International Information and Engineering Technology Association
Advancing the World of Information and Engineering

Mathematical Modelling of Engineering Problems
Vol. 8, No. 4, August, 2021, pp. 527-537
Journal homepage: http://iieta.org/journals/mmep

Approximations for the Concentration and Effectiveness Factor in Porous Catalysts of Arbitrary Shape: Taylor Series and Akbari-Ganji's Methods

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https://doi.org/10.18280/mmep.080405

Received: 27 February 2021
Accepted: 14 July 2021

Keywords:
mathematical modeling, nonlinear diffusion, reaction equation, Michaelis-Menten kinetic, Taylor series, Akbari-Ganji's method

ABSTRACT

A mathematical model of reaction-diffusion problem with Michaelis-Menten kinetics in catalyst particles of arbitrary shape is investigated. Analytical expressions of the concentration of substrates are derived as functions of the Thiele modulus, the modified Sherwood number, and the Michaelis constant. A Taylor series approach and the Akbari-Ganji's method are utilized to determine the substrate concentration and the effectiveness factor. The effects of the shape factor on the concentration profiles and the effectiveness factor are discussed. In addition to their simple implementations, the proposed analytical approaches are reliable and highly accurate, as it will be shown when compared with numerical simulations.

1. INTRODUCTION

Nonlinear differential equations in general and reaction-diffusion equations, in particular, arise as mathematical models of various phenomena sciences and engineering, where solutions of theoretical and experimental problems are often steady-state reaction-diffusion equations with nonlinear chemical kinetics. Of these problems, we mention as examples mathematical models in immobilized enzymes [1, 2], microbial cells [3-5], respiring tissue [6], and artificial kidney system [7]. Various analytical and numerical approaches have been utilized to find approximate solutions to these models. For example, Tosaka and Miyake [8] analyzed a mathematical model for oxygen diffusion in a spherical cell using an integral equation method. Maalmi et al. [9] presented the mathematical expressions for the steady-state reaction rate and the associated reactant concentration profiles using semi-analytical and numerical methods. Indira and Rajendran studied a mathematical model based on polyphenol oxidase catechol as a prototype enzymatic electro system [10]. Do and Greenfield used a finite integral transformation approach to solve a nonlinear kinetics problem in a general solid shape [11]. Bucolo and Tripathi studied the governing equations for the exchange of substrate between vascular and extravascular compartments on a steady-state condition [12]. Napper and Schubert investigated a mathematical Michaelis-Menten kinetics model of oxygen delivery to heart tissue [13]. Rajendran et al. used a homotopy perturbation approach for deriving an analytical expression of mediated bioelectrocatalysis concentration [14].

It is almost impossible to find exact solutions to nonlinear differential equations. Therefore, many numerical and analytical methods have been developed to find approximate solutions of nonlinear models that arise in real applications in almost all branches of sciences and engineering [15].

Although there are many effective numerical methods to solve nonlinear equations, finding approximate analytical solutions remains an ultimate goal to obtain a profound understanding of the effect of different parameters on the governing system. In addition, some serious drawbacks come along with numerical solutions, such as achieving numerical stabilities and the difficulty of adjusting parameters to match the numerical data [16]. Of the most used analytical methods, we mention the homotopy perturbation method [17, 18], homotopy analysis method [19], variational iteration method [20], Akbari-Ganji's method [21], Green's function method [22], Adomian decomposition method [23], and Taylor series method [24].

In addition to being largely accessible to researchers with a moderate mathematical background, recent applications of the Taylor series method (TSM) and Akbari-Ganji's method (AGM) have proved to be efficient and highly accurate for solving nonlinear models arise in various fields of sciences and engineering. For example, TSM has been employed in solving fractal Bratu equation [24], Lane–Emden equation [25], nonlinear reaction-diffusion equation in the electroactive polymer film [26], nonlinear equation in mass transfer [27], nonlinear concentration equation in electroanalytical chemistry [28], nonlinear reaction-diffusion problem in electrostatic interaction [29] and a nonlinear Poisson–Boltzmann equations [30]. The Akbari-Ganji's method (AGM) has also been utilized for deriving semi-analytic solutions of nonlinear models. For example, Berkan [21] used AGM to study the steady three-dimensional problem of condensation film on an inclined rotating. Nirmala et al. [31] derived the steady-state substrate and product concentrations for non-Michaelis-Menten kinetics in an amperometric biosensor using the hyperbolic function method, which is a particular case of the Akbari-Ganji method. Manimegalai et al. [32] used AGM to obtain approximate analytical solutions for the nonlinear equations that describe diffusion-limited reaction within the film. Dharmalingam et al. [33] solved nonlinear reaction-diffusion equations that determine the substrate concentration in the electroactive polymer film using AGM. More applications of the AGM method can be found in ref. [34-36].

In the present work, we employ both the Taylor series and Akbari-Ganji's methods to investigate a nonlinear diffusion model of oxygen in general geometry. The aim is to obtain simple closed-form approximate expressions of substrate concentration and effectiveness factor using for all Thiele modulus values, Michaelis constant, and modified Sherwood numbers in a solid of general shape.

2. MATHEMATICAL FORMULATION OF THE PROBLEM

A cell generally consists of a surface membrane and protoplasm. In the protoplasm, some organelles compartmentalize enzymes. The sequential metabolic reactions catalyzed by these enzymes provide the necessary energy for the cells. Therefore, the oxygen, which serves as the substrate for the metabolic reactions, plays an essential role in modulating these reactions. The oxygen tension gradient in a cell even governs the distribution of different organelles. The oxygen consumption rate in cells and tissues is a complex function of oxygen tension.

The purpose of the present work is to predict the oxygen tension in a slap, cylindrical and spherical cell using an oxygen uptake kinetics of the Michaelis-Menten type. This kinetics is rigorous because it predicts reasonably well the observed oxygen uptake rates. In addition, an unsteady state oxygen diffusion model is considered here, and transients of oxygen tension may give a better understanding of the oxygen diffusion characteristics.

