A New Approximate Analytical Expression of Non-Isothermal Diffusion Model

J. MALA, G. SUGANYA, M. MALLIKARJUNA, R. SENTHAMARAI*
Department of Mathematics,
College of Engineering and Technology, SRM Institute of Science and Technology,
Kattankulathur 603203, Tamilnadu,
INDIA

*Corresponding Author

Abstract: - In this study, we've addressed the Lane-Emden boundary value problem that appears in biochemical, scientific, and chemical applications. We've used the Taylor series approach to solve the non-isothermal reaction-diffusion equation in a planar catalyst. We've derived the approximate analytical expression for concentration and effectiveness factors. The collected results are illustrated using appropriate graphs. The presented analysis proves the applicability of the utilized method's dependability and effectiveness. We've also solved the equation numerically by using MATLAB software to compare our approximate analytical solutions. Our analytical results of concentration and effectiveness factor are most appropriately matched with the numerical results. We've also discussed the influence of the parameters on concentration and effectiveness factors.

Key-Words: - Mathematical modeling; Lane–Emden equation; Taylor series method; Catalyst; Non-linear reaction-diffusion equation, Iso-thermal reaction; Numerical simulation.

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1 Introduction

The planar shape factor for Lane-Emden equation is as follows:

$$v''(x) - f(v(x)) = 0 \tag{1}$$

The Lane-Emden equation has many applications in many branches of chemistry, physics, and other sciences. Astrophysicists Jonathan Homer Lane and Robert Emden first investigated the Lane-Emden equation, which examined how a spherical cloud of gas behaved thermally while subject to the laws of classical thermodynamics and functioning under the mutual attraction of its molecules. Numerous phenomena in mathematical physics and astronomy, including stellar structure theory, isothermal gas spheres, thermionic current theory, the thermal behavior of a spherical cloud of star gas, and modeling of galactic clusters have been simulated using Lane- Emden's equation. The equation also explains temperature and solves the solitary behavior that happens at $x = 1$. A large amount of research has been conducted on these types of structural issues. Many researchers have employed numerical and analytic methods to solve Lane-Emden type equations with initial and boundary conditions [1], [2], [3], [4], [5], [6].

There is a vast industrial application of the packed catalytic pellets with heterogeneous reaction kinetics. Namely, emission control in HVAC (Heating, Ventilation, and Air Conditioning) systems, air purification, temperature control, and heat transfer enchantment of HVAC systems, can be used in the catalytic heating and cooling system. The obtained approximate analytical results will be helpful for a better understanding of the reactor and optimizing the batch reactor system by considering the various effects of the system parameters.

Many analytical approaches such as the Homotopy Perturbation method, Adomian decomposition method, Variational Iteration method, and other methods as well applied to solve nonlinear equations. The variational iteration method has been used to solve the non-isothermal reaction-diffusion model, [7]. This method has been applied to solve prey-predator equations and nonlinear coupled reaction-diffusion systems at conducting polymer-modified ultra microelectrodes [8], [9], [10]. The homotopy perturbation method has been applied to solve immobilized enzyme reactions and prey-predator systems, [11], [12], [13]. Adomian decomposition method has been utilized by the researchers to solve non-linear reaction-diffusion equation, [14], [15] and epidemic models, [16].

Utilizing the Taylor series method, we were able to solve the nonlinear equation. Taylor series approach to analyse the Lane-Emden equation was studied by He JH, Ji FY, [17]. Taylor series method has been applied to solve many systems like nonlinear reaction-diffusion equations, [18], [19]. The goal of this research is to use Taylor's series method to obtain a simple, closed approximate expression of the effectiveness factor and substrate concentration in a given system for planar shape. Our obtained analytical expression gives the most accurate result for all values of parameters in the given boundary. To validate the analytical results, the graphs are presented.

