$

The unknown coefficients l and m are obtained by solving the non-linear differential equations as follows:

$$y(x) = le^{a\alpha} + me^{-a\alpha} = y_{\alpha}$$

$$y'(x) = le^{a\beta} - me^{-a\beta} = y_{\beta}$$
(27)
(28)

Eqs. (27) and (28) may be used to get the unknown parameters l and m.

The following non-linear differential equations are obtained by substituting an Eq. (26) into the Eq. (24)

$$q: f(y(x, l, m, a, c, d), y'(x, l, m, a, c, d), y''(x, l, m, a, c, d)) = 0$$
(29)

This equation is valid at  $x = x_0$ . Solving the Eq. (29), the unknown parameter a can be obtained in terms of given parameters c and d.

## 3.1 Approximate Analytical Solution of the Spherical Catalyst by using ASM

The approximate analytical solution for the dimensionless concentration of chemical species in a spherical catalyst is given:

$$u(x) = \frac{e^{mx} + e^{-mx}}{e^m + e^{-m}}$$
(30)

The effectiveness factor  $\eta$  for a spherical pellet

$$\eta = \frac{3}{\varphi^2} tanh(m) \tag{31}$$

Where:

$$m = 1.0723$$
 (32)

#### 3.2 Approximate Analytical Solution of the Spherical Biocatalyst by using ASM

The approximate analytical solution for the dimensionless concentration of chemical species in a spherical biocatalyst is given as:

$$u(x) = \frac{e^{ax} + e^{-ax}}{e^a + e^{-a}}$$
(33)

The effectiveness factor  $\eta$  for a spherical pellet

$$\eta = \frac{3}{\varphi^2} tanh(a) \tag{34}$$

Where

$$a = -1.1220$$
 (35)

(26)

#### 4. Numerical Simulation

The approximate analytical solutions for the dimensionless concentration of the spherical catalyst and spherical biocatalyst for the steady state have been derived using Ananthaswamy-Sivasankari method (ASM). The solutions are derived using ASM for steady-state is explained in section (a) and (b), respectively. The derived semi-analytical expression along with the numerical simulation obtained using MATLAB have been plotted in Figure 1 and Figure 2. The MATLAB programming is given in section (c) for Eq. (12) and Section (d) for Eq. (20). The specific application of numerical simulation was described in depth by Jamal Ghoulish *et al.*, [53].

a) Approximate analytical solution of the Eq. (12) for the dimensionless concentration of the spherical catalyst by using Ananthaswamy-Sivasankari method (ASM)

However, the proposed new method is applicable to boundary value issues. For the differential equation and its derivatives, additional boundary conditions can be generated. The semi-analytical solution of the dimensionless concentration of the spherical catalyst is obtained approximately by using ASM is described below.

The following is an approximate analytical solution to Eq. (12) that satisfies the boundary condition as follows:

$$u(x) = Ae^{mx} + Be^{-mx}$$

$$\frac{du}{dx} = mAe^{mx} - mBe^{-mx}$$
(36)
(37)

Utilizing the boundary conditions in Eq. (13), we obtain the value of the parameters A &B as follows:

$$A = B, B = \frac{1}{e^m + e^{-m}}$$
(38)

Thus, Eq. (36), becomes:

$$u(x) = \frac{e^{mx} + e^{-mx}}{e^m + e^{-m}}$$
(39)

Now by using Eq. (39) in Eq. (12) and on simplification, we get:

$$m^{2}\left(\frac{e^{mx} + e^{-mx}}{e^{m} + e^{-m}}\right) + \frac{2}{x}m\left(\frac{e^{mx} - e^{-mx}}{e^{m} + e^{-m}}\right) - \sigma^{2}\left(\frac{e^{mx} + e^{-mx}}{e^{m} + e^{-m}}\right)exp\left[\frac{\gamma\beta\left(1 - \left(\frac{e^{mx} + e^{-mx}}{e^{m} + e^{-m}}\right)\right)}{1 + \beta\left(1 - \left(\frac{e^{mx} + e^{-mx}}{e^{m} + e^{-m}}\right)\right)}\right] = 0$$
(40)

Now taking x = 0, Eq. (40) becomes:

$$m^{2}\left(\frac{2}{e^{m}+e^{-m}}\right) - \sigma^{2}\left(\frac{2}{e^{m}+e^{-m}}\right)exp\left[\frac{\gamma\beta\left(1-\sec h\left(m\right)\right)}{1+\beta\left(1-\sec h\left(m\right)\right)}\right] = 0$$
(41)

$$m^{2} - \sigma^{2} \exp\left[\frac{\gamma\beta\left(1 - \sec h\left(m\right)\right)}{1 + \beta\left(1 - \sec h\left(m\right)\right)}\right] = 0$$
(42)