The particle shape is assumed to have a strong symmetry to make the composition at any point in space as a function of a single spatial variable (e.g., slab, cylinder, and spherical enzyme support). Following Lin et al. [5], the diffusion of oxygen in general geometry is expressed as follows:

$$D\left(\frac{d^2S}{dX^2}+\frac{n}{X}\frac{dS}{dX}\right)-\frac{V_mS}{S+k_m}=0 \quad (1)$$

$$X=0; \frac{dS}{dX}=0 \quad (2)$$

$$X=d; D\frac{dS}{dX}=h(S_0-S) \quad (3)$$

where, S is the concentration of oxygen, D is the diffusion coefficients of oxygen, V_m is the maximum reaction rate, k_m is the Michaelis constant, respectively. The variable d represents the radius of the cell. S_0 is the concentration of oxygen outside the cell membrane n is a shape factor. By introducing the following dimensionless variables

$$A=\frac{S}{S_0}, x=\frac{X}{d}, S_h=\frac{hd}{D}, K_m=\frac{k_m}{S_0}, \alpha=\left(\frac{V_m d^2}{DS_0}\right) \quad (4)$$

Eq. (1) can be expressed in the form

$$\frac{d^2A(x)}{dx^2}+\frac{n}{x}\frac{dA(x)}{dx}-\frac{\alpha A(x)}{K_m+A(x)}=0 \quad (5)$$

The boundary conditions are

$$x=0, \frac{dA}{dx}=0 \text{ (Symmetry condition)}, \quad (6)$$

$$x=1, \frac{dA}{dx}=S_h(1-A) \text{ (Mixed boundary condition)}, \quad (7)$$

where, A is the dimensionless concentration of oxygen, S_h is the modified Sherwood number, and x is the radial coordinate.

The variable n characterizes the immobilized catalyst shape with n=0, 1, 2 for the slab, cylindrical and spherical particle, respectively. The geometry factor can be generalized to other non-standard catalysts particles [37, 38]. The shape parameter of the arbitrary geometry can be computed from the equation $n=(LS_a/V)-1$, where L is the characteristic length for the chosen geometry, S_a is the surface area of the catalyst particle, and V is its volume. Non-integer values for geometries other than regular ones can also be used [39]. The effectiveness factor is given by

$$Ef=\frac{(1+K_m)}{\alpha}\left[\frac{dA}{dx}\right]_{x=1}. \quad (8)$$

From Eq. (4), it is evident that with large values of Thiele modulus α, the rate term dominates, and the reaction is fast while slow diffusion limits the overall rate. Smaller values of the Thiele modulus represent slow reactions with rapid diffusion.

Michaelis-Menten constant K_m reflects the enzyme's affinity for its substrate. The smaller the value of K_m, the more strongly the enzyme binds the substrate. If the K_m value is known, it becomes possible to predict the cell needs (enzymes or substrate) to speed up the enzymatic reaction. The K_m value approximately measures the concentration of the substrate in the cell where a reaction is occurring.

3. CONCENTRATION OF SUBSTRATE USING THE TAYLOR SERIE METHOD (TSM)

This section uses TSM to solve the nonlinear boundary value problem (5)-(7). As discussed in the introduction, the TSM yields a semi-analytical solution in the form of a rapidly convergent series without a need for linearization.

The analytical expression for the concentration using the TSM is given by

$$A(x)=\sum_{i=0}^{\infty}\frac{x^i}{i!}\frac{d^iA}{dx^i}\bigg|_{x=0} = A(0)+\frac{x}{1!}\frac{dA}{dx}\bigg|_{x=0}+\frac{x^2}{2!}\frac{d^2A}{dx^2}\bigg|_{x=0}+\frac{x^3}{3!}\frac{d^3A}{dx^3}\bigg|_{x=0}+ \quad (9)$$

The successive derivatives of the function $A(x)$ (see Appendix A) are computed at 0 and denoted by $A_1(0)$, $A_2(0)$, $A_3(0)$, etc. Therefore,

$$A(x)=A(0)+A_1(0)x^2+A_2(0)x^4+A_3(0)x^6, \quad (10)$$

where,

$$A_1(0) = \frac{\alpha A(0)}{(n+1)\big(K_m + A(0)\big)} \frac{1}{2!},$$

$$A_2(0) = \frac{3\alpha^2 A(0)}{(n+1)(n+3)(K_m+A(0))^3} \frac{1}{4!}, \tag{11}$$

$$A_3(0) = \frac{15\alpha^3 A(0) K_m[(n+1)K_m - 2A(0)(n+3)]}{6!\ (n+1)^2(n+3)(n+5)(K_m+A(0))^5}$$

From boundary condition (7), we get

$$S_h A(0) - S_h + A_1(0)(2+S_h) + A_2(0)(4+S_h) + A_3(0)(6+S_h) = 0 \tag{12}$$

The unknown quantity $A(0)$ can be obtained by solving Eq. (12). For example, for the values S_h=1, K_m=0.5, n=0, and α=1, we obtain:

$$A(0)^6 + 3A(0)^5 + 3A(0)^4 + 1.10417A(0)^3 - 0.1125A(0)^2 - 0.159028A(0) - 0.03125 = 0,$$

which leads to $A(0)$=0.47119, and hence the substrate concentration, given by Eq. (10), becomes

$$A(x) = 0.339599 + 0.2022388069x^2 + 0.1195389474x^4 - 0.0008691325663x^6.$$

Using Eq. (8), the effectiveness factor is reduced to

$$Ef = \frac{(1+K_m)}{\alpha}(2A_1(0) + 4A_2(0) + 6A_3(0)), \tag{13}$$

where, $A_1(0), A_2(0),$ and $A_3(0)$ are given in Eq. (11).