2 Mathematical Formulation

Many industrial reactors use packed catalytic pellets with heterogeneous reaction kinetics. We consider the Lane-Emden BVP for the normalized concentration $v(x)$ in [7] and is as follows:

$$v''(x) - \varphi^2 v(x)\, exp\left[\frac{\alpha\beta\big(1-v(x)\big)}{1+\beta\big(1-v(x)\big)}\right] = 0 \qquad (2)$$

with the boundary conditions:

$$v(1) = 1, v'(0) = 0 \qquad (3)$$

In Eq. (2), dimensionless activation energy is α, φ is the Thiele modulus and the dimensionless heat of reaction is β.

$$x = \frac{f}{F},\ v = \frac{E_A}{E_{As}},\ \alpha = \frac{P}{F_g R_s},$$
$$\beta = \frac{(-\Delta H)GC_{As}}{TR_s}, \phi^2 = \frac{T_{ref}R^2}{G} \qquad (4)$$

The effectiveness factor η for a planar pellet is defined as:

$$\eta = \frac{3}{\varphi^2}\frac{dy}{dx}\Big|_{x=1} \qquad (5)$$

3 Concentration of Substrate using Taylor Series Method

This method, widely recognized and established, has been employed for the formal solution of ordinary differential equations (ODEs), [20].

Suppose the function $u(z)$ satisfies the 2^{nd} order ODE:

$$F(u'', u', u, z) = 0 \qquad (6)$$

As the general solution involves two arbitrary constants, the objective of the boundary value problem (BVP) is to identify a solution (if exists) within a specified range of $z \in [m, n]$ that satisfies, for instance, the two given boundary conditions:

$$u(m) = M, \qquad u(n) = N \qquad (7)$$

where A and B represent predetermined constants. It becomes more straightforward to ascertain the solution when two conditions are provided at a single boundary, as in the case of the Cauchy problem. For instance:

$$u(m) = M, \qquad u'(m) = a \qquad (8)$$

In fact, solving problem (2) involves resolving the Cauchy problem (3) for an undetermined value $a*$ of a to ensure the fulfillment of the condition $u(n) = N$. If a singular solution is attainable, numerical techniques, such as a shooting method combined with a Newton–Raphson adjustment procedure, can be employed for resolution. However, the current focus lies on exploring quasi-analytical methods that leverage the representation of the solution through Taylor series.

For this purpose, an initial step involves expanding the solution using a Taylor series around the boundary a.

$$u(z) = \sum_{i=0}^{\infty} p_i (z-m)^i \qquad (9)$$

and derives the coefficients p_n in relation to M and a, ensuring Eq. is satisfied successively in powers of $(z-m)$. This process yields the set $p_n(M, a)$ (where $p_0 = M, p_1 = a$, and so on). The next step involves summation of the obtained series to meet the condition at the second boundary, determining the value $a*$ for a:

$$\sum_{i=0}^{\infty} p_i(M, a^*)(n-m)^i = N \qquad (10)$$

Ultimately, the comprehensive solution to the problem is formally expressed as:

$$u^*(z) = \sum_{i=0}^{\infty} p_i(M, a^*)(a-m)^i \qquad (11)$$

Taylor's series method is employed to solve the nonlinear system of equations in this work. The TSM produces an approximate solution in terms of a fast convergent series without linearization. We compute the concentration using proposed method (Appendix-A) as follows:

$$v(x) = \sum_{i=0}^{\infty} \frac{x}{i!}\frac{dv}{dx}\Big|_{x=0} \qquad (12)$$

$$= v(0) + \frac{x}{1!}\frac{dv}{dx}\bigg|_{x=0} + \frac{x^2}{2!}\frac{d^2v}{dx^2}\bigg|_{x=0} + \frac{x^3}{3!}\frac{d^3v}{dx^3}\bigg|_{x=0} \quad (13)$$

$$v(0) = v(0) \quad (14)$$

By boundary condition:

$$v'(0) = 0 \quad (15)$$

$$v''(x) = \varphi^2 v(x)\, exp\left[\frac{\alpha\beta\big(1 - v(x)\big)}{1 + \beta\big(1 - v(x)\big)}\right] \quad (16)$$

$$v'''(x)\varphi^2\, exp\left[\frac{\alpha\beta\big(1 - v(x)\big)}{1 + \beta\big(1 - v(x)\big)}\right]\left[v'(x) - \frac{\alpha\beta v(x) v'(x)}{\Big(1 + \beta\big(1 - v(x)\big)\Big)^2}\right] \quad (17)$$