On solving Eq. (42) by substituting the values of  $\gamma = 0.5$ ,  $\beta = 1$ ,  $\sigma = 1$ , we get:

$$m^{2} - e^{\left(0.5000\frac{\cosh(m)-1}{2\cosh(m)-1}\right)} = 0$$
(43)

By solving the above Eq. (43), we get the value of the parameter m as follows:

$$m = 1.0723$$
 (44)

Similarly, we get the values of m by changing the values of  $\gamma$ ,  $\beta$  and  $\sigma$ .

Hence an approximate analytical solution of the dimensionless substrate concentration of the spherical catalyst u(x) Eq. (12) is obtained as:

$$u(x) = \frac{e^{mx} + e^{-mx}}{e^m + e^{-m}}$$
(45)

(b) Approximate analytical solution of the Eq. (20) for the dimensionless concentration of the spherical biocatalyst by using Ananthaswamy-Sivasankari method (ASM)

However, the proposed new method is applicable to boundary value issues. For the differential equation and its derivatives, additional boundary conditions can be generated. The semi-analytical solution of the dimensionless concentration of the spherical biocatalyst is obtained approximately by using ASM is described below.

The following is an approximate analytical solution to Eq. (20) that satisfies the boundary condition as follows:

$$u(x) = le^{ax} + me^{-ax}$$

$$\frac{du}{dx} = ale^{ax} - ame^{-ax}$$
(46)
(47)

Utilizing the boundary conditions in Eq. (21), we obtain the value of the parameters l & m as follows:

$$l = m, l = \frac{1}{e^a + e^{-a}}$$
(48)

$$u(x) = \frac{e^{ax} + e^{-ax}}{e^a + e^{-a}}$$
(49)

Now by using Eq. (49) in Eq. (20) and on simplification, we get

$$a^{2}\left(\frac{e^{ax} + e^{-ax}}{e^{a} + e^{-a}}\right) + \frac{2}{x}a\left(\frac{e^{ax} - e^{-ax}}{e^{a} + e^{-a}}\right) - \sigma^{2}\left[\frac{(1+\beta)\left(\frac{e^{ax} - e^{-ax}}{e^{a} + e^{-a}}\right)}{1+\beta\left(1 - \left(\frac{e^{ax} + e^{-ax}}{e^{a} + e^{-a}}\right)\right)}\right]$$

$$= 0$$
(50)

Now taking x = 0, Eq. (50) becomes:

$$a^{2}\left(\frac{2}{e^{a}+e^{-a}}\right) - \sigma^{2}\left[\frac{\left(1+\beta\right)\left(\frac{2}{e^{a}+e^{-a}}\right)}{1+\beta\left(\frac{2}{e^{a}+e^{-a}}\right)}\right] = 0$$
(51)

$$a^{2} - \sigma^{2} \exp\left[\frac{(1+\beta)}{1+\beta \operatorname{sec} h(a)}\right] = 0$$
(52)

On solving Eq. (52) by substituting the values of  $\beta = 1, \sigma = 1$ , we get:

$$\frac{a^2 \cosh(a) + m^2 - 2 \cosh(a)}{\cosh(a) + 1} = 0$$
(53)

By solving the above Eq. (53), we get the value of the parameter m as follows:

$$a = -1.1220$$
 (54)

Similarly, we get the values of a by changing the values of  $\beta$  and  $\sigma$ .

Hence an approximate analytical solution of the dimensionless substrate concentration of the spherical biocatalyst u(x) Eq. (20) is obtained as

$$u(x) = \frac{e^{ax} + e^{-ax}}{e^a + e^{-a}}$$
(55)

(c) Matlab Programming for Eq. (12)

```
function pdex4
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('Distance x')
ylabel('u1(x,2)')
%-----
                                      -----
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
```

```
sigma=1;
beta=1;
gamma=0.5;
F =(-sigma^2*u(1))*exp((gamma*beta*(1-u(1)))/(1+beta*(1-u(1))));
s = F;
%-----
function u0 = pdex4ic(x);
%create a initial conditions
u0 = 1;
%------
function[pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)
%create a boundary conditions
pl = 0;
ql = 1;
pr = ur-1;
qr = 0;
(d) Matlab Programming for Eq. (20)
function pdex4
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('Distance x')
ylabel('u1(x,2)')
%------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = DuDx;
sigma=1;
beta=1;
F = ((-sigma^2)^*(1+beta)^*u(1))/(1+beta^*u(1));
s = F;
%------
function u0 = pdex4ic(x);
%create a initial conditions
u0 = 1;
%-----
function[pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)
%create a boundary conditions
pl = 0;
ql = 1;
```