Using the dimensionless variables in Eq. (4), the effectiveness factor is computed from Eq. (13), where

$$K_m = \frac{k_m}{S_0},$$

$$A_1(0) = \frac{\frac{1}{2}\left(\frac{V_m d^2}{DS_0}\right)A(0)}{(n+1)\left(\frac{k_m}{S_0} + A(0)\right)},$$

$$A_2(0) = \frac{\frac{3}{4!}\left(\frac{V_m d^2}{DS_0}\right)^2 A(0)}{(n+1)(n+3)\left(\frac{k_m}{S_0} + A(0)\right)^3},$$

$$A_3(0) = \frac{\frac{15}{6!}\left(\frac{V_m d^2}{DS_0}\right)^3 A(0)\frac{k_m}{S_0}\left((n+1)\frac{k_m}{S_0} - 2A(0)(n+3)\right)}{(n+1)^2(n+3)(n+5)\left(\frac{k_m}{S_0} + A(0)\right)^5}.$$

4. CONCENTRATION SUBSTRATE USING THE AKBARI-GANJI'S AND TAYLOR SERIES METHODS

As discussed in the introduction, Akbari-Ganji's method is a powerful algebraic approach that produces semi-analytic approximate solutions of nonlinear differential equations. The method requires no linearization and gives solutions in terms of convergent series. The AGM begins by assuming the solution to Eq. (5) is in the form of the hyperbolic function:

$$A(x) = B_1\cosh(mx) + B_2\sinh(mx) \tag{14}$$

Substituting boundary conditions (6)-(7) in Eq. (15) gives

$$B_1 = \frac{S_h}{m\sinh m + S_h\cosh m}, B_2 = 0 \tag{15}$$

$$A(x) = A(0)\cosh(mx) \tag{16}$$

where, $A(0) = B_1 = \frac{S_h}{m\sinh m + S_h\cosh m}$.

From Eq. (17), we obtain

$$m = \cosh^{-1}\left(\frac{A(1)}{A(0)}\right). \tag{17}$$

Therefore, a derived analytical expression of the concentration is given by

$$A(x) = A(0)\cosh\left[x\cosh^{-1}\left[\frac{A(1)}{A(0)}\right]\right] \tag{18}$$

and the effectiveness factor is

$$Ef = \frac{(1+K_m)A(1)}{\alpha}\sinh\left[\cosh^{-1}\left[\frac{A(1)}{A(0)}\right]\right] = \frac{(1+K_m)A(1)}{\alpha}\sqrt{\frac{\big(A(1)\big)^2 - A(0)^2}{A(0)^2}} \tag{19}$$

As pointed out earlier, notice that $A(0)$ can be obtained from Eq. (12) for given parameters values. When $n = \frac{L\,S_a}{V} - 1$, both the concentration and effectiveness factor of a substrate of arbitrary shape can be obtained from Eq. (10).

5. PREVIOUS RESULT

Devi et al. [40] used the Adomian decomposition method (ADM) to find the following analytical expressions for the concentration of substrate and effectiveness factor.

5.1 Slab

The concentration of substrate and the effectiveness factor are given by

$$A(x) = 1 + l(\alpha) + m(\alpha)x^2 - 2\frac{m(\alpha)K_m}{(K_m+1)}\left[\frac{3l(\alpha)}{2} + \frac{5m(\alpha)}{12} - \frac{l(\alpha)x^2}{2} - \frac{m(\alpha)x^4}{12}\right] \tag{20}$$

$$Ef = \frac{(1+K_m)}{\alpha}\left(2m(\alpha) + 2\frac{m(\alpha)K_m}{(K_m+1)}\left[l(\alpha) + \frac{m(\alpha)}{3}\right]\right) \tag{21}$$

5.2 Spherical

The concentration of substrate and the effectvenes factor are given by in spherical is

$$A(x) = 1 + \frac{1}{3}[l(\alpha) + m(\alpha)] - 2\frac{m(\alpha)K_m}{S_h(K_m+1)}\left[\frac{l(\alpha)}{9} + \frac{m(\alpha)}{15} + \frac{S_h l(\alpha)}{18} + \frac{S_h m(\alpha)}{18} + \frac{S_h l(\alpha)x^2}{2} + \frac{S_h m(\alpha)x^4}{12}\right] \tag{22}$$

where

$$l(\alpha) = -\left[\frac{1}{2}\frac{\alpha}{K_m+1} + \frac{\alpha}{S_h(K_m+1)}\right], m(\alpha) = \frac{1}{2}\left[\frac{\alpha}{K_m+1}\right]. \tag{23}$$

$$Ef = \frac{(1+K_m)}{\alpha}\left(-2\frac{m(\alpha)K_m}{S_h(K_m+1)}\left[S_h l(\alpha) + \frac{S_h m(\alpha)}{3}\right]\right)$$

It is to be mentioned here that the Adomian decomposition method usually fails to provide any meaningful information beyond a finite interval [41].

6. ESTIMATION OF PARAMETERS

From Eq. (5), the reaction rate can be written in the form:

$$\frac{1}{R} = \frac{K_m + A}{\alpha A} \tag{24}$$

that is, $RA = \alpha A - K_m R$, where K_m and α are unknown parameters. Using the method of least squares, the normal equation, in a matrix form can be written as

$$\begin{pmatrix} \sum A_i & -\sum R_i \\ \sum A_i R_i & -\sum {R_i}^2 \end{pmatrix} \begin{pmatrix} \alpha \\ K_m \end{pmatrix} = \begin{pmatrix} \sum A_i R_i \\ \sum A_i {R_i}^2 \end{pmatrix} \tag{25}$$

By solving the above system, we can obtain Thiele module (α) and Michaela's constant (K_m). Eq. (25) may also be written in the form

$$\frac{1}{R} = \frac{K_m}{\alpha}\frac{1}{A} + \frac{1}{\alpha} \tag{26}$$

By plotting $1/R$ versus $1/A$, we can obtain the slope K_m/α and the intercept $1/\alpha$ and hence the kinetic parameters K_m and α can be deduced.

7. NUMERICAL SIMULATIONS

The nonlinear differential Eq. (5) subject to boundary conditions (6) and (7) is solved numerically by using the MATLAB function "pdex4". Figure 1 shows that the analytical TSM solution (Eqs. (10)), AGM solution (Eq. (20)), ADM solution [26], and the numerical solution are in strong agreement.

For Figures 1(a)-(d), the following values of $A(0)$ were used to generate the dimensionless concentrations:

Figure 1(a): $A(0)$= 0.02166, 0.37910, 0.69631, 0.98651,
Figure 1(b): $A(0)$=0.11800, 0.38558, 0.67532, 0.99950,
Figure 1(c): $A(0)$=0.02609, 0.26651, 0.36167, 0.46493,
Figure 1(d): $A(0)$= 0.26651, 0.45986, 0.58199.

