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Theoretical Analysis of Nonlinear Reaction-diffusion Equation on Immobilised Alpha-Chymotrypsin in Acetonitrile Solvent

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Abstract:
The study focuses on immobilised Alpha-chymotrypsin operating under kinetic constraints. This model incorporates equations representing the inherent kinetics of four distinct reactions, along with the experimentally analysed physical properties of three different support materials, to estimate the immobilised biocatalyst's initial activity and nucleophile selectivity. Approximate analytical solutions of acyl donor and nucleophile substrate concentrations under steady-state conditions are derived concerning all diffusion parameters using Akbari Ganji and homotopy perturbation methods. We examine our analytical results with numerical data obtained using MATLAB software to assess accuracy. It is shown that the derived analytical results closely match the numerical results. The model reliably replicates experimentally observed trends in initial rate and nucleophile selectivity across varying enzyme loadings.

Keywords: Nonlinear reaction-diffusion equation, Akbari Ganji Method, Homotopy perturbation Method, acyl donor and nucleophile

1. Introduction

In recent pasts, advancements in comprehending enzyme behaviour in organic environments and their practical applications in synthesis have progressively enhanced the ability of using biocatalysts in single-phase organic solvents [1]. Enzymes function as heterogeneous catalytic systems primarily because they are generally insoluble in such systems unless deliberately engineered to be soluble. Immobilising enzymes within porous carrier particles has proven effective in preventing the aggregation and compaction of suspended enzyme powders. Additionally, this process gives the biocatalyst particles several beneficial properties, including homogeneous particle size, effective substrate and water distribution, improved accessibility to enzyme active sites, and mechanical, solid, and hydrodynamic resistance. The immobilisation procedure also makes the enzyme suitable for use in continuous-flow systems, such as stirred tank reactors, packed bed reactors, or systems that recover the biocatalyst for reuse after batch operations [2-4].

The rate at which substrates may reach the active sites on solid particles ultimately determines the efficiency of faster catalysts, similar to other heterogeneous catalytic systems. It is anticipated that most reasonably rapid heterogeneous catalytic systems, if not all of them, will have both internal and external diffusional limits [5-7]. When mass transfer is the limiting factor, simple modifications to the

biocatalyst particles—like decreasing their size or choosing a more porous matrix for immobilisation—significantly affect the reaction rate more than changes to the enzyme or its surroundings. Higher agitation rates in stirred tanks or higher flow rates surrounding catalyst particles in fixed beds may lower external diffusional limitations. However, internal diffusional constraints are more difficult to circumvent and typically have a huge impact [8-11].

The model of simultaneous diffusion and reaction is essential for optimizing the catalytic system, as confirmed by many reports dealing with this phenomenon's description and mathematical modelling. Vikram M. Paradkar and Jonathan S. Dordick developed a model of alpha-Chymotrypsin Dissolved in Organic Solvents both theoretically and experimentally [12]. When working with immobilised enzymes in organic media, mass transfer limits can be a significant consideration was proposed by Raul J. Barros et al [13]. M. Veeramuni et al. published a Mathematical modelling of immobilised α-Chymotrypsin in acetonitrile medium [14]. Raul J Barrros et al. build a mathematical model explaining the a-chymotrypsin synthesis in acetonitrile medium with spherical Geometry [15].

Previously, there were no analytical solutions for the acyl donor and nucleophile molar concentrations in planar coordinates. This report introduces a novel analytical expression for these concentrations and presents analytical formulations for the consumption rates of each substrate. Furthermore, we compare our analytical results for acyl donor and nucleophile substrate concentrations with numerical simulations conducted using the Matlab program. The comparisons demonstrate a high level of agreement.

2. Mathematical model of the problem

In an acetonitrile solvent under kinetic control, the enzymatic synthesis di-tripeptides or tripeptides alpha-chymotrypsin can be illustrated below. In this setting, the substrates undergo the enzymatic reactions as follows:

Creation of a product:

$$AcD + Nuc \rightarrow Pep + LG \tag{2.1}$$

This process entails an acyl donor (AcD) reacting with a nucleophile (Nuc) to produce a peptide (Pep) and a leaving group (LG).
Hydrolysis of the acyl donor:

$$AcD + H_2O \rightarrow Hyp + LG \tag{2.2}$$

In this reaction, the acyl donor (AcD) undergoes hydrolysis with water (H_2O), resulting in the formation of a hydrolysis product (Hyp) and a leaving group (LG).

