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Mathematical Modelling of Immobilized α-Chymotrypsin Enzyme in Acetonitrile Medium Under Kinetic Control Using Rajendran-Joy Approach

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ABSTRACT

A mathematical model of reaction-diffusion processes in immobilized chymotrypsin enzyme in an acetonitrile medium under kinetic control is discussed. The model is developed using a system of reaction-diffusion equations with a nonlinear component associated with the enzymatic reaction's kinetics. The Rajendran-Joy approach gives the general analytical expressions of acyl donor and nucleophile concentrations in spherical biocatalyst particles. The initial rate of consumption of each substrate is also reported. The effect of reaction and diffusion parameters on substrate concentration and consumption rate is also discussed. A numerical solution of nonlinear equations was compared with theoretical results. There is a good degree of agreement between the two results.

1. INTRODUCTION

Recently, there has been a lot of interest in enzymes and biological catalysts, especially for monophasic chemical solvents [1-5]. When enzymes are compressed into cellular organelles or enzyme chains, catalytic activity can occur [6]. The catalytic systems generated here are heterogeneous, and most enzymes are insoluble. When evaluating enzyme activity, it is critical to consider the roles of external and internal diffusion of non-aqueous enzyme systems [7]. These problems could be resolved using immobilized enzymes. By immobilization, the structure of the enzymes is often maintained, permitting their usage even under extreme environments [8, 9].

Theories concerning biocatalyst behaviour are based on fundamental physical or chemical analyses. It is advantageous to apply thermodynamic approaches that consider the components' distribution throughout the different phases and their solvent in the bulk phase [10, 11]. Enzymes are beneficial in various applications, including food-related conversions, analysis, and chemical processing [12]. One area where enzymes have proven particularly useful is in producing optically active intermediates. These are chemical compounds that rotate the plane of polarized light. Studying simultaneous diffusion and reaction is essential for optimizing the catalytic system, as demonstrated by the many articles that describe and numerically simulate these processes [13-18]. A model was developed to describe the kinetic regulation of immobilized a-chymotrypsin's production in an acetonitrile medium [19].

The simple analytical expression of the acyl donor and nucleophile molar concentrations has not been published using simple mathematical concepts. In this work, we developed a new analytical expression concentration using Rajendran-Joy method. Furthermore, each substrate's analytical expression of rate consumption has been provided. With analytical data support, comprehending the physical influence of each parameter will be simple. The theoretical results will help to understand the physical impact of parameters, which will be useful in analysing the rate of consumption of substrates and optimising the processes. Additionally, we compare our analytical results for the molar concentrations with the numerical simulations using the MATLAB program.

2. MATHEMATICAL FORMULATION

We can consider the function of immobilized chymotrypsin in an acetonitrile medium under kinetic control. Also, the enzymes have been distributed evenly in the spherical biocatalyst particles. External mass transfer limitations were considered negligible. Under these conditions, the chemical reaction in enzyme-catalyzed reactions may be described as follows [19]:

$$AcD + Nuc \rightarrow Pep + LG \tag{1}$$

Hydroylsis of acyl donor:

$$AcD + H_2O \rightarrow Hyp + LG \tag{2}$$

The mass balance equations for peptide and hydrolysis products can be expressed for the above intrinsic kinetics as follows:

$$\frac{d^2[AcD]}{dr^2} + \frac{2}{r}\frac{d\,[AcD]}{dr} = \frac{\left(k_{Synth}[Nuc] + k_{Hydr}\right)[AcD][E_0]}{D_{Aeff}(k_N + [Nuc])} \tag{3}$$

$$\frac{d^2[Nuc]}{dr^2}+\frac{2}{r}\frac{d\,[Nuc]}{dr}=\frac{k_{Synth}[Nuc]\,[AcD][E_0]}{D_{Neff}(k_N+[Nuc])} \quad (4)$$

The boundary conditions are:

$$At\ r=0, \qquad \frac{d[AcD]}{d\,r}=0, \qquad \frac{d[Nuc]}{d\,r}=0 \quad (5)$$

$$At\ r=R,\ [AcD]=[AcD]_B,\ [Nuc]=[Nuc]_B \quad (6)$$

where, $[AcD]$ and $[Nuc]$ are the molar concentration of acyl donor and nucleophile. The other parameters are defined in the nomenclature. For every substrate, the initial rate of consumption is:

$$Rate_A=\frac{4\,\pi\,R^2D_{Aeff}}{M_p}\left(\frac{d[AcD]}{d\,r}\right)_{r=R} \quad (7)$$

$$Rate_N=\frac{4\,\pi\,R^2D_{Neff}}{M_p}\left(\frac{d[Nuc]}{d\,r}\right)_{r=R} \quad (8)$$

By introducing the dimensionless variables:

$$u=\frac{[AcD]}{[AcD]_B}, v=\frac{[Nuc]}{[Nuc]_B}$$
$$x=\frac{r}{R}, \gamma_1=\frac{R^2k_{Hydr}[AcD]_BE_0}{D_{Aeff}k_N}$$
$$\gamma_2=\frac{R^2k_{Synth}[AcD]_B[Nuc]_BE_0}{D_{Neff}k_N}$$

$$\alpha_1=\frac{k_{Synth}\,[Nuc]_B}{k_{Hydr}}, \alpha_2=\frac{[Nuc]_B}{k_N} \quad (9)$$

The Eqs. (3) and (4) reduce to the following dimensionless form:

$$\frac{d^2u(x)}{dx^2}+\frac{2}{x}\frac{du(x)}{dx}=\frac{\gamma_1\,u(x)(1+\alpha_1\,v(x))}{1+\,\alpha_2\,v(x)} \quad (10)$$

$$\frac{d^2v(x)}{dx^2}+\frac{2}{x}\frac{dv(x)}{dx}=\frac{\gamma_2\,u(x)v(x)}{1+\,\alpha_2\,v(x)} \quad (11)$$