Tables 1-2 represent give a closer comparison between numerical results and analytical results (Taylor's series method, Akbari-Ganji's method and Adomian decomposition method). The average relative errors at discrete points show that TSM and AGM are superior to the ADM, which is valid only for small values of parameters.

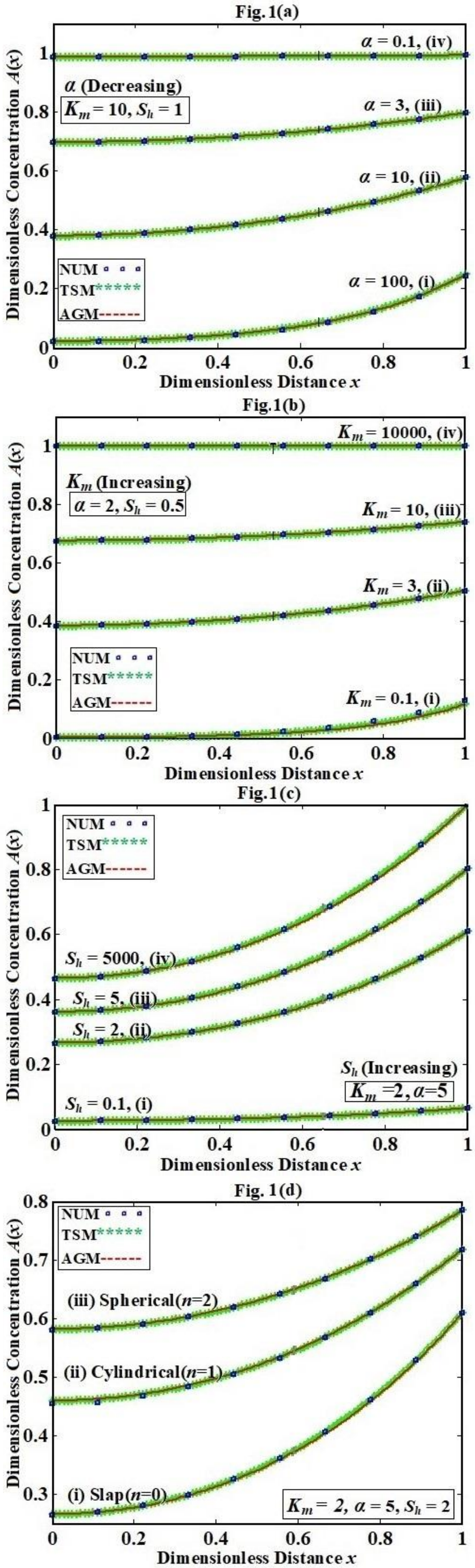

Figure 1. Dimensionless concentration substrate $A(x)$ versus dimensionless distance x for different values of $A(0)$

Tables 3-6 show that the analytical values of the effective factor computed by the proposed TSM are equal to the numerical values for various kinetic parameters unlike the analytical values computed by the ADM where some variations are evident.

Table 1. Comparison of numerical solution of the concentration of substrate $A(x)$ with the analytical solutions by TSM, AGM, and ADM methods for K_m=1, S_h=0.5 and different values of α (Slab, n=0)

α=0.1, $A(0)$= 0.882322							
x	Num	TSM Eq. (10)	TSM Error (%)	AGM Eq. (18)	AGM Error (%)	ADM Eq.(20)	ADM Error (%)
0.0	0.9851	0.9851	0	0.9851	0.00	0.9851	0.00
0.2	0.9853	0.9853	0.00	0.9853	0.00	0.9853	0.00
0.4	0.9859	0.9859	0.00	0.9859	0.00	0.9859	0.00
0.6	0.9869	0.9869	0.00	0.9869	0.00	0.9869	0.00
0.8	0.9883	0.9883	0.00	0.9883	0.00	0.9883	0.00
1.0	0.9901	0.9901	0.00	0.9901	0.00	0.9901	0.00
	Average Error		**0.00**		**0.00**		**0.00**

α=0.2, $A(0)$= 0.779004							
x	Num	TSM Eq. (10)	TSM Error (%)	AGM Eq. (18)	AGM Error (%)	ADM Eq.(20)	ADM Error (%)
0.0	0.6872	0.6872	0	0.6872	0.00	0.6888	0.23
0.2	0.6914	0.6913	0.01	0.6913	0.01	0.6929	0.22
0.4	0.7039	0.7036	0.04	0.7034	0.07	0.7051	0.17
0.6	0.7248	0.7241	0.10	0.7239	0.12	0.7255	0.10
0.8	0.7544	0.753	0.19	0.7528	0.21	0.7543	0.01
1.0	0.7905	0.7905	0.00	0.7905	0.00	0.7917	0.15
	Average Error		**0.06**		**0.07**		**0.15**

α=0.7, $A(0)$= 0.545345							
x	Num	TSM Eq. (10)	TSM Error (%)	AGM Eq. (18)	AGM Error (%)	ADM Eq.(20)	ADM Error (%)
0.0	0.4889	0.4889	0	0.4889	0.00	0.5101	4.34
0.2	0.4954	0.4953	0.02	0.4952	0.04	0.5163	4.22
0.4	0.5153	0.5147	0.12	0.5143	0.19	0.535	3.82
0.6	0.5487	0.5475	0.22	0.5468	0.35	0.5665	3.24
0.8	0.5964	0.5942	0.37	0.5935	0.49	0.6113	2.50
1.0	0.6555	0.6555	0.00	0.6555	0.00	0.6701	2.23
	Average Error		**0.12**		**0.18**		**3.39**

Table 2. Comparison of numerical solution of the concentration of substrate $A(x)$ with the analytical solutions by TSM, AGM, and ADM for K_m=1, α=0.5 for different values of S_h (Spherical, n=2)