$$v^{iv}(x) = \varphi^2\, exp\left[\frac{\alpha\beta\big(1 - v(x)\big)}{1 + \beta\big(1 - v(x)\big)}\right]\left[\left(v''(x) - \frac{\begin{pmatrix}1 + \beta\big(1 - v(x)\big)\left(\alpha\beta v'^2(x) + \alpha\beta v(x) v''(x)\right) \\ +2\alpha\beta^2 v(x) v'^2(x)\end{pmatrix}}{\Big(1 + \beta\big(1 - v(x)\big)\Big)^3}\right)\right] + \left[\left(\frac{\alpha\beta v(x) v'(x)}{\Big(1 + \beta\big(1 - v(x)\big)\Big)^2}\right) exp\left(\frac{\alpha\beta\big(1 - v(x)\big)}{1 + \beta\big(1 - v(x)\big)}\right)\left(\frac{-\alpha\beta v'(x)}{\Big(1 + \beta\big(1 - v(x)\big)\Big)^2}\right)\right] \quad (18)$$

Using Taylor's series expansion about $x = 0$, the concentration of substrates is as follows:

$$v(x) = v(0) + v'(0)\frac{x}{1!} + v''(0)\frac{x^2}{2!} + v'''(0)\frac{x^3}{3!} + \ldots \quad (19)$$

At $x = 0$ we get,

$$v(x) = v(0) + \frac{x^2}{2!}\varphi^2 v(0)\left[exp\left(\frac{\alpha\beta\big(1 - v(0)\big)}{1 + \beta\big(1 - v(0)\big)}\right)\right] + \frac{x^4}{4!}\varphi^4 v(0)\left[exp\left(\frac{\alpha\beta\big(1 - v(0)\big)}{1 + \beta\big(1 - v(0)\big)}\right)\right]^2\left[1 - \frac{\alpha\beta v(0)}{\Big(1 + \beta\big(1 - v(0)\big)\Big)^2}\right] \quad (20)$$

where $v(0)$ is obtained as follows using the boundary condition:

$$1 = v(0) + \frac{1}{2!}\varphi^2 v(0)\left[exp\left(\frac{\alpha\beta\big(1 - v(0)\big)}{1 + \beta\big(1 - v(0)\big)}\right)\right] + \frac{1}{4!}\varphi^4 v(0)\left[exp\left(\frac{\alpha\beta\big(1 - v(0)\big)}{1 + \beta\big(1 - v(0)\big)}\right)\right]^2\left[1 - \frac{\alpha\beta v(0)}{\Big(1 + \beta\big(1 - v(0)\big)\Big)^2}\right] \quad (21)$$

The pellet's effectiveness factor is specified as follows:

$$\eta = \frac{3}{\varphi^2}\frac{dv}{dx}\bigg|_{x=1} \quad (22)$$

$$\eta = \frac{3}{\varphi^2}\left[\varphi^2 v(0)\left[exp\left(\frac{\alpha\beta\big(1 - v(0)\big)}{1 + \beta\big(1 - v(0)\big)}\right)\right] + \frac{1}{6}\varphi^4 v(0)\left[exp\left(\frac{\alpha\beta\big(1 - v(0)\big)}{1 + \beta\big(1 - v(0)\big)}\right)\right]^2\left[1 - \frac{\alpha\beta v(0)}{\Big(1 + \beta\big(1 - v(0)\big)\Big)^2}\right]\right] \quad (23)$$

4 Validation of Analytical Results

The numerical simulation for nonlinear equation (2) along with the boundary conditions (3) and (4) is carried out in MATLAB using the function pdex4. The approximate analytical solution has been derived for the Lane-Emden equation (2) using Taylor series method. The analytical solutions have been compared with the numerical simulation and the results are shown in Figure 1, Figure 2 and Figure 3. The analytical approximation using Taylor's series is the most successful way to obtain the analytical expression for steady-state substrate concentration.