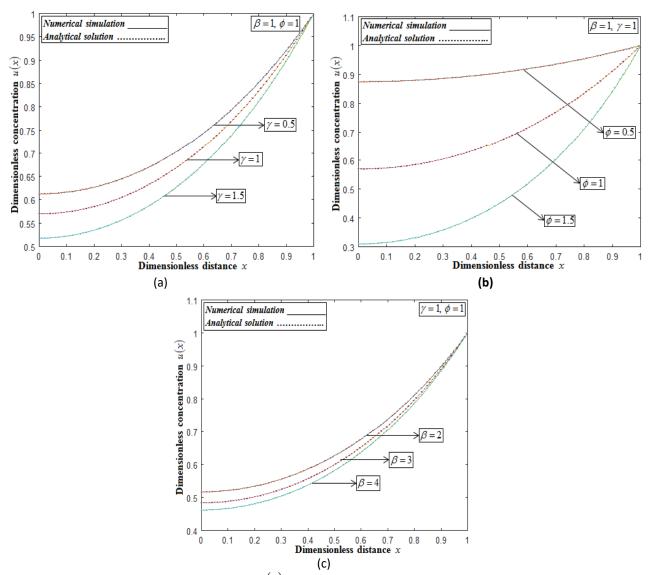
pr = ur-1; qr = 0;

## 5. Results and Discussion

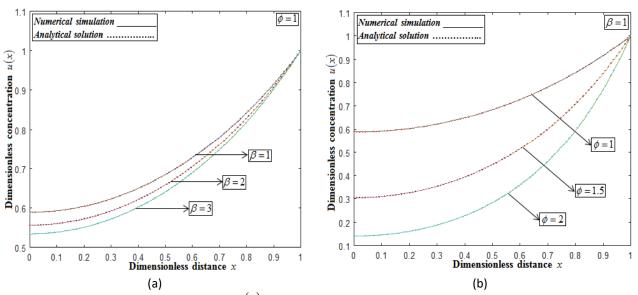
The semi-analytical solutions for the dimensionless concentration of the spherical catalyst and spherical biocatalyst for the steady state are given in the section (a) and section (b). Figure 1 shows that dimensionless concentration u(x) versus the dimensionless distance x by utilizing Eq. (30). From the Figures 1(a) - 1(c) it is noted that, when the values of dimensionless activation energy  $\gamma$ , Thiele modulus  $\phi$  and dimensionless heat of reaction  $\beta$  increases, the corresponding dimensionless concentration u(x) decreases respectively for certain values of the remaining dimensionless parameters. Figure 2 shows that dimensionless concentration u(x) versus the dimensionless concentration u(x) versus the dimensionless distance x by using Eq. (33). From the Figures 2(a) - 2(b) it depicts that, when Thiele modulus  $\phi$  and dimensionless heat of reaction  $\beta$  increases, the corresponding dimensionless concentration of spherical biocatalyst u(x) decreases respectively for certain values of the the the dimensionless distance x by using Eq. (33). From the Figures 2(a) - 2(b) it depicts that, when Thiele modulus  $\phi$  and dimensionless heat of reaction  $\beta$  increases, the corresponding dimensionless concentration of spherical biocatalyst u(x) decreases respectively for certain values of the further dimensionless parameters.

Figures 3(a)-3(b) shows that the effectiveness factor  $\eta$  versus Thiele modulus  $\phi$  by using Eq. (31). From this Figures, it cleared that, when the values of dimensionless heat of reaction  $\beta$  and dimensionless activation energy  $\gamma$  increases, their corresponding effectiveness factor  $\eta$  also increases respectively. Figures 3(c)-3(d) shows that the effectiveness factor  $\eta$  versus dimensionless activation energy  $\gamma$  by using Eq. (12). From the Figure 3(c) it noted that, when the value of dimensionless heat of reaction  $\beta$  increases, their corresponding effectiveness factor  $\eta$  decreases. Also, from the Figure 3(d) it depicts that when the value of dimensionless heat of reaction  $\beta$  increases factor  $\eta$  also increases respectively. Figures 3(e)-3(f) shows that the effectiveness factor  $\eta$  versus dimensionless heat of reaction  $\beta$  shows that the effectiveness factor  $\eta$  also increases, their corresponding Eq. (31). From the Figure 3(e) it observed that, when the values of Thiele modulus  $\phi$  increases, their corresponding effectiveness factor  $\eta$  also increases factor  $\eta$  decreases. Also, from the Figure 3(e) it observed that, when the values of Thiele modulus  $\phi$  increases, their corresponding effectiveness factor  $\eta$  decreases. Also, from the Figure 3(f) it observed that, when the values of Thiele modulus  $\phi$  increases, their corresponding effectiveness factor  $\eta$  also increases factor  $\eta$  also increases respectively.