S_h=1, m=0.881506							
x	Num	TSM Eq. (10)	TSM Error (%)	AGM Eq. (18)	AGM Error (%)	ADM Eq.(22)	ADM Error (%)
0.0	0.8815	0.8815	0	0.8815	0.00	0.9232	4.73
0.2	0.8831	0.8831	0.00	0.8831	0.00	0.9233	4.55
0.4	0.8879	0.8876	0.03	0.8877	0.02	0.9236	4.02
0.6	0.8959	0.8956	0.03	0.8956	0.03	0.9241	3.15
0.8	0.9071	0.9066	0.06	0.9066	0.06	0.9547	5.25
1.0	0.9208	0.9208	0.00	0.9208	0.00	0.9255	0.51
	Average Error		**0.02**		**0.02**		**3.70**
S_h=2, m=0.919362							
x	Num	TSM Eq. (10)	TSM Error (%)	AGM Eq. (18)	AGM Error (%)	ADM Eq.(22)	DM Error (%)
0.0	0.9194	0.9194	0	0.9194	0.00	0.961	4.52
0.2	0.921	0.921	0.00	0.921	0.00	0.9611	4.35
0.4	0.9259	0.9258	0.01	0.9258	0.01	0.9613	3.82
0.6	0.9341	0.9338	0.03	0.9338	0.03	0.9616	2.94
0.8	0.9455	0.945	0.05	0.945	0.05	0.962	1.75
1.0	0.9595	0.9595	0.00	0.9595	0.00	0.9625	0.31
	Average Error		**0.02**		**0.02**		**2.95**
S_h=3, m= 0.932364							
x	Num	TSM Eq. (10)	TSM Error (%)	AGM Eq. (18)	AGM Error (%)	ADM Eq.(22)	ADM Error (%)
0.0	0.9324	0.9324	0	0.9324	0.00	0.974	4.46
0.2	0.934	0.934	0.00	0.934	0.00	0.9741	4.29
0.4	0.9389	0.9388	0.01	0.9388	0.01	0.9743	3.77
0.6	0.9472	0.9469	0.03	0.9469	0.03	0.9745	2.88
0.8	0.9587	0.9582	0.05	0.9582	0.05	0.9749	1.69
1.0	0.9728	0.9728	0.00	0.9728	0.00	0.9752	0.25
	Average Error		**0.02**		**0.02**		**2.89**

Table 3. Comparison between simulation results and analytical results (TSM and ADM) for effective factor with fixed values of K_m=0.1 and S_h=5 and various values α

α	Num	TSM Eq. (13)	% TSM Error	ADM Eq. (21)	% ADM Error
0	0.995	0.995	0.00	0.9952	0.02
0.1	0.9954	0.9954	0.00	0.9956	0.02
0.2	0.9904	0.9904	0.00	0.9912	0.08
0.3	0.9848	0.9848	0.00	0.9868	0.20
0.4	0.9787	0.9787	0.00	0.9824	0.38
0.5	0.9718	0.9718	0.00	0.978	0.64
0.6	0.9641	0.9641	0.00	0.9736	0.99
0.7	0.9553	0.9553	0.00	0.9691	1.44
0.8	0.9451	0.9451	0.00	0.9647	2.07
0.9	0.9331	0.9331	0.00	0.9603	2.92
1	0.9188	0.9188	0.00	0.9559	4.04
Avg. Error			**0.00**		**1.16**

Table 4. Comparison between simulation results and analytical results (TSM and ADM) for effective factor with fixed values of K_m=50 and S_h=5 and various values α

α	Num	TSM Eq. (13)	% TSM Error	ADM Eq. (21)	% ADM Error
0	0.9995	0.9995	0.00	0.9995	0.00
0.1	0.999	0.999	0.00	0.999	0.00
0.2	0.998	0.998	0.00	0.998	0.00
0.3	0.9969	0.9969	0.00	0.9969	0.00
0.4	0.9959	0.9959	0.00	0.9959	0.00
0.5	0.9948	0.9948	0.00	0.9948	0.00
0.6	0.9939	0.9939	0.00	0.9939	0.00
0.7	0.9929	0.9929	0.00	0.9929	0.00
0.8	0.9919	0.9919	0.00	0.9919	0.00
0.9	0.9909	0.9909	0.00	0.9909	0.00
1	0.9899	0.9899	0.00	0.9899	0.00
Avg. Error			**0.00**		**0.00**

Table 5. Comparison between simulation results and analytical results (TSM and ADM) for effective factor with fixed values of α=0.1 and S_h=5 and various values K_m

K_m	Num	TSM Eq. (13)	% TSM Error	ADM Eq. (21)	% ADM Error
0	0.995	0.995	0.00	0.995	0.00
0.1	0.9954	0.9954	0.00	0.9954	0.00
0.2	0.9923	0.9923	0.00	0.9923	0.00
0.3	0.9903	0.9903	0.00	0.9903	0.00
0.4	0.9889	0.9889	0.00	0.9889	0.00
0.5	0.988	0.988	0.00	0.988	0.00
0.6	0.9874	0.9874	0.00	0.9874	0.00
0.7	0.987	0.987	0.00	0.987	0.00
0.8	0.9868	0.9868	0.00	0.9868	0.00
0.9	0.9867	0.9867	0.00	0.9867	0.00
1	0.9867	0.9867	0.00	0.9867	0.00
Avg. Error			**0.00**		**0.00**

Table 6. Comparison between simulation results and analytical results (TSM and ADM) for effective factor with fixed values of α=1 and S_h=5 and various values K_m

K_m	Num	TSM Eq. (13)	% TSM Error	ADM Eq. (21)	% ADM Error
0	0.92	0.92	0.00	0.9559	3.90
0.1	0.9188	0.9188	0.00	0.9359	1.86
0.2	0.8933	0.8933	0.00	0.9259	3.65
0.3	0.8799	0.8799	0.00	0.9053	2.89
0.4	0.8726	0.8726	0.00	0.8912	2.13
0.5	0.8705	0.8705	0.00	0.8815	1.26
0.6	0.8685	0.8685	0.00	0.8750	0.75
0.7	0.8670	0.8670	0.00	0.8708	0.44
0.8	0.8655	0.8655	0.00	0.8683	0.32
0.9	0.8640	0.8640	0.00	0.867	0.35
1	0.8620	0.8620	0.00	0.8667	0.55
Avg. Error			**0.00**		**1.65**

8. RESULTS AND DISCUSSION

The nonlinear Eq. (5) is solved using two simple, efficient, and reliable approaches: The Taylor series and the Akbari-Ganji methods. Semi-analytical approximate concentrations were obtained for all values of parameters using Taylor series (Eq. (10)) and AGM (Eq. (18)). Figures 1 and 2 show that there is a strong agreement between the analytical and numerical results. From Tables 1 and 2, it is confirmed that the accuracy of the proposed methods (TSM and AGM) significantly surpasses the accuracy of AGM.