5 Results and Discussion

The closed form of the approximate analytical solution has been derived for the Lane-Emden equation (2) by applying the Taylor series method. The MATLAB tool is used to perform the numerical simulation. Figure 1 implies, that increasing the value of Thiele modulus φ decreases the concentration of substrate $v(x)$. Figure 2 infers that, the increase in the dimensionless activation energy has the inverse effect on the system as it decreases the concentration of the substrate $v(x)$. Figure 3 shows that, increasing the dimensionless heat of reaction β decreases the concentration of substrate $v(x)$. The effectiveness factor for different values of φ is shown in Figure 4. Figure 5 depicts various values of dimensionless activation energy. The effects of φ, and β on the effectiveness factor are inferred from these two figures. The value of Thiele modulus φ decreases η and the activation energy increases the effectiveness factor. Surface plot of concentration of substrate $v(x)$, Figure 6 indicates the effect of activation energy and dimensionless distance x, Figure 7 indicates the effect of heat of reaction β and dimensionless distance x, Figure 8 Thiele modulus φ and dimensionless distance x. Table 1 represents the value of $v(0)$ which is obtained from the boundary condition. The values of $v(0)$ are obtained corresponding to the boundary condition (3) and are applied in the approximate solution. Table 2 represents the values of $v(0)$ which are used in finding the effectiveness factor.

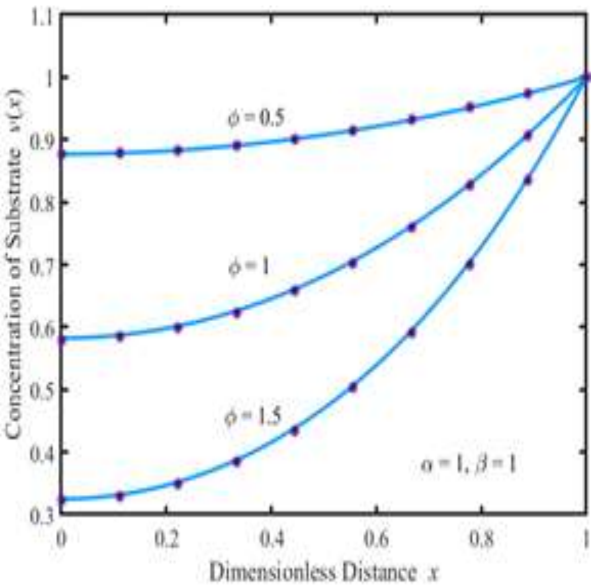

Fig. 1: Plot of $v(x)$ versus x, (numerical results represented by —— and TSM represented by ***. The curves are plotted using Eqn. (20) for different values of φ.

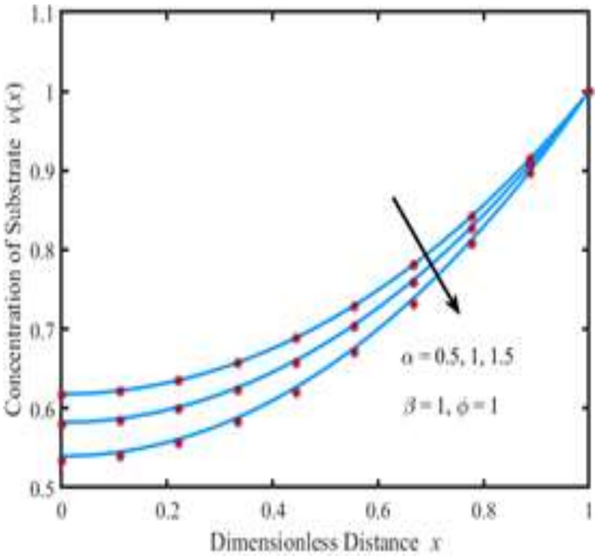

Fig. 2: Plot of $v(x)$ versus x, (numerical results represented by —— and TSM represented by ***. The curves are plotted using Eqn. (20) for different values of α.