The boundary condition becomes:

$$At\ x=0, \qquad \frac{d\,u}{d\,x}=0, \qquad \frac{d\,v}{d\,x}=0 \quad (12)$$

$$At\ x=1, \qquad u=1, \qquad v=1 \quad (13)$$

The dimensionless form of initial rate of consumption each substrate is:

$$\frac{Rate_A}{\mu}=\left(\frac{d\,u}{d\,x}\right)_{x=1} \quad (14)$$

$$\frac{Rate_N}{\eta}=\left(\frac{d\,v}{d\,x}\right)_{x=1} \quad (15)$$

where,

$$\mu=\frac{4\,\pi\,R^2D_{Aeff}[AcD]_B}{M_p}, \eta=\frac{4\,\pi\,R^2D_{Neff}[Nuc]_B}{M_p} \quad (16)$$

3. RESULT AND DISCUSSION

3.1 Analytical expression of concentration and initial rate of consumption

There are several asymptotic techniques for solving nonlinear reaction-diffusion equations. Recently, the homotopy perturbation [20-24]. Tayor series [25-28], variational iteration [29-31], Pade approximations [32]. Akbari-Ganji [33-37], Rajendran-Joy [38-40], Adomian decomposition [41, 42], and homotopy analysis methods [43] have been used to solve nonlinear equations.

Although the homotopy perturbation method solves some issues with the traditional perturbation method, it is not always possible to expect a compact answer. The presumed solution in the Akbari-Ganji method is expressed in the algebraic form (i. e., $u(x)=a+bx+cx^2+\cdots$). This approach is inapplicable for the semi-infinite boundary value problems i.e., $x\epsilon[0,\infty]$. The solutions derived from the Taylor series and the variational iteration approach are inconsistently convergent. Although Adomian decomposition method is often efficient, the convergence of the series only sometimes results in a compact solution. This method also has the disadvantage of requiring the computation of Adomian polynomials, which may be challenging. Homotopy analysis approaches have limitations, such as the incorporation of auxiliary operators, parameters, and functions.

In the Rajendran-Joy approach, an initial solution is considered an exponential function with unknown coefficients. The number of unknown coefficients in the initial solution is greater than the order of the differential equation. These unknown constant coefficients, which are the key to solving the linear/nonlinear differential equation, can be obtained from the initial conditions and the differential equation. The basic concept of the Rajendran-Joy method (RJM) is given in Appendix A. Consider the following exponential function to solve Eqs. (10) and (11):

$$u(x)=A_0e^{mx}+B_0e^{-mx} \quad (17)$$

$$v(x)=A_1e^{nx}+B_1e^{-nx} \quad (18)$$

where, A_0, B_0, A_1, B_1, m and n are constant. Determining the constant values using boundary conditions (12) and (13) is simple:

$$A_0=\frac{1}{\cosh(m)}, A_1=\frac{1}{\cosh(n)}, \quad B_0=0, \text{and } B_1=0 \quad (19)$$

As a result, Eqs. (17) and (18) become:

$$u(x)=\frac{\cosh\,(m\,x)}{\cosh(m)} \quad (20)$$

$$v(x)=\frac{\cosh\,(n\,x)}{\cosh(n)} \quad (21)$$

We consider the generalized version of Eqs. (10) and (11) to find the constant m and n in Eqs. (20) and (21) as follows:

$$F(x)=\frac{d^2u(x)}{dx^2}+\frac{2}{x}\frac{du(x)}{dx}-\frac{\gamma_1\,u(x)(1+\alpha_1\,v(x))}{1+\,\alpha_2\,v(x)}=0 \quad (22)$$

$$G(x) = \frac{d^2v(x)}{dx^2} + \frac{2}{x}\frac{dv(x)}{dx} - \frac{\gamma_2\, u(x)v(x)}{1 + \alpha_2\, v(x)} = 0 \qquad (23)$$

Applying L-Hospitals' rule in the Eqs. (22) and (23), and at $x = 0$, we get:

$$F(x)|_{x=0} = 3m^2 - \frac{\gamma_2\,(1 + \alpha_1\, sechn)}{1 + \alpha_2\, sechn} = 0 \qquad (24)$$

$$G(x)|_{x=0} = 3n^2 - \frac{\gamma_2 sechm}{1 + \alpha_2\, sechn} = 0 \qquad (25)$$

From the above result we get:

$$m = \sqrt{\frac{\gamma_1(1 + \alpha_1 \operatorname{sech} n)}{3\,(1 + \alpha_2 \operatorname{sech} n)}}$$
$$n = \sqrt{\frac{\gamma_2 \operatorname{sech}\left(\sqrt{\frac{\gamma_1(1 + \alpha_1 \operatorname{sech} n)}{3\,(1 + \alpha_2 \operatorname{sech} n)}}\right)}{3\,(1 + \alpha_2 \operatorname{sech} n)}} \qquad (26)$$

When m and n are very small, $sechn = 1$. Now m and n become:

$$m = \sqrt{\frac{\gamma_1(1+\alpha_1)}{3\,(1+\alpha_2)}} \text{ and } n = \sqrt{\frac{\gamma_2}{3\,(1+\alpha_2)}} \qquad (27)$$