The obtained concentration depends on the Michaelis constant (K_m), Thiele module (α), and the modified Sherwood number (S_h). The Thiele modulus, which is used for the determination of the effectiveness factor, describes the relationship between diffusion and reaction as follows:

$$\alpha = \sqrt{\frac{V_m L^2}{2DS_0}} = \frac{\text{Diffusion Time}}{\text{Reaction Time}}$$

The Sherwood number S_h, which is also known as the mass transfer Nusselt number represents the ratio of convective to diffusive mass transfer coefficients, that is

$$S_h = \frac{K_m L}{D} = \frac{\text{Convective mass transfer coefficient}}{\text{Diffusion mass transfer coefficient}}$$

where, L is a characteristic length, D is the mass diffusivity, k_m is the mass transfer coefficient. Figure 1 represents the substrate's concentration for various Michaelis-Menten values of the constant K_m, Thiele modulus α, and Sherwood number S_h for planar, cylindrical, and spherical particles. It is inferred from Figure 1 that the concentration of the substrate increases when Michaelis's constant (K_m) and Sherwood number (S_h) increase or the Thiele modulus (α) decreases for all geometries. The concentration curves for the spherical, cylindrical, and planar particles are plotted in Figure 1(d). It is observed that the substrate concentration for a spherical particle is greater than that of a planar or a cylindrical particle.

To measure variations in reaction rates throughout the process, a parameter for the effectiveness factor, which is the ratio of the pellet's overall reaction rate to the reaction rate at the pellet's external surface, is introduced.

The effectiveness factor is an essential indicator of pore diffusion and reactions on pore walls in porous catalytic pellets and solid fuel particles. It is established by Thiele [35] that the reaction rate in a particle may be expressed by the product of its rate under surface conditions and the effectiveness factor.

Figure 2 demonstrates the effects of Thiele modulus, Michaelis constant, modified Sherwood number, and shape factors (slap, cylindrical and spherical) on the effectiveness factor. When the reaction rate controls the process, the effectiveness factor approaches unity. However, the effectiveness factor decreases rapidly when Thiele modulus's value increases (Figures 2(a)-2(c)) for all other parameters' values.

At high Sherwood number values (S_h), the mass transfer limitations are the dominating factors in determining the substrate conversion. Figure 2(a) shows the effects of S_h on the internal effectiveness factor. The effectiveness factor continues to increase slowly as S_h increases. When S_h, however, becomes larger than 1000, the effectiveness factor becomes independent of it.

From Figure 2(b), it is inferred that the effectiveness factor is uniform for high Michaelis constant due to the intraparticle diffusion.

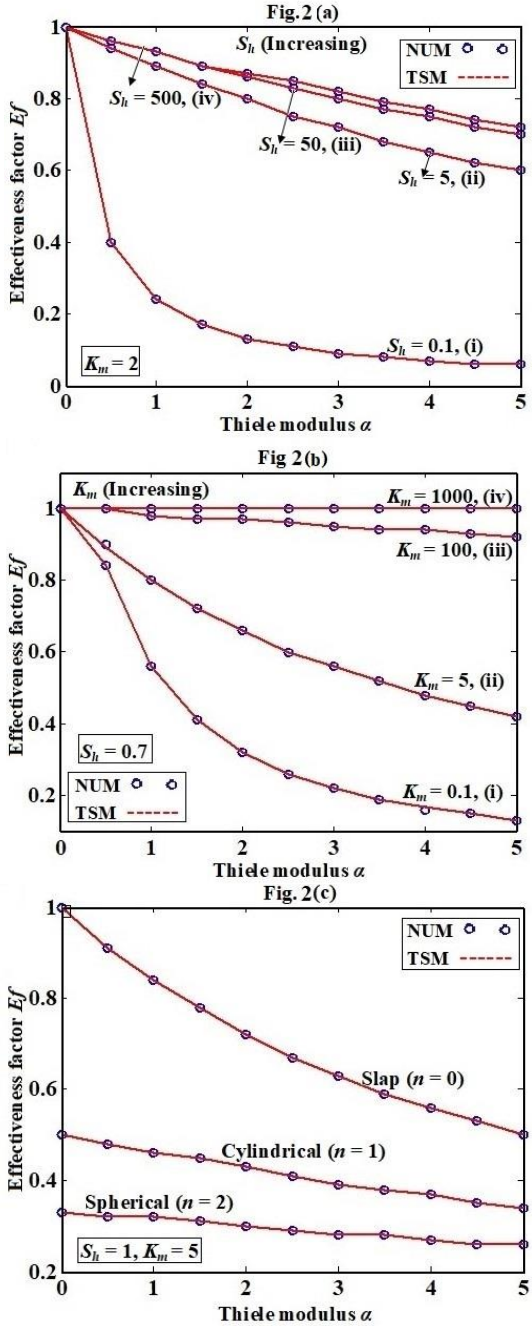

Figure 2. Comparison of analytical expression of effective factor with simulation results for various values of K_m, α and S_h

The effectiveness factor curves for the spherical, cylindrical, and slap particles are plotted in Figure 2(c). From these figures, it is observed that the effectiveness factor for slap particle is more significant than a planar, cylindrical, and spherical particle.

Figures 3(a)-(b) illustrate the influence of shape factor on the concentration and effectiveness factor for various parameters' values. From these figures, it is inferred that slab shape gave better results on the effectiveness factor than those of the other shapes. A better diffusion mass transfer in the slab shape leads to a better yield.

The limiting cases for saturated (zero-order) catalytic kinetics and un-saturated (first-order) catalytic kinetics are discussed in Appendix B.