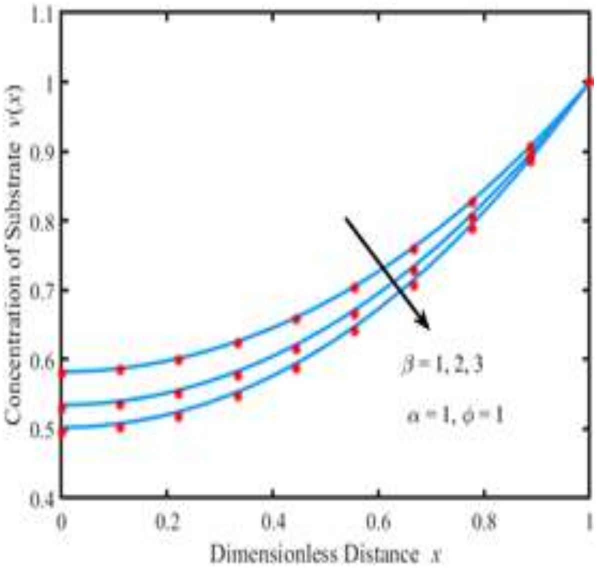

Fig. 3: Plot of $v(x)$ versus x, (numerical results represented by —— and TSM represented by ***. The curves are plotted using Eqn. (20) for different values of β.

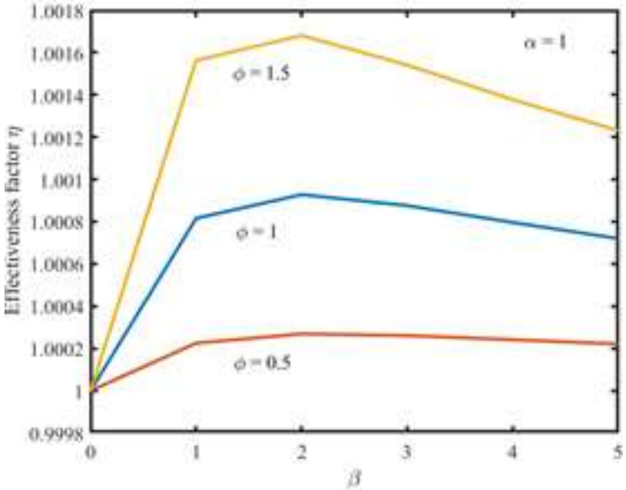

Fig. 4: Plot of effectiveness factor η versus dimensionless heat reaction β for various values of Thiele modulus φ [φ = 0.5, 1, 1.5]

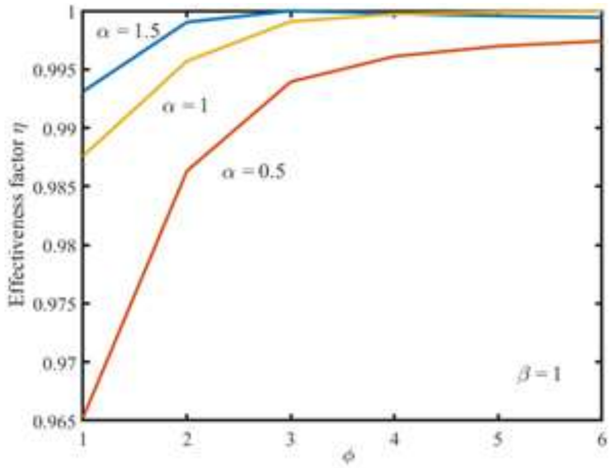

Fig. 5: Plot of effectiveness factor η versus Thiele modulus φ for various values of dimensionless activation energy [= 0.5, 1, 1.5].

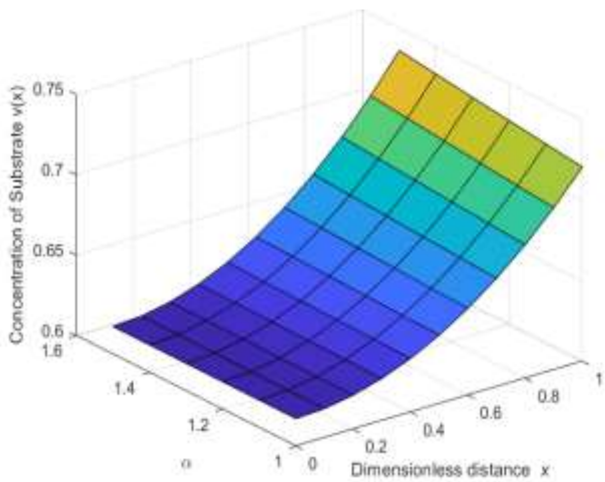

Fig. 6: Surface plot of $v(x)$ concerning (a) activation energy and dimensionless distance x