The initial rate of consumption of each substrate is:

$$\frac{Rate_A}{\mu} = \left(\frac{d\,u}{d\,x}\right)_{x=1} = \left(\sqrt{\frac{\gamma_1(1 + \alpha_1)}{3\,(1 + \alpha_2)}}\right) tanh\left(\sqrt{\frac{\gamma_1(1 + \alpha_1)}{3\,(1 + \alpha_2)}}\right) \qquad (28)$$

$$\frac{Rate_N}{\eta} = \left(\frac{d\,v}{d\,x}\right)_{x=1} = \left(\sqrt{\frac{\gamma_2}{3\,(1 + \alpha_2)}}\right) \tanh\left(\sqrt{\frac{\gamma_2}{3\,(1 + \alpha_2)}}\right) \qquad (29)$$

3.2 Previous analytical results

Veeramuni et al. [9] solved Eqs. (10) and (11) using boundary conditions (12) and (13), employing the Adomian decomposition method. Adomian [44] created the Adomian decomposition technique (ADM) between the 1970s and the 1990s. This technique is not only efficient but also versatile, capable of resolving various linear, nonlinear, ordinary, and partial differential equations, as well as integral transforms. They obtained the analytical equation for the concentration as follows:

$$u(x) = 1 - \frac{(A - 6l_1)(x^2 - 1)}{36} + \frac{A\,(x^4 - 1)}{120} \qquad (30)$$

$$v(x) = 1 - \frac{(B - 6m_1)(x^2 - 1)}{36} + \frac{B\,(x^4 - 1)}{120} \qquad (31)$$

where,

$$l_1 = \frac{\gamma_1(1 + \alpha_1)}{(1 + \alpha_2)}, m_1 = \frac{\gamma_2}{(1 + \alpha_2)}$$
$$A = l_1^2 + \frac{m_1^2}{\gamma_2}(\gamma_1\alpha_1 - \alpha_2 l_1) \text{ and } B = m_1\left(\frac{m_1^2}{\gamma_2} + l_1\right) \qquad (32)$$

The initial rate of consumption of each substrate is:

$$\frac{Rate_A}{\mu} = \left(\frac{d\,u}{d\,x}\right)_{x=1} = -\frac{(A - 6l_1)}{18} + \frac{A}{30} \qquad (33)$$

$$\frac{Rate_N}{\eta} = \left(\frac{d\,v}{d\,x}\right)_{x=1} = -\frac{(B - 6m_1)}{18} + \frac{B}{30} \qquad (34)$$

The ADM has limitations, however. The first is that the approach produces a series of solutions that need to be shortened for practical use. Also, it is challenging to find Adomian polynomials. However, using the RJM approach, we can quickly determine the coefficients. Also, ADM method fail to provide some significant information beyond a finite interval [45].

3.3 Validation of the analytical methods

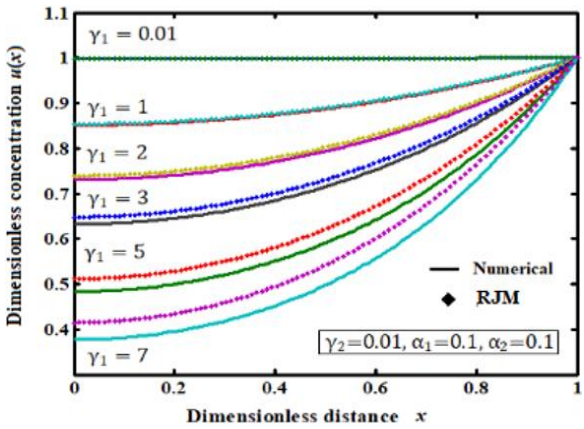
The nonlinear Eqs. (10) and (11) are also numerically solved using MATLAB program. In Tables 1 and 2, the numerical outcomes are compared with our new analytical and prior findings. The average error difference percentage between the numerical results and our new findings across all parameter values is 0.8598. The greatest average error variation between the numerical and prior results (ADM method) is 1.3752. Tables 1 and 2 indicate that the nucleophile concentration near the particle centre consistently exceeds that of the acyl donor. This is because limits on mass transfer have more impact on the acyl donor than on the nucleophilic substrate.

3.4 Effects of the parameters on concentration and initial rate of consumption

The substrate concentrations depend upon the diffusion parameters γ_1 and $\gamma_2$and reaction parameters α_1 and α_2.

The diffusion parameters are directly propositional to enzyme load and inversely proportional to diffusion coefficients. The kinetics rate constant and the reaction parameters have an inverse relationship. In Figures 1(a)-(b), the substrate's concentration profile for various diffusion parameter γ_1 and α_1 is plotted using Eq. (21). These figures show that the concentration value is close to 1 ($u(x) \approx 1$) or uniform for all small values of the parameters. The concentration consequently declines as the diffusion parameters γ_1 and α_1 decreased (Figures 1(c)-(d)).

The concentration $v(x)$ for various diffusion parameter values γ_1 and γ_2 is displayed using Eq. (21) in Figure 2. This figure illustrates that the concentration value is uniform for all small values of the parameters α_1 and α_2.The concentration is uniform for the lowest diffusion parameter values. Concentration decreases as the diffusion parameter values increase. In all of these cases, the concentration gradients are steeper for the acyl donor than for the nucleophile. As the enzyme loading increases (γ_1 or γ_2 increases), the concentration slopes get steeper for both the acyl donor and the nucleophile. This means that mass transfer is more limited, as expected.