The rate equation describing the formation of peptides and hydrolysis products in the aforementioned inherent kinetics can be formulated as[15]:

$$\frac{d^2[AcD]}{dr^2} = \frac{1}{D_{Aeff}} \frac{(k_{Synth}[Nuc]+k_{Hydr})[AcD][E_0]}{k_N+[Nuc]} \tag{2.3}$$

$$\frac{d^2[Nuc]}{dr^2} = \frac{1}{D_{Neff}} \frac{k_{Synth}[Nuc][AcD][E_0]}{k_N+[Nuc]} \tag{2.4}$$

Where $[AcD]$ and $[Nuc]$, are the acyl donor and nucleophile's molar concentrations, D_{Neff} and $D_{Aeff}$are the nucleophile and acyl donor's effective diffusion coefficients and E_0 is the amount of

enzyme, k_{Synth}, k_{Hydr} and k_N are the kinetic constants. The nonlinear reaction-diffusion equations system mentioned above has the following boundary conditions:

$$r = 0; \quad \frac{d[AcD]}{dr} = 0, \quad \frac{d[Nuc]}{dr} = 0 \tag{2.5}$$

$$r = R: \quad [AcD] = [AcD]_B, \quad [Nuc] = [Nuc]_B \tag{2.6}$$

Where R is the radius of the particle, $[AcD]_B$ and $[Nuc]_B$ are the bulk molar concentrations.

$x = \frac{r}{R}, \gamma_1 = \frac{R^2 k_{Hydr}[AcD]_B E_0}{D_{Aeff} k_N}$, $\gamma_2 = \frac{R^2 k_{Synth}[AcD]_B [Nuc\}_B}{D_{Neff} K_N}$, $\alpha_1 = \frac{k_{Synth}[Nuc]_B}{k_{Hydr}}$, $\alpha_2 = \frac{[Nuc]_B}{k_N}$,

$U = \frac{[AcD]}{[AcD]_B}$, V= $\frac{[Nuc]}{[Nuc]_B}$

By applying above dimensionless parameters in equation (2.3) and (2.4) we get nonlinear equations as

$$\frac{d^2U(x)}{dx^2} = \frac{\gamma_1 U(x)(1+\alpha_1 V(x))}{(1+\alpha_2 V(x))} \tag{2.7}$$

$$\frac{d^2V(x)}{dx^2} = \frac{\gamma_2 U(x) V(x)}{(1+\alpha_2 V(x))} \tag{2.8}$$

The following are the boundary conditions expressed in dimensionless form

$$\frac{dU(x)}{dx} = 0, \frac{dV(x)}{dx} = 0 \; at \; x = 0 \tag{2.9}$$

$$U(x) = 1, V(x) = 1 \; at \; x = 1 \tag{2.10}$$

Each substrate's initial rate of consumption is indicated by

$$Rate_A = \frac{4\pi R^2}{M_P} D_{Aeff} \left(\frac{d[AcD]}{dr}\right)_{r=R} \tag{2.11}$$

$$Rate_N = \frac{4\pi R^2}{M_P} D_{Neff} \left(\frac{d[Nuc]}{dr}\right)_{r=R} \tag{2.12}$$

The following is the dimensionless form of equations (2.11) and (2.12) above:

$$\frac{Rate_A}{\mu} = \left(\frac{dU}{dx}\right)_{x=1} \tag{2.13}$$

$$\frac{Rate_N}{\eta} = \left(\frac{dV}{dx}\right)_{x=1} \tag{2.14}$$

3. Analytical Expressions

Various numerical techniques [16] are helpful for approximating solutions to nonlinear systems, but certain disadvantages are frequently disregarded. Achieving numerical stability and altering settings to meet the numerical data precisely might take a lot of work. Therefore, researchers prefer analytical solutions because they provide better insights into the effects of model parameters. In the last forty years, many dependable and highly accurate analytical techniques have been developed and effectively used to solve many nonlinear models in a wide range of scientific fields. Several methods are mentioned, including homotopy analysis [17,18], variational iteration method [19,20], differential transformation method [21,22], Adomian decomposition method [23], homotopy perturbation method (HPM) [24,25,26], Akbari-Ganji method [27,28] and Taylor series method [29,30].