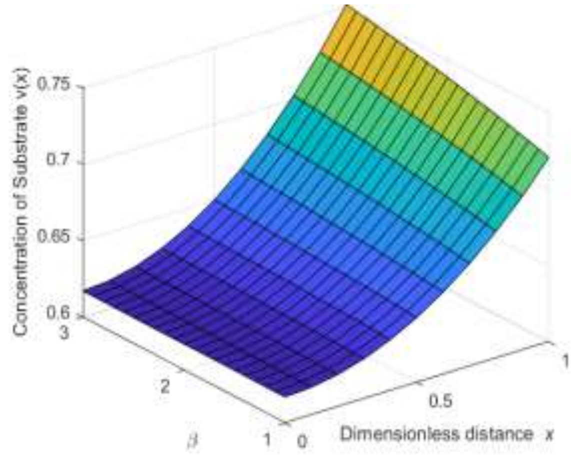

Fig. 7: Surface plot of $v(x)$ concerning heat of reaction β and dimensionless distance x

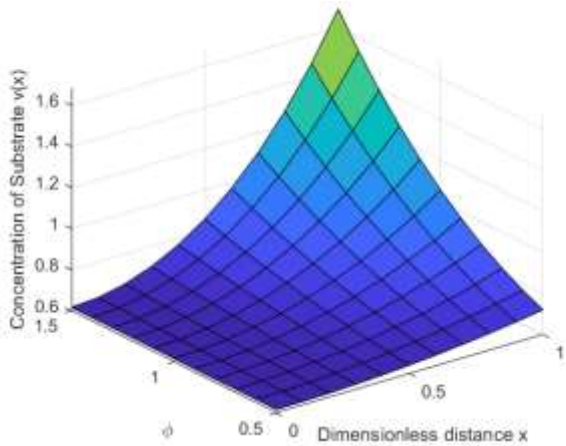

Fig. 8: Surface plot of $v(x)$ concerning Thiele modulus φ and dimensionless distance x.

Table 1. Values of $v(0)$ obtained from boundary condition for finding an approximate solution

φ =1, β =1		φ =1, α =1		α =1, β =1	
α	$v(0)$	β	$v(0)$	φ	$v(0)$
0.5	0.6171765173	1	0.5794129538	0.5	0.8768262735
1	0.5794129538	2	0.5287661678	1	0.5794129538
1.5	0.5338434064	3	0.4952518262	1.5	0.3223155775

Table 2**.** Values of v(0) obtained from boundary condition for finding the effectiveness factor

φ	$v(0)$			β	$v(0)$		
	α = 0.5, β =1	α =1, β =1	α =1.5, β =1		φ = 0.5, α =1	φ =1, α =1	φ =1.5, α =1
1	1.688378892	1.535205995	1.423380174	0	0.3199999999	2/7	0.2424242424
2	1.460144243	1.265019903	1.119925727	1	0.2016024318	0.1696820466	0.1333484486
3	1.349034161	1.133847190	0.9855548782	2	0.1661115386	0.1359529519	0.1037610596
4	1.298013871	1.078740841	0.9333240600	3	0.1501994254	0.1210603704	0.9863497655
5	1.271545517	1.051443375	0.9082945921	4	0.1412753769	0.1127809599	0.9469214318
6	1.256310953	1.036123967	0.8944808641	5	0.1355856563	0.1075321122	0.9265548149

6 Conclusion

In this paper, we have addressed the Lane-Emden boundary value problem. An analytical approximate solution has been derived by using the Taylor series for the non-isothermal reaction-diffusion equation. The effectiveness factor has been obtained and a graphical representation is shown. Our analytical solution is compared with numerical simulation using MATLAB. There seems to be a good agreement between both the results which proved this method to be a powerful one.

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Contribution of Individual Authors to the Creation of a Scientific Article (Ghostwriting Policy)

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Conflict of Interest

The authors have no conflicts of interest to declare.