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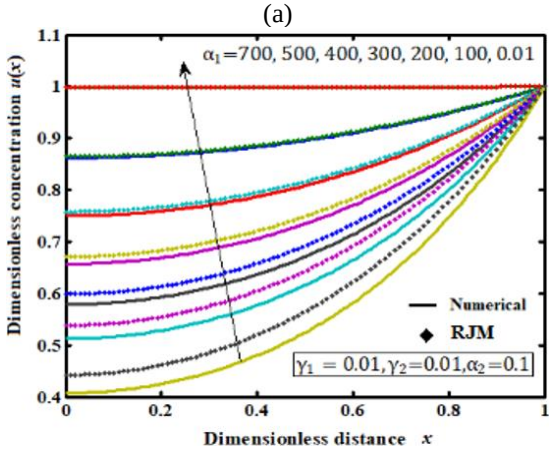

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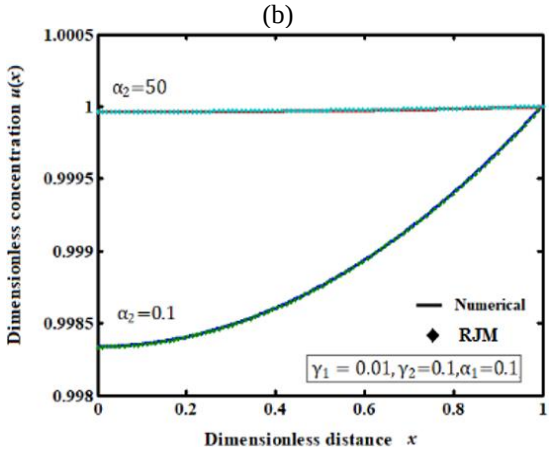

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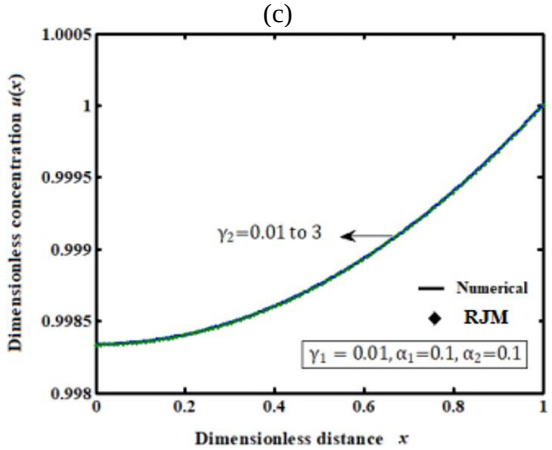
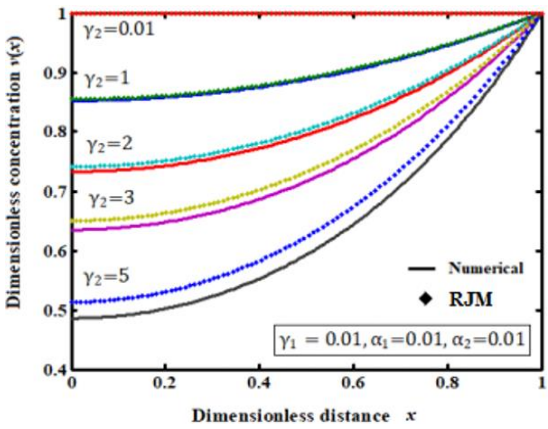


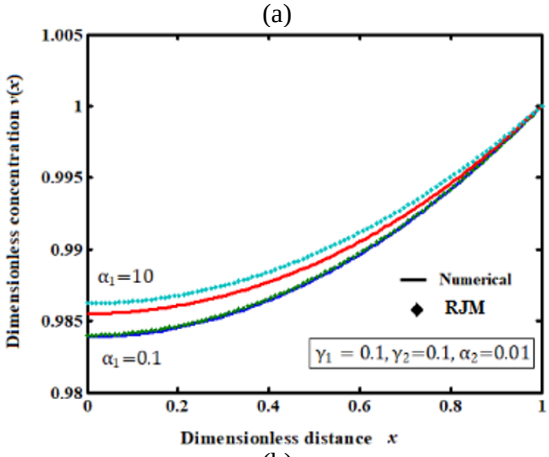
(d)

Note: The dotted line shows the Eq. (16), while the solid line is the numerical outcomes.

Figure 1. Comparison of analytical result for concentration of acyl donor $u(x)$ with simulation result for various value for γ_1, γ_2, α_1 and α_2



(a)



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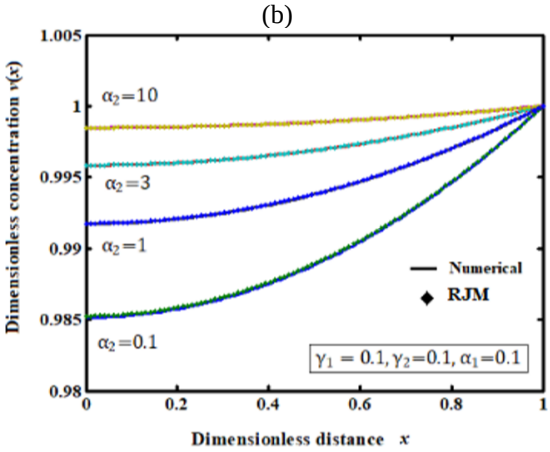

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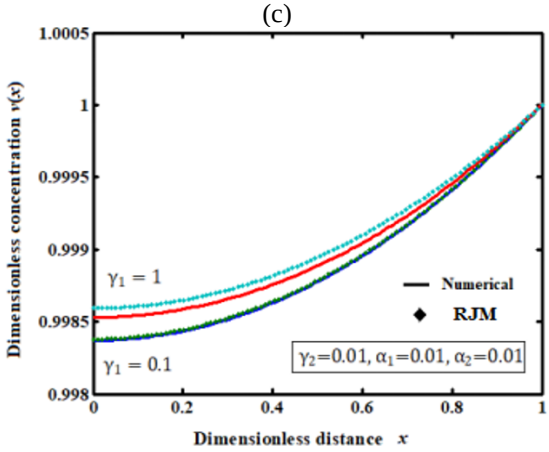


(d)

Note: The dotted line indicates the Eq. (16), while the solid line represents the numerical findings.