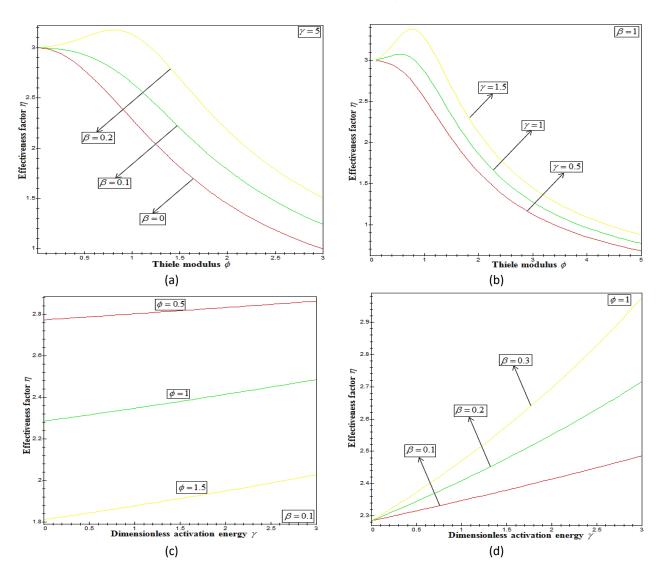
Figure 4(a) shows that the effectiveness factor  $\eta$  versus Thiele modulus  $\phi$  by using Eq. (34). From the Figure 4(a) it is evident that, when the values of dimensionless heat of reaction  $\beta$  increases, their corresponding effectiveness factor  $\eta$  increases respectively. Also, Figure 4(b) shows that the effectiveness factor  $\eta$  versus dimensionless heat of reaction  $\beta$ . From the Figure 4(b) it represents that when the values of Thiele modulus  $\phi$  increases, their corresponding effectiveness factor  $\eta$  decreases.

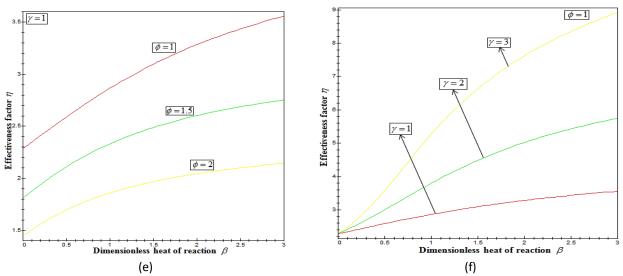


**Fig. 1.** (a) Dimensionless concentration u(x) versus dimensionless distance x by utilizing Eq. (30) for distinct values of dimensionless activation energy  $\gamma$  and certain value of Thiele modulus  $\phi$  and dimensionless heat of reaction  $\beta$ , (b) Dimensionless concentration u(x) versus dimensionless distance x by utilizing Eq. (30) for distinct values of Thiele modulus  $\phi$  and certain value of dimensionless activation energy  $\gamma$  and dimensionless heat of reaction  $\beta$ , (c) Dimensionless concentration versus u(x) dimensionless distance x by utilizing Eq. (30) for distinct values of reaction  $\beta$ , (c) Dimensionless heat of reaction  $\beta$  and certain value of dimensionless heat of reaction  $\beta$  and certain value of dimensionless activation energy  $\gamma$  and Thiele modulus  $\phi$ .