3.1 Approximate Analytical solution for the concentration of acyl donor and nucleophile using Akbari Ganji Method

The Akbari-Ganji approach, a numerical technique for solving nonlinear systems and equations, was named after its authors, M.R. Akbari and D.D. Ganji. It became a component of the larger area of

analytical approaches that approximate solutions without requiring sophisticated discretization methods or much processing power. The approach provides accurate solutions to nonlinear problems. It has received recognition for its effectiveness in various scientific and engineering applications. Iteratively improving solutions through mathematical techniques frequently outperforms traditional numerical methods regarding accuracy and processing economy. The approximate analytical solution of substrate concentration of acyl donor and substrate concentration of nucleophile obtained by using the Akbari Ganji Method is

$$U(x) = \frac{\cosh(mx)}{\cosh(m)} \tag{3.1}$$

$$V(x) = \frac{\sinh(nx)}{\sinh(n)} \tag{3.2}$$

Where $m = \sqrt{\frac{\gamma_1(1+\alpha_1)}{1+\alpha_2}}$ and

$$n = \sqrt{\frac{\gamma_2}{1+\alpha_2}}$$

3.2 Approximate Analytical solution for the substrate concentration of acyl donor and nucleophile using homotopy perturbation method

Ji Huang He initially proposed the homotopy perturbation method, which effectively tackles a wide range of nonlinear issues. Numerous scientific disciplines, including engineering sciences, physics, and applied mathematics, are fully aware of this. The problem of solving nonlinear ordinary and partial differential equations, and the nonlinear differential equation method is a constant challenge for researchers in these domains. Although the HPM methodology has several limitations, it can be seen as an extension of homotopy and basic perturbation techniques. For instance, the HPM technique only requires a few iterations to yield accurate results; neither linearization nor a tiny parameter are needed. The approximate analytical solution of substrate concentration of acyl donor and nucleophile is obtained by homotopy perturbation method is

$$U(x) = 1 + \frac{\gamma_1(1+\alpha_1)}{2(1+\alpha_2)}(x^2 - 1) \tag{3.3}$$

$$V(x) = 1 + \frac{\gamma_2}{2(1+\alpha_2)}x^2 - \frac{\gamma_2}{2(1+\alpha_2)} \tag{3.4}$$

The analytical expressions for rate consumption of acyl donor and nucleophile substrate concentrations are

$$Rate_A/\mu = \left(\frac{dU}{dx}\right)_{x=1} = \frac{\gamma_1(1+\alpha_1)}{(1+\alpha_2)} \tag{3.5}$$

$$Rate_N/\eta = \left(\frac{dV}{dx}\right)_{x=1} = \frac{\gamma_2}{(1+\alpha_2)} \tag{3.6}$$

4. Validation of Analytical Results

Numerical methods were employed to solve the nonlinear reaction-diffusion equations (2.7) and (2.8) with the boundary conditions (2.9) and (2.10). The MATLAB function, designed for solving boundary value problems for nonlinear differential equations, was utilized for the numerical solution of these equations. The numerical solutions agreed with those obtained using the HPM and AGM methods. Specifically, two iterations of the HPM and straightforward algebraic calculations of AGM were employed to estimate the approximate concentration. The analytical expression of the acyl donor and nucleophile concentration obtained from the AGM and HPM methods is compared with the numerical results. Satisfactory agreement is noticed. Tables (1-4) compare the analytical results (AGM, HPM) derived in this study and the numerical results obtained through MATLAB software. Significantly, the

AGM results demonstrate closer agreement with the numerical results in comparison to the HPM results. Table 1 shows the maximum average error percentage difference between AGM and HPM for the acyl donor substrate concentration is 0.02 and 0.31. Table 2 reveals the average error percentages for AGM and HPM as 0.11 and 0.39. In contrast, Table 3 indicates that the average error percentage for the nucleophile substrate concentration is 0.02 and 0.43 for AGM and HPM. Finally, Table 4 notes that error percentages for both AGM and HPM for nucleophile substrate are 0.01 and 0.03.

Table 1: Compares the dimensionless concentration of acyl donor substrate with AGM and HPM with numerical results for fixed parameters $\gamma_2, \alpha_1, \alpha_2 = 1$ and different values of $\gamma_1 = 0.1,0.7,0.9$