Figure 2. Comparison of analytical expression of concentration of nucleophile $v(x)$ with simulation result for various value for γ_1, γ_2, α_1 and α_2

Table 1. Comparison of dimensionless substrate concentration $u(x)$ for different parameter values of γ_2 when γ_1= 0.01, α_1 = 0.01, and α_2 = 0.01 with simulation results and previous analytical results

x	$\gamma_1 = 1, m = 0.5773503$					$\gamma_1 = 2, m = 0.8164966$				
	Numerical	RJM Eq. (16) This Work	ADM [41] Eq. (21)	Error % RJM Eq. (16) This Work	Error % ADM [41] Eq. (21)	Numerical	RJM Eq. (16) This Work	ADM [41] Eq. (21)	Error % RJM Eq. (16) This Work	Error % ADM [41] Eq. (21)
0	0.8509	0.8537	0.8539	0.3291	0.3527	0.7308	0.7395	0.7444	1.1905	1.8610
0.2	0.8567	0.8595	0.8597	0.3268	0.3501	0.7408	0.7496	0.7536	1.1879	1.7279
0.4	0.8743	0.8771	0.8770	0.3203	0.3088	0.7713	0.7801	0.7816	1.1409	1.3354
0.6	0.9040	0.9065	0.9067	0.2765	0.2986	0.8237	0.8319	0.8306	0.9955	0.8377
0.8	0.9466	0.9483	0.9489	0.1795	0.2430	0.9006	0.9064	0.9038	0.6440	0.3553
1	1.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000
Average error (%)				0.2387	0.2587	Average error (%)			0.8598	1.0195

Table 2. Comparison of dimensionless substrate concentration $v(x)$ for different parameter values of γ_1 when γ_2= 0.01, α_1 = 0.1, and α_2 = 0.1 with simulation results and previous analytical result

x	$\gamma_2 = 1, n = 0.574419$					$\gamma_2 = 2, n = 0.81281$				
	Numerical	RJM Eq. (17) This Work	ADM [41] Eq. (22)	Error % RJM Eq. (17) This Work	Error % ADM [41] Eq. (22)	Numerical	RJM Eq. (17) This Work	ADM [41] Eq. (22)	Error % RJM Eq. (17) This Work	Error % ADM [41] Eq. (22)
0	0.8523	0.8550	0.8554	0.3168	0.3637	0.7328	0.7413	0.7458	1.1599	1.7740
0.2	0.8580	0.8608	0.8609	0.3263	0.3263	0.7427	0.7513	0.7549	1.1579	1.6426
0.4	0.8754	0.8782	0.8791	0.3198	0.4223	0.7730	0.7817	0.7829	1.1255	1.2807
0.6	0.9049	0.9074	0.9075	0.2763	0.2873	0.8250	0.8331	0.8316	0.9818	3.2242
0.8	0.9471	0.9488	0.9490	0.1795	0.2006	0.9014	0.9071	0.9044	0.6323	0.3328
1	1.0000	1.0000	1.0000	0.0000	0.0000	1.0000	1.0000	1.0000	0.0000	0.0000
Average error (%)				0.2364	0.2667	Average error (%)			0.8429	1.3752

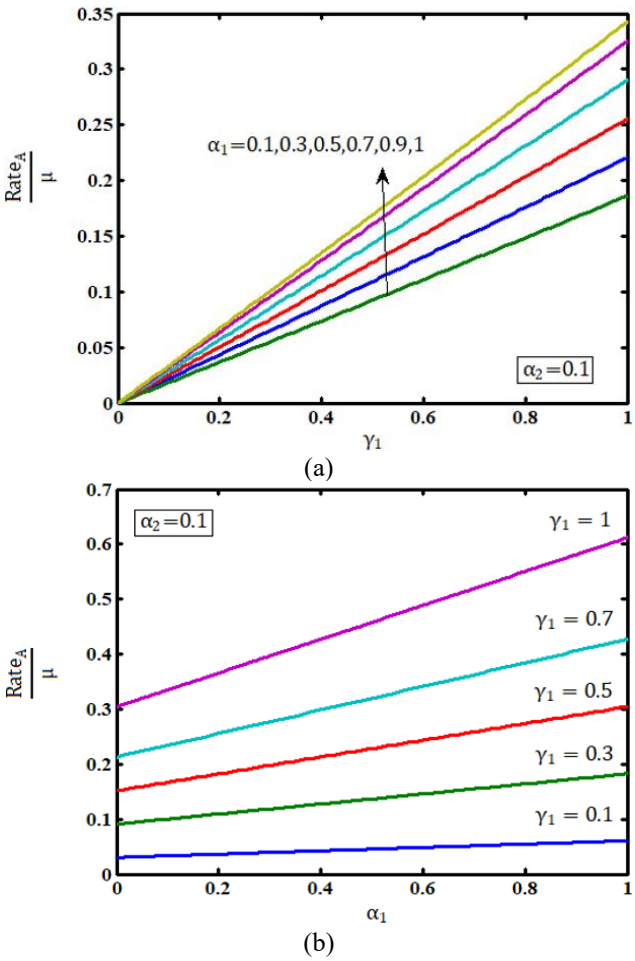


Figure 3. Effect of initial rate of substrate consumption $\frac{\text{Rate}_A}{\mu}$ for different values of γ_1, α_1 and α_2 using Eq. (19)