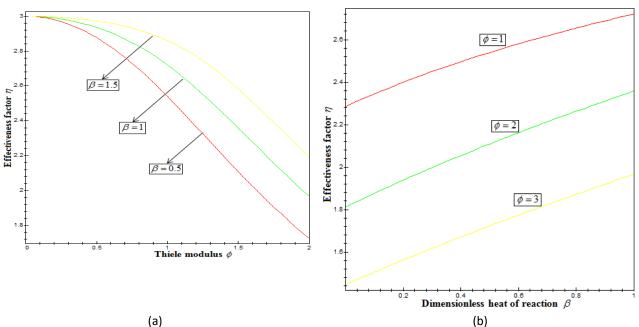


**Fig. 2.** (a) Dimensionless concentration u(x) versus dimensionless distance x by utilizing Eq. (33) for distinct values of dimensionless heat of reaction  $\beta$  and certain value of Thiele modulus  $\phi$ . (b) Dimensionless concentration u(x) versus dimensionless distance x by utilizing Eq. (33) for distinct values of Thiele modulus  $\phi$  and certain value of dimensionless heat of reaction  $\beta$ .





**Fig. 3.** (a) Effectiveness factor versus Thiele modulus by utilizing Eq. (31) for distinct values of dimensionless heat of reaction and certain value of dimensionless activation energy. (b) Effectiveness factor versus Thiele modulus by utilizing Eq. (31) for distinct values of dimensionless activation energy and certain value of dimensionless heat of reaction. (c) Effectiveness factor versus dimensionless activation energy by utilizing Eq. (31) for distinct values of Thiele modulus and certain value of dimensionless heat of reaction. (d) Effectiveness factor versus dimensionless activation energy by utilizing Eq. (31) for distinct values of Thiele modulus and certain value of dimensionless heat of reaction. (d) Effectiveness factor versus dimensionless activation energy by utilizing Eq. (31) for distinct values of reaction and certain value of Thiele modulus. (e) Effectiveness factor versus dimensionless heat of reaction versus dimensionless heat of reaction by utilizing Eq. (31) for distinct values of dimensionless activation energy. (f) Effectiveness factor versus dimensionless activation energy. and certain value of Thiele modulus.



**Fig. 4.** (a) Effectiveness factor  $\eta$  versus Thiele modulus  $\phi$  by utilizing Eq. (34) for distinct values of dimensionless heat of reaction  $\beta$ , (b) Effectiveness factor  $\eta$  versus dimensionless heat of reaction  $\beta$  by utilizing Eq. (34) for distinct values of Thiele modulus  $\phi$ .

# 6. Conclusions

The two Lane-Emden type Boundary Value Problems that describes the diffusion of reactants in an idealized spherical porous catalytic pellet and in spherical porous biocatalyst pellet was examined. The new analytical method called Ananthaswamy- Sivasankari method (ASM) employed for both models, which greatly enhances the computational efficiency while overcoming the difficulty of the singular behaviour at the spherical origin x=0 of the pellets. For all parameter values, the results are in good agreement with the numerical simulation.