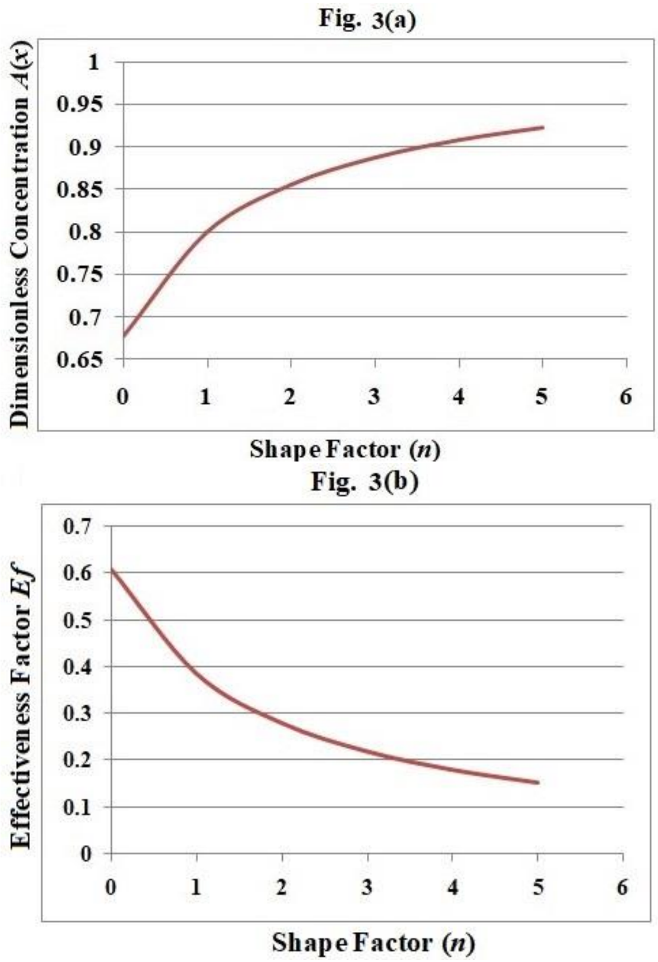

Figure 3. Concentration of substrate and effectiveness factor versus shape factor

9. CONCLUSION

Two approximate semi-analytical methods for solving reaction-diffusion problems inside catalyst particles were discussed. Analytical expressions for the substrate's concentration and the effectiveness factor for all parameters are obtained using Taylor series and Akbari-Ganji's methods. The effects of Michaelis constant, Thiele module, and modified Sherwood number, and the shape factor on the concentration profiles were discussed. The sensitivity analysis and estimation of the kinetics parameter were also reported. It was concluded that a lower shape factor results in a stronger effectiveness factor. In terms of mass diffusion transfer, the other form is inferior to the slab shape, leading to a lower yield. The analytical results derived by the proposed methods produced less relative error than the results of the Adomian decomposition method when compared to numerical simulation results. The proposed approximation approach can be applied to several multicomponent reactions in various catalyst geometries with adequate precision.

ACKNOWLEDGMENT

This work was supported by the Academy of Maritime Education and Training (AMET), Deemed to be University, Chennai. The authors are thankful to Shri J. Ramachandran, Chancellor, Col. and Dr. G. Thiruvasagam, Vice-Chancellor of AMET, Chennai, Tamil Nadu, for their immense support.

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NOMENCLATURE

Symbols	Name	Unit
S	Substrate concentration	mol/cm^3
S_0	Bulk-substrate concentration	mol/cm^3
k_m	Michaelis – Menten constant	mol/cm^3
D	Effective diffusivity inside the particle	cm^{2}s^{-1}
V_m	Maximum reaction rate	mol/cm^{3}s
x	Spatial variable	cm
h	Permeability of the membrane at X=d	cm/s
d	Radius of the cell	cm
α	Dimensionless reaction rate	
X	Dimensionless Spatial Variable	
K_m	Dimensionless Michaelis -Menten constant	
S_h	Modified Sherwood number	
A	Dimensionless substrate concentration (=S/S_0)	
n	Shape factor (n = 0 for slab, n=1 for cylindrical and n = 2 for spherical particle, n=(LS_a/V)-1 for general geometry), L is the characteristic length for the chosen geometry, S_a is the surface area of the catalyst particle, and V is the volume	

APPENDIX A. APPROXIMATE ANALYTICAL SOLUTION OF EQ. (5) USING TAYLOR SERIES

The Taylor series solution of Eq. (5) is given in the form

$$A(x) = A(0) + A'(0)\frac{x}{1!} + A''(0)\frac{x^2}{2!} + \cdots \tag{A1}$$

From the boundary condition Eq. (6), we have

$$A'(0) = 0 \tag{A2}$$

and Eq. (5) can be rewritten as follows:

$$[xA''(x) + nA'(x)]\big(K_m + A(x)\big) - x\alpha A(x) = 0 \tag{A3}$$

Differentiate the above equation with respect to x we get

$$\begin{aligned}&[xA'''(x) + (n+1)A''(x)]\big(K_m + A(x)\big)\\ &= -A'(x)[nA'(x) + xA''(x)] + \alpha x A'(x) + \alpha A(x)\end{aligned} \tag{A4}$$

When x=0, Eq. (A4) results in

$$[(n+1)A''(0)]\big(K_m + A(0)\big) = \alpha A(0), \tag{A5}$$

and hence

$$A''(0) = \frac{\alpha A(0)}{(n+1)\big(K_m + A(0)\big)} \tag{A6}$$

Differentiating Eq. (A7) with respect to x and substituting x=0 gives

$$\begin{aligned}&(n+2)A'''(0)(K_m + A(0))\\ &= 2\alpha A'(0) - nA'(0)A''(0)\\ &- 2A'(0)[nA''(0) + A''(0)\end{aligned}$$

Using initial condition in Eq. (7) gives

$$A'''(0) = 0,\ A^{(5)}(0) = 0 \tag{A7}$$

$$A^{(4)}(0) = \frac{3\alpha^2 A(0)}{(n+1)(n+3)(K_m + A(0))^3} \tag{A8}$$

$$\begin{aligned}&A^{(6)}(0)\\ &= \frac{15\alpha^3 A(0)K_m[(n+1)K_m - 2A(0)(n+3)]}{(n+1)^2(n+3)(n+5)(K_m + A(0))^5}\end{aligned} \tag{A9}$$

Substituting (A2) and (A6-A9) into (A1) gives the explicit concentration form.