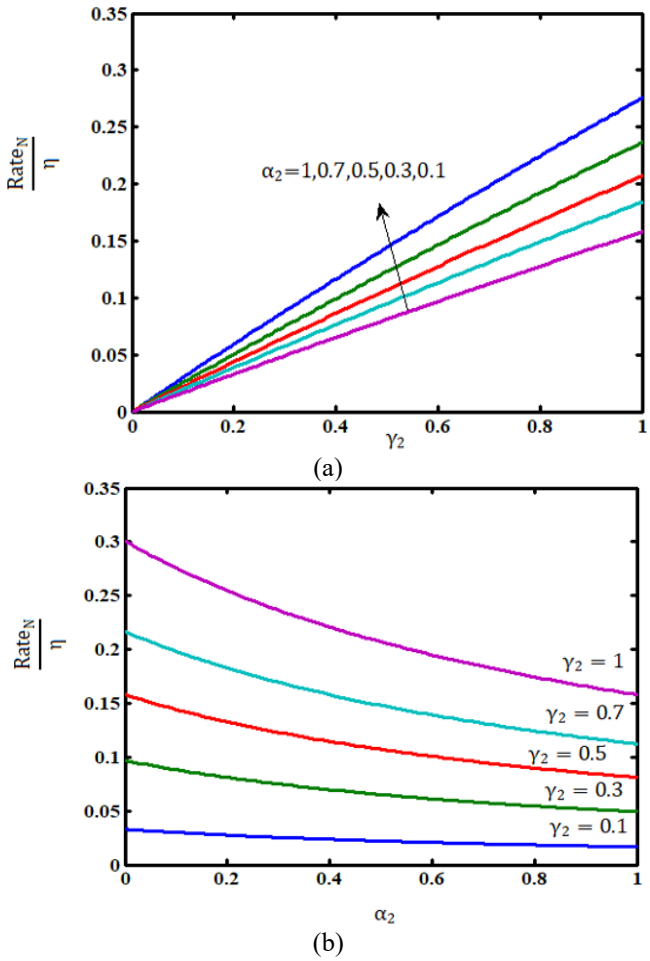


Figure 4. Effect of initial rate of substrate consumption $\frac{\text{Rate}_N}{\eta}$ for different values of γ_2 and α_2 using Eq. (20)

Figures 3 and 4 demonstrate the dimensionless consumption rate vs dimensionless variables γ_1, α_1 and α_2 for the substrates *u* and *v*, respectively. From these figures, it is observed that the consumption rate rises as the values of α_1 and α_2 increase for certain fixed values of other parameters. The data show that the rate consumption remains constant for all values of the parameter γ_1 as the dimensionless parameter γ_2 grows. The consumption rate increases as enzyme loading E_0 increases.

4. EXTENSIONS TO THE THEORETICAL MODEL

The following section describes further improvements to the theoretical model offered in this work. In this section, the general geometry of the electrode was addressed. The reaction-diffusion equations for immobilized enzyme systems have the following form:

$$\frac{d^2[AcD]}{dr^2} + \frac{N}{r}\frac{d[AcD]}{dr} = \frac{(k_{Synth}[Nuc] + k_{Hydr})[AcD][E_0]}{D_{Aeff}(k_N + [Nuc])} \quad (35)$$

$$\frac{d^2[Nuc]}{dr^2} + \frac{N}{r}\frac{d[Nuc]}{dr} = \frac{k_{Synth}[Nuc][AcD][E_0]}{D_{Neff}(k_N + [Nuc])} \quad (36)$$

where, the shape factor $N = 0$ (planar electrode), $N = 1$ (cylindrical electrode) and $N = 2$ (spherical electrode). The boundary conditions are:

$$At\ r = 0, \quad \frac{d[AcD]}{dr} = 0, \quad \frac{d[Nuc]}{dr} = 0 \quad (37)$$

$$At\ r = R,\ [AcD] = [AcD]_B,\ [Nuc] = [Nuc]_B \quad (38)$$

The Eqs. (37) and (38) reduce to the following dimensionless form.

$$\frac{d^2u(x)}{dx^2} + \frac{N}{x}\frac{du(x)}{dx} = \frac{\gamma_1\, u(x)(1 + \alpha_1\, v(x))}{1 + \alpha_2\, v(x)} \quad (39)$$

$$\frac{d^2v(x)}{dx^2} + \frac{N}{x}\frac{dv(x)}{dx} = \frac{\gamma_2\, u(x)v(x)}{1 + \alpha_2\, v(x)} \quad (40)$$

The boundary condition becomes:

$$At\ x = 0, \frac{du}{dx} = 0, \frac{dv}{dx} = 0 \quad (41)$$

$$At\ x = 1, u = 1, v = 1 \quad (42)$$

The approximate analytical expressions of acyl donor and nucleophile concentration are:

$$u(x) = \frac{cosh(m\,x)}{cosh(m)} \quad (43)$$

$$v(x) = \frac{cosh(n\,x)}{cosh(n)} \quad (44)$$

where, m and n:

$$m = \sqrt{\frac{\gamma_1(1 + \alpha_1\,\mathrm{sech}\,n)}{(N+1)(1 + \alpha_2 \mathrm{sech} n)}}$$
$$n = \sqrt{\frac{\gamma_2\,\mathrm{sech}\left(\sqrt{\frac{\gamma_1(1 + \alpha_1\,\mathrm{sech}\,n)}{(N+1)\,(1 + \alpha_2 \mathrm{sech} n)}}\right)}{(N+1)(1 + \alpha_2 \mathrm{sech} n)}} \quad (45)$$