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## References

- [1] Duggan, R. C., and A. M. Goodman. "Pointwise bounds for a nonlinear heat conduction model of the human head." *Bulletin of mathematical biology* 48 (1986): 229-236.<u>https://doi.org/10.1007/BF02460025</u>
- [2] Lin, S. H. "Oxygen diffusion in a spherical cell with nonlinear oxygen uptake kinetics." *Journal of Theoretical Biology* 60, no. 2 (1976): 449-457.<u>https://doi.org/10.1016/0022-5193(76)90071-0</u>
- [3] Rach, Randolph, Jun-Sheng Duan, and Abdul-Majid Wazwaz. "Solving coupled Lane–Emden boundary value problems in catalytic diffusion reactions by the Adomian decomposition method." *Journal of Mathematical Chemistry* 52 (2014): 255-267.<u>https://doi.org/10.1007/s10910-013-0260-6</u>
- [4] Rach, Randolph, Jun-Sheng Duan, and Abdul-Majid Wazwaz. "On the solution of non-isothermal reaction-diffusion model equations in a spherical catalyst by the modified Adomian method." *Chemical Engineering Communications* 202, no. 8 (2015): 1081-1088.<u>https://doi.org/10.1080/00986445.2014.900054</u>
- [5] Van Gorder, Robert A. "Exact first integrals for a Lane–Emden equation of the second kind modeling a thermal explosion in a rectangular slab." New Astronomy 16, no. 8 (2011): 492-497. <u>https://doi.org/10.1016/j.newast.2011.04.006</u>
- [6] Wazwaz, Abdul-Majid. "Solving the non-isothermal reaction-diffusion model equations in a spherical catalyst by the variational iteration method." *Chemical Physics Letters* 679 (2017): 132-136. <u>https://doi.org/10.1016/j.cplett.2017.04.077</u>
- [7] Duan, Jun-Sheng, Randolph Rach, and Abdul-Majid Wazwaz. "Steady-state concentrations of carbon dioxide absorbed into phenyl glycidyl ether solutions by the Adomian decomposition method." *Journal of Mathematical Chemistry* 53 (2015): 1054-1067. <u>https://doi.org/10.1007/s10910-014-0469-z</u>
- [8] Wazwaz, Abdul-Majid. "Solving systems of fourth-order Emden–Fowler type equations by the variational iteration method." *Chemical Engineering Communications* 203, no. 8 (2016): 1081-1092. https://doi.org/10.1080/00986445.2016.1141094
- [9] Wazwaz, Abdul-Majid. "The variational iteration method for solving new fourth-order Emden–Fowler type equations." *Chemical Engineering Communications* 202, no. 11 (2015): 1425-1437. <u>https://doi.org/10.1080/00986445.2014.952814</u>
- [10] Das, Nilima, Randhir Singh, Abdul-Majid Wazwaz, and Jitendra Kumar. "An algorithm based on the variational iteration technique for the Bratu-type and the Lane–Emden problems." *Journal of Mathematical Chemistry* 54 (2016): 527-551. <u>https://doi.org/10.1007/s10910-015-0575-6</u>
- [11] Kanth, ASV Ravi, and K. Aruna. "He's variational iteration method for treating nonlinear singular boundary value problems." *Computers & Mathematics with Applications* 60, no. 3 (2010): 821-829. <u>https://doi.org/10.1016/j.camwa.2010.05.029</u>
- [12] Singh, Randhir, Jitendra Kumar, and Gnaneshwar Nelakanti. "Numerical solution of singular boundary value problems using Green's function and improved decomposition method." *Journal of Applied Mathematics and Computing* 43 (2013): 409-425. <u>https://doi.org/10.1007/s12190-013-0670-4</u>
- [13] Singh, Randhir, Nilima Das, and Jitendra Kumar. "The optimal modified variational iteration method for the Lane-Emden equations with Neumann and Robin boundary conditions." *The European Physical Journal Plus* 132 (2017): 1-11. <u>https://doi.org/10.1140/epip/i2017-11521-x</u>
- [14] Singh, Randhir, and Jitendra Kumar. "An efficient numerical technique for the solution of nonlinear singular boundary value problems." *Computer Physics Communications* 185, no. 4 (2014): 1282-1289. <u>https://doi.org/10.1016/j.cpc.2014.01.002</u>