Substituting x=1 in the derived concentration and its derivative gives

$$\begin{aligned}&A(1)\\ &= A(0) + \frac{\alpha A(0)}{(n+1)\big(K_m + A(0)\big)}\frac{1}{2!}\\ &+ \frac{3\alpha^2 A(0)}{(n+1)(n+3)(K_m + A(0))^3}\frac{1}{4!}\\ &+ \frac{15\alpha^3 A(0)K_m[(n+1)K_m - 2A(0)(n+3)]}{(n+1)^2(n+3)(n+5)(K_m + A(0))^5}\frac{1}{6!}\end{aligned} \tag{A10}$$

$$\begin{aligned}&A'(1)\\ &= A(0) + \frac{\alpha A(0)}{(n+1)\big(K_m + A(0)\big)}\frac{2}{2!}\\ &+ \frac{12\alpha^2 A(0)}{(n+1)(n+3)(K_m + A(0))^3}\frac{1}{4!}\\ &+ \frac{90\alpha^3 A(0)K_m[(n+1)K_m - 2A(0)(n+3)]}{(n+1)^2(n+3)(n+5)(K_m + A(0))^5}\frac{1}{6!}\\ &+ \cdots\end{aligned} \tag{A11}$$

where, A(0) can be obtained from boundary condition (6). Now Eqs. (A10) and (A11) can be used in the boundary condition

$$A'^{(1)} = S_h\big(1 - A(1)\big). \tag{A12}$$

From Eq. (A10), we can obtain the value of $A(0)$ and hence. we can obtain the concentration of substrate for slap, spherical, and cylindrical cases by using $n = 0, 1,$ and 2, respectively.

APPENDIX B. LIMITING CASES

B.1 Saturated (zero order) catalytic kinetics

We initially consider the situation where the substrate concentration of oxygen $A(x)$ is much greater than the Michaelis constant K_m, that is, $A(x) \gg K_m$. In such a case, Eq.

(5) takes on the simple linear form

$$xA''(x) + nA'(x) - \alpha x = 0 \qquad (B1)$$

The boundary conditions are

$$x = 0, \frac{dA}{dx} = 0 \qquad (B2)$$

$$x = 1, \frac{dA}{dx} = S_h(1 - A) \qquad (B3)$$

The solution is readily obtained for the following cases:
For n=0, Eq. (B1) becomes

$$A''(x) - \alpha = 0 \qquad (B4)$$

In this case the concentration and the effectiveness factor are, respectively,

$$A(x) = \frac{1}{2}\left(\frac{2S_h - \alpha(2 + S_h)}{S_h} + \alpha x^2\right) \qquad (B5)$$

$$Ef = \frac{(1 + K_m)}{\alpha}\left[\frac{dA}{dx}\right]_{x=1} = \frac{1}{\alpha}(\alpha) = 1 \qquad (B6)$$

For $n = 1$, Eq. (B1) becomes

$$xA''(x) + A'(x) - \alpha x = 0 \qquad (B7)$$

and in this case, the concentration and the effictiveness factor are, respectively,

$$A(x) = \frac{1}{4}\left(\frac{4S_h - \alpha(2 + S_h)}{S_h} + \alpha x^2\right) \qquad (B8)$$

$$Ef = \frac{(1 + K_m)}{\alpha}\left[\frac{dA}{dx}\right]_{x=1} = \frac{1}{\alpha}\left(\frac{\alpha}{2}\right) = \frac{1}{2} \qquad (B9)$$

For n=2, Eq. (B4) becomes

$$xA''(x) + 2A'(x) - \alpha x = 0 \qquad (B10)$$

In this case, the concentration and the effictiveness factor are, respectively,

$$A(x) = \frac{1}{6}\left(\frac{6S_h - \alpha(2 + S_h)}{S_h} + \alpha x^2\right) \qquad (B11)$$

$$Ef = \frac{(1 + K_m)}{\alpha}\left[\frac{dA}{dx}\right]_{x=1} = \frac{1}{\alpha}\left(\frac{\alpha}{3}\right) = \frac{1}{3} \qquad (B12)$$

B.2 Unsaturated (first order) catalytic kinetics

Here we consider the case when the substrate concentration in the film is less than the Michaelis constant. That is, we assume that $A(x)$<<1. In this case, Eq. (5) can be written as follows

$$xA''(x) + nA'(x) - \frac{\alpha x A(x)}{K_m} = 0 \qquad (B13)$$

Assume a solution of the form

$$A(x) = B_1 \cosh(mx) + B_2 \sinh(mx) \qquad (B14)$$

By using boundary conditions (B2) and (B3), we obtain

$$B_1 = \frac{S_h}{m \sinh m + S_h \cosh m}, B_2 = 0 \qquad (B15)$$

and hence,

$$A(x) = \frac{S_h \cosh(mx)}{m \sinh m + S_h \cosh m} \qquad (B16)$$

$$A'(x) = \frac{mS_h \sinh(mx)}{m \sinh m + S_h \cosh m} \qquad (B17)$$

$$A''(x) = \frac{m^2 S_h \cosh(mx)}{m \sinh m + S_h \cosh m} \qquad (B18)$$

If we substitute these into Eq. (B14), we have

$$\frac{m^2 S_h \cosh(mx)}{m \sinh m + S_h \cosh m} + \frac{n}{x}\frac{mS_h \sinh(mx)}{m \sinh m + S_h \cosh m} - \frac{\alpha}{K_m}\frac{m^2 S_h \cosh(mx)}{m \sinh m + S_h \cosh m} = 0 \qquad (B19)$$

Using L'Hospital's rule in Eq. (B21) at $x = 0$ leads to

$$\frac{m^2(1 + n)S_h \cosh(mx)}{m \sinh m + S_h \cosh m} - \frac{\alpha}{K_m}\frac{S_h \cosh(mx)}{m \sinh m + S_h \cosh m} = 0 \qquad (B20)$$

$$m^2(1 + n) - \frac{\alpha}{K_m} = 0 \qquad (B21)$$

which implies

$$m = \pm\sqrt{\frac{\alpha}{K_m(1 + n)}} \qquad (B22)$$

Substituting this value in (B16) gives the explicit concentration of the substrate. The effictive factor is given by

$$Ef = \frac{(1 + K_m)}{\alpha}\frac{mS_h \sinh(mx)}{m \sinh m + S_h \cosh m} \qquad (B23)$$