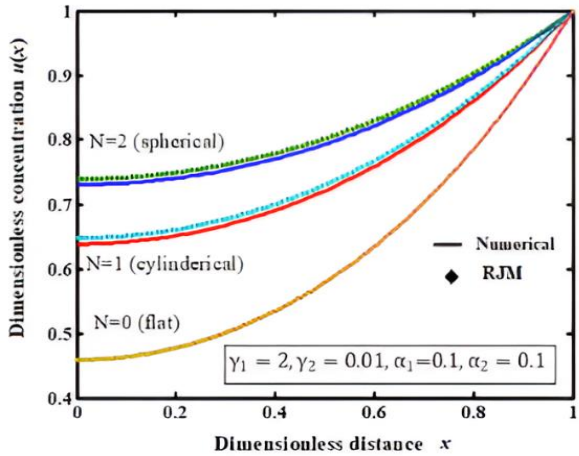
When m and n are very small, $sechn = 1$. Now m and n become:

$$m = \sqrt{\frac{\gamma_1(1+\alpha_1)}{(N+1)\,(1+\alpha_2)}} \text{ and } n = \sqrt{\frac{\gamma_2}{(N+1)\,(1+\alpha_2)}}$$

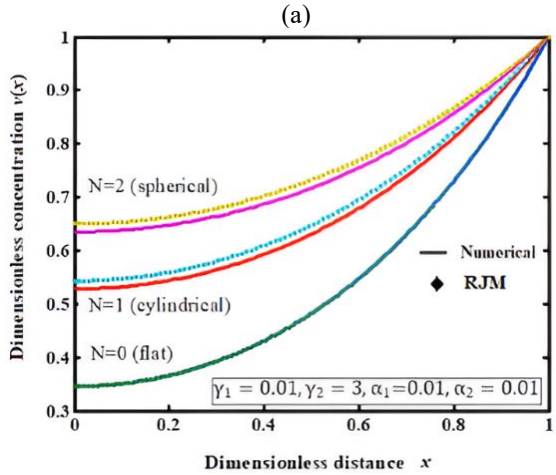
The initial rate of consumption of each substrate is:

$$\frac{Rate_A}{\mu} = \left(\frac{du}{dx}\right)_{x=1} = \left(\sqrt{\frac{\gamma_1(1+\alpha_1)}{(N+1)\,(1+\alpha_2)}}\right) tanh\left(\sqrt{\frac{\gamma_1(1+\alpha_1)}{(N+1)\,(1+\alpha_2)}}\right) \quad (46)$$

$$\frac{Rate_N}{\eta} = \left(\frac{dv}{dx}\right)_{x=1} = \left(\sqrt{\frac{\gamma_2}{(N+1)\,(1+\alpha_2)}}\right) \tanh\left(\sqrt{\frac{\gamma_2}{(N+1)\,(1+\alpha_2)}}\right) \quad (47)$$



(a)



(b)

Note: Dotted line: analytical and solid line: numerical

Figure 5. The effect of parameter N on concentrations

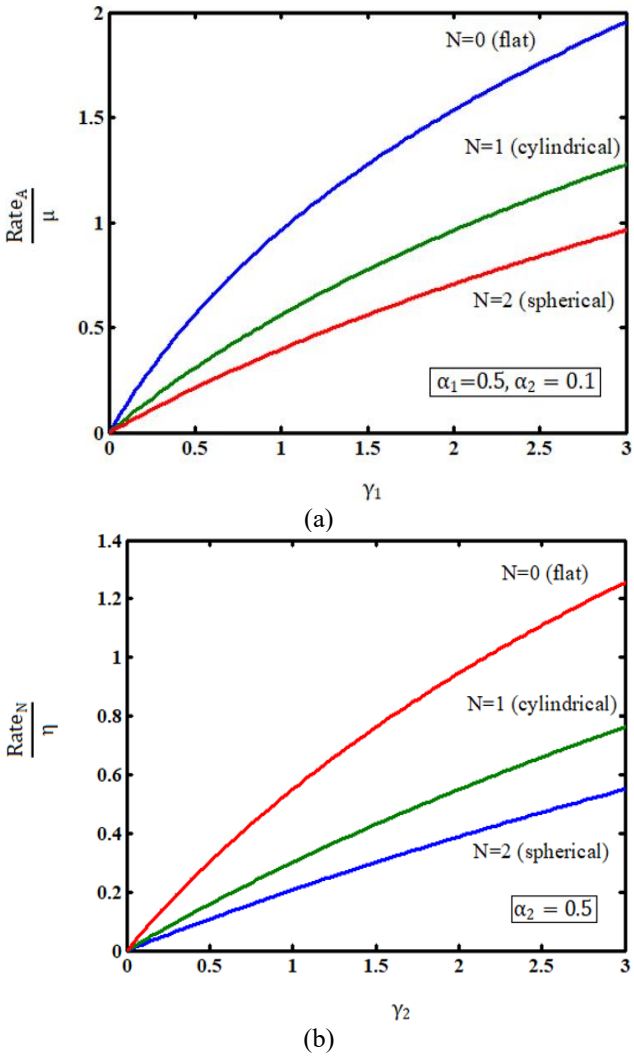


Figure 6. Effect of initial rate of substrate consumption $\frac{\text{Rate}_A}{\mu}$ and $\frac{\text{Rate}_N}{\eta}$ for various values of γ_1, α_1, γ_2 and α_2

The analytical expression of concentration of acyl donor and nucleophile $u(x)$ and $v(x)$ with simulation result for various N in Figure 5. From the Figures, it is observed that the concentration is high in spherical electrode compared to flat and cylindrical electrode.

Figure 6 depicts the analytical expression of acyl donor and nucleophile consumption rates and the simulation results for varying N. It is discovered that consumption is higher in spherical electrodes than in flat and cylindrical electrodes.