- [15] Singh, Randhir, Jitendra Kumar, and Gnaneshwar Nelakanti. "Approximate series solution of nonlinear singular boundary value problems arising in physiology." *The Scientific World Journal* 2014 (2014). <u>https://doi.org/10.1155/2014/945872</u>
- [16] Singh, Randhir, and Jitendra Kumar. "The Adomian decomposition method with Green's function for solving nonlinear singular boundary value problems." *Journal of Applied Mathematics and Computing* 44 (2014): 397-416. <u>https://doi.org/10.1007/s12190-013-0699-4</u>
- [17] Singh, Randhir, Sukhjit Singh, and Abdul-Majid Wazwaz. "A modified homotopy perturbation method for singular time dependent Emden–Fowler equations with boundary conditions." *Journal of Mathematical Chemistry* 54 (2016): 918-931. <u>https://doi.org/10.1007/s10910-016-0594-y</u>
- [18] Singh, Randhir, Abdul-Majid Wazwaz, and Jitendra Kumar. "An efficient semi-numerical technique for solving nonlinear singular boundary value problems arising in various physical models." *International Journal of Computer Mathematics* 93, no. 8 (2016): 1330-1346. <u>https://doi.org/10.1080/00207160.2015.1045888</u>
- [19] Singh, Randhir, and Abdul-Majid Wazwaz. "Numerical solution of the time dependent Emden–Fowler equations with boundary conditions using modified decomposition method." *Appl. Math. Inf. Sci* 10, no. 2 (2016): 403-408.<u>doi:10.18576/amis/100203</u>
- [20] Wazwaz, Abdul-Majid, and Randolph Rach. "Comparison of the Adomian decomposition method and the variational iteration method for solving the Lane-Emden equations of the first and second kinds." *Kybernetes* (2011). <u>https://doi.org/10.1108/03684921111169404</u>
- [21] Richardson, Owen Willans. *The emission of electricity from hot bodies*. Vol. 4. Longmans, Green and Company, 1921.
- [22] Sun, Yan-Ping, Shi-Bin Liu, and Scott Keith. "Approximate solution for the nonlinear model of diffusion and reaction in porous catalysts by the decomposition method." *Chemical Engineering Journal* 102, no. 1 (2004): 1-10. <u>https://doi.org/10.1016/S1385-8947(03)00060-3</u>
- [23] Wazwaz, Abdul-Majid, Randolph Rach, and Jun-Sheng Duan. "A study on the systems of the Volterra integral forms of the Lane–Emden equations by the Adomian decomposition method." *Mathematical Methods in the Applied Sciences* 37, no. 1 (2014): 10-19. <u>https://doi.org/10.1002/mma.2776</u>
- [24] Wazwaz, Abdul-Majid. "A new algorithm for solving differential equations of Lane–Emden type." *Applied mathematics and computation* 118, no. 2-3 (2001): 287-310. <u>https://doi.org/10.1016/S0096-3003(99)00223-4</u>
- [25] Wazwaz, Abdul-Majid. "A new method for solving singular initial value problems in the second-order ordinary differential equations." *Applied Mathematics and computation* 128, no. 1 (2002): 45-57. https://doi.org/10.1016/S0096-3003(01)00021-2
- [26] Wazwaz, Abdul-Majid. "Adomian decomposition method for a reliable treatment of the Bratu-type equations." *Applied Mathematics and Computation* 166, no. 3 (2005): 652-663. https://doi.org/10.1016/j.amc.2004.06.059
- [27] Wazwaz, Abdul-Majid, and Abdul-Majid Wazwaz. "Solitary waves theory." Partial Differential Equations and Solitary Waves Theory (2009): 479-502. <u>https://doi.org/10.1007/978-3-642-00251-9\_12</u>
- [28] Wazwaz, Abdul-Majid, Randolph Rach, and Jun-Sheng Duan. "Adomian decomposition method for solving the Volterra integral form of the Lane–Emden equations with initial values and boundary conditions." *Applied Mathematics and Computation* 219, no. 10 (2013): 5004-5019. <u>https://doi.org/10.1016/j.amc.2012.11.012</u>
- [29] Flockerzi, Dietrich, and Kai Sundmacher. "On coupled Lane-Emden equations arising in dusty fluid models." In Journal of physics: conference series, vol. 268, no. 1, p. 012006. IOP Publishing, 2011. doi:10.1088/1742-6596 /268/1/012006
- [30] Muatjetjeja, Ben, and Chaudry Masood Khalique. "Noether, partial Noether operators and first integrals for the coupled Lane-Emden system." *Mathematical and Computational Applications* 15, no. 3 (2010): 325-333. <u>https://doi.org/10.3390/mca15030325</u>
- [31] Talwalkar, S., Mankar, S., Katariya, A., Aghalayam, P., Ivanova, M., Sundmacher, K. and Mahajani, S. "Selectivity engineering with reactive distillation for dimerization of C4 olefins: experimental and theoretical studies." *Industrial and Engineering Chemistry Research* 46, (2007): 3024–3034. <u>https://doi.org/10.1021/ie060860+</u>
- [32] Zou, Henghui. "A priori estimates for a semilinear elliptic system without variational structure and their applications." *Mathematische Annalen* 323 (2002): 713-735. <u>https://doi.org/10.1007/s002080200324</u>
- [33] Connors, Kenneth Antonio. *Chemical kinetics: the study of reaction rates in solution*. Wiley-VCH Verlag GmbH, 1990.
- [34] Wazwaz, Abdul-Majid. "The variational iteration method for solving systems of equations of Emden–Fowler type." *International Journal of Computer Mathematics* 88, no. 16 (2011): 3406-3415. https://doi.org/10.1080/00207160.2011.587513
- [35] Wazwaz, Abdul-Majid. "The variational iteration method for solving the Volterra integro-differential forms of the Lane–Emden equations of the first and the second kind." *Journal of Mathematical Chemistry* 52, no. 2 (2014): 613-626. <u>https://doi.org/10.1007/s10910-013-0281-1</u>