5. CONCLUSIONS

The mathematical modelling of immobilized enzyme systems is examined. The closed analytical expressions of concentration are obtained using the RJM approach. This method offers a straightforward solution for concentration in planar, cylindrical, and spherical electrodes. The impact of the parameters on concentration is also discussed. There is good agreement between the theoretical and numerical results. This theoretical model helps in the analysis and comprehension of the system's dynamics, as well as parameter optimization. This technique may be applied to solve nonlinear equations in microbial fuel cell and biosensor for real-time environmental monitoring.

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NOMENCLATURE

E_0	Amount of enzyme, mg ml^{-1}
$[AcD]_B$	Bulk molar concentration of acyl donor, mM
$[Nuc]_B$	Bulk molar concentration of nucleophile, mM
$[AcD]$	Concentration of acyl donor, mM
$[Nuc]$	Concentration of nucleophile, mM
$[Pep]$	Concentration of peptide product, mM
$[Hyp]$	Concentration of hydrolysis product, mM
D_{Aeff}	Effective diffusion coefficient of acyl donor, cm^2/s
D_{Neff}	Effective diffusion coefficient of nucleophile, cm^2/s
k_{Hydr}	Kinetic constant, μ mol min^{-1} mg C T^{-1}
k_N	Kinetic constant, mM
k_{Synth}	Kinetic constant, μ mol min^{-1} mg C T^{-1}
r	Distance from the centre of the particle, cm
R	Particle radius, cm
LG	Leaving group (ethanol or methanol)
$u(x)$	Dimensionless concentration of substrate
$v(x)$	Dimensionless concentration of substrate
x	Dimensionless distance
$\gamma_1, \gamma_2, \alpha_1, \alpha_2$	Dimensionless parameters

APPENDIX

A basic concept of Rajendran-Joy method (RJM)

Suppose that the nonlinear second-order differential equation with one independent variable *x* is given by:

$$p_s: f(u_s, u_s', u_s'') = 0; s = 1,2, \dots, r \tag{A1}$$

where, p_s is a polynomial of $u_s = u_s(x, a, b)$ and its derivatives. In this case, *a* and *b* represent the parameters, and *x* is within the interval [L, U], which may be either finite or semi-infinite, subject to the following boundary constraints.

$$\begin{cases} At\ x = L, u_s(x) = u_{sL_0}\ or\ u_s'(x) = u_{sL_1} \\ At\ x = U, u_s(x) = u_{sU_0}\ or\ u_s'(x) = u_{sU_1} \end{cases} \tag{A2}$$

Consider that the solution to the nonlinear equations is an exponential function of the given form.

$$u_s(x) = l_s \exp(n_s x^n) + m_s \exp(-n_s x^n) \tag{A3}$$

The exponential function is chosen because of its applicability to both finite and semi-infinite boundary conditions. The value of *n* is either 1 or 2, depending upon the defined boundary constraints. The unknown coefficients l_s, m_s and n_s are obtained by solving the nonlinear equations as follows:

$$\begin{cases} u_s(L) = l_s \exp(n_s L^n) + m_s \exp(-n_s L^n) = u_{sL_0} \\ or \\ u_s'(L) = n\, l_s \exp(n_s L^n) - n\, m_s \exp(-n_s L^n) = u_{sL_1} \end{cases} \tag{A4}$$

and

$$\begin{cases} u_s(U) = l_s \exp(n_s U^n) + m_s \exp(-n_s U^n) = u_{sU_0} \\ or \\ u_s'(U) = n\, l_s \exp(n_s U^n) - n\, m_s \exp(-n_s U^n) = u_{sU_1} \end{cases} \tag{A5}$$

The following algebraic nonlinear equations are obtained by substituting Eq.(A3) into Eq. (A1).

$$\begin{cases} p_1 = f(u_1(x, l_s, m_s, n_s, n, a, b), \\ \quad u_1'(x, l_s, m_s, n_s, n, a, b), \\ \quad u_1''(x, l_s, m_s, n_s, n, a, b)) = 0 \\ \quad . \\ \quad . \\ \quad . \\ p_r = f(u_r(x, l_s, m_s, n_s, n, a, b), \\ \quad u_r'(x, l_s, m_s, n_s, n, a, b), \\ \quad u_r''(x, l_s, m_s, n_s, n, a, b)) = 0 \end{cases} \tag{A6}$$

The above equation is valid when $x \in [L, U]$. Now we take any value of x in this interval.

At $x = \beta$, where $L \le \beta \le U$, from the above Eq. (A6), we can obtain the following linear or nonlinear algebraic equations.

$$\begin{cases} p_1 = f(u_1(\beta, l_s, m_s, n_s, n, a, b), \\ \quad u_1'(\beta, l_s, m_s, n_s, n, a, b), \\ \quad u_1''(\beta, l_s, m_s, n_s, n, a, b)) = 0 \\ \quad . \\ \quad . \\ \quad . \\ p_r = f(u_r(\beta, l_s, m_s, n_s, n, a, b), \\ \quad u_r'(\beta, l_s, m_s, n_s, n, a, b), \\ \quad u_r''(\beta, l_s, m_s, n_s, n, a, b)) = 0 \end{cases} \tag{A7}$$

Now the differential equation is transformed into algebraic nonlinear equation. By solving the algebraic nonlinear Eqs. (A4), (A5) and (A7) using wolframealpha.com46or Ying Buzu or regular false algorithms 47, we can obtain the unknown parameter l_s, m_s and n_s for the given values of parameters a and b. While the Taylor series, Adomian decomposition, Akbari-Ganji, and homotopy analysis techniques are limited to finite domains, the Rajendran-Joy methodology may be used in both finite and semi-infinite domains. For some strong nonlinear problems with complex and mixed boundary conditions, this RJM cannot be applied.