- [36] Saadatmandi, Abbas, Nafiseh Nafar, and Seyed Pendar Toufighi. "Numerical study on the reaction cum diffusion process in a spherical biocatalyst." (2014): 47-61. <u>https://doi.org/10.22052/IJMC.2014.5539</u>
- [37] Randhir Singh. "Optimal homotopy analysis method for the non-isothermal reaction–diffusion model equations in a spherical catalyst." *Journal of Mathematical Chemistry* 56, no. 9 (2018): 2579-2590. https://doi.org/10.1007/s10910-018-0911-8
- [38] Ananthaswamy, V., Shanthakumari, R. and Subha, M. "Simple analytical expressions of the non–linear reaction diffusion process in an immobilized biocatalyst particle using the new homotopy perturbation method." *Review of Bioinformatics and Biometrics* 3, (2014): 23–28.
- [39] He, Ji-Huan. "Variational iteration method for autonomous ordinary differential systems." *Applied mathematics and computation* 114, no. 2-3 (2000): 115-123. <u>https://doi.org/10.1016/S0096-3003(99)00104-6</u>
- [40] Liao, Shijun, Jian Su, and Allen T. Chwang. "Series solutions for a nonlinear model of combined convective and radiative cooling of a spherical body." *International Journal of Heat and Mass Transfer* 49, no. 15-16 (2006): 2437-2445. <u>https://doi.org/10.1016/j.ijheatmasstransfer.2006.01.030</u>
- [41] Weisz, P. B., and J. S. Hicks. "The behaviour of porous catalyst particles in view of internal mass and heat diffusion effects." *Chemical Engineering Science* 17, no. 4 (1962): 265-275. <u>https://doi.org/10.1016/0009-2509(62)85005-2</u>
- [42] Chitra, J., Ananthaswamy, V., Sivasankari, S. and Seenith 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) (ISSN: 2041-3065) 14, no. 1 (2023): 53-69.
- [43] Sivasankari, S., Ananthaswamy,V. and Seenith Sivasundaram. "A new approximate analytical method for solving some non-linear initial value problems in physical sciences." Mathematics in Engineering, Science and Aerospace (MESA) (ISSN: 2041-3065) 14, no. 1 (2023): 145-162.
- [44] Ala'yed, O., Saadeh, R., & Qazza, A. (2023). Numerical solution for the system of Lane-Emden type equations using cubic B-spline method arising in engineering. AIMS Mathematics, 8(6), 14747-14766. <u>https://doi:10.3934/math.203754</u>
- [45] Omaba, M. E. (2022). New analytical method of solution to a nonlinear singular fractional Lane–Emden type equation. AIMS Mathematics, 7(10), 19539-19552. <u>https://doi:10.3934/math.20221072</u>
- [46] Rach, R., Duan, J. S., & Wazwaz, A. M. (2015). On the solution of non-isothermal reaction-diffusion model equations in a spherical catalyst by the modified Adomian method. *Chemical Engineering Communications*, 202(8), 1081-1088. <u>https://doi.org/10.1080/00986445.2014.900054</u>
- [47] Fogler, H. S. (1999). Elements of chemical reaction engineering, 3rd.
- [48] Danish, M., Kumar, S., & Kumar, S. (2011). OHAM solution of a singular BVP of reaction cum diffusion in a biocatalyst. *IAENG International Journal of Applied Mathematics*, *41*(3), 223-227.
- [49] Fogler, H.S. (1997). Elements of Chemical Reaction Engineerring: 2<sup>nd</sup> Edition. New Jersey: Prentice-Hall Inc.
- [50] Skrzypacz, P., Andreev, V. V., & Golman, B. (2020). Dead-core and non-dead-core solutions to diffusion-reaction problems for catalyst pellets with external mass transfer. *Chemical Engineering Journal*, 385, 123927. <u>https://doi.org/10.1016/j.cej.2019.123927</u>
- [51] Golman, B., Andreev, V. V., & Skrzypacz, P. (2020). Dead-core solutions for slightly non-isothermal diffusionreaction problems with power-law kinetics. *Applied Mathematical Modelling*, 83, 576-589. <u>https://doi.org/10.1016/j.apm.2020.03.016</u>
- [52] Crasta, A., Pathan, K. A., & Khan, S. A. (2023). Analytical and Numerical Simulation of Surface Pressure of an Oscillating Wedge at Hypersonic Mach Numbers and Application of Taguchi's Method. *Journal of Advanced Research in Applied Sciences and Engineering Technology 30*, no. 1 (2023): 15-30. <u>https://doi.org/10.37934/araset.30.1.1530</u>
- [53] Jamal Ghouizi, Mohamed Nabou, Mohammed Elmir, Mohamed Douha, and Mehdi Berramdane. "Numerical Simulation of Natural Convetion in A Cavity Filled with A Nanofluid Who's Wall Containing the Heat source is Inclined." Journal of Advanced Research in Fluid Mechanics and Termal Sciences 76, no. 1, (2020): 1-16. <u>https://doi.org/10.37934/arfmts.76.1.116</u>