X	$\gamma_1 = 0.1$					$\gamma_1 = 0.7$					$\gamma_1 = 0.9$				
	NUM	**AGM**	**HPM**	**ERR % AGM**	**ERR % HPM**	**NUM**	**AGM**	**HPM**	**ERR % AGM**	**ERR % HPM**	**NUM**	**AGM**	**HPM**	**ERR % AGM**	**ERR % HPM**
0	0.952	0.9518	0.9523	0.02	0.03	0.7294	0.7293	0.7292	0.01	0.02	0.6481	0.648	0.6408	0.01	0.73
0.25	0.955	0.9549	0.9525	0.01	0.25	0.7458	0.7455	0.7437	0.03	0.21	0.6688	0.6686	0.6678	0.02	0.1
0.5	0.9642	0.9641	0.9590	0.01	0.52	0.7955	0.7953	0.7943	0.02	0.12	0.7325	0.7324	0.7313	0.01	0.12
0.75	0.9795	0.9793	0.9789	0.02	0.06	0.8809	0.8808	0.8789	0.01	0.2	0.8431	0.8432	0.843	0.01	0.01
1	1	0.9997	0.9991	0.03	0.09	1	0.9998	0.9852	0.02	1.48	1	0.9989	0.9923	0.11	0.77
	AVG ERR %			0.018	0.19	**AVG ERR %**			0.018	0.406	**AVG ERR %**			0.032	0.346

Table 2: Compares the dimensionless concentration of acyl donor substrate with AGM and HPM with numerical results for fixed parameters $\gamma_1, \gamma_2, \alpha_2 = 0.1$ and different values of $\alpha_1 = 5, 10, 20$

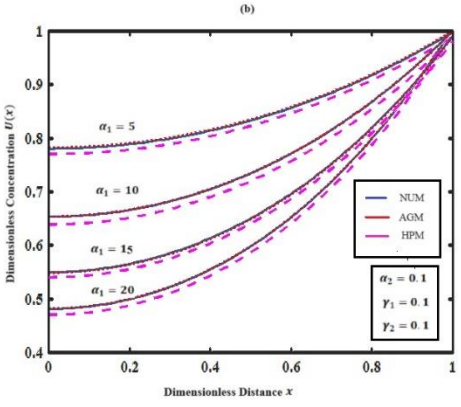
X	$\alpha_1 = 5$					$\alpha_1 = 10$					$\alpha_1 = 20$				
	NUM	**AGM**	**HPM**	**ERR % AGM**	**ERR % HPM**	**NUM**	**AGM**	**HPM**	**ERR % AGM**	**ERR % HPM**	**NUM**	**AGM**	**HPM**	**ERR % AGM**	**ERR % HPM**
0	0.7821	0.7822	0.7811	0.01	0.01	0.6534	0.6352	0.6542	0.02	0.08	0.4777	0.4772	0.4667	0.05	1.1
0.25	0.7953	0.7943	0.7933	0.1	0.2	0.6738	0.6733	0.6728	0.05	0.1	0.5064	0.5063	0.5054	0.01	0.1
0.5	0.8357	0.8356	0.9355	0.01	0.02	0.7363	0.7363	0.7253	0	1.1	0.5962	0.5958	0.5932	0.04	0.3
0.75	0.9046	0.9044	0.9036	0.02	0.1	0.8452	0.845	0.8472	0.02	0.2	0.7581	0.7580	0.7579	0.01	0.02
1	1	0.999	0.9902	0.1	0.98	1	1	0.9886	1.01	1.14	1	0.9987	0.9957	0.13	0.43
	AVG ERR %			0.048	0.28	**AVG ERR %**			0.22	0.524	**AVG ERR %**			0.048	0.39

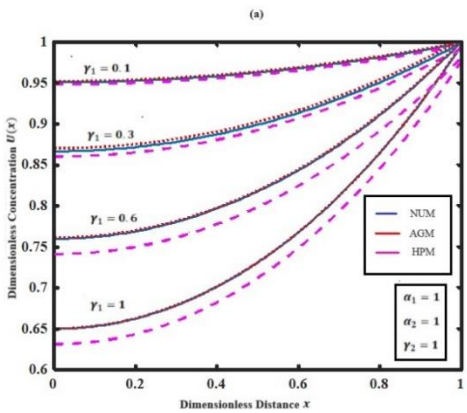
Table 3: Examine the dimensionless concentration of nucleophile substrate with AGM and HPM with numerical results for fixed parameters $\gamma_1, \alpha_1, \alpha_2 = 0.1$ and different values of $\gamma_2 = 0.1, 0.3, 0.9$

X	$\gamma_2 = 0.1$					$\gamma_2 = 0.3$					$\gamma_2 = 0.9$				
	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM
0	0.9578	0.9574	0.9567	0.04	0.11	0.881	0.8811	0.8794	0.01	0.16	0.6995	0.6994	0.6991	0.01	0.04
0.25	0.9604	0.9603	0.9512	0.01	0.92	0.8884	0.8878	0.8763	0.06	1.21	0.7174	0.7171	0.7172	0.03	0.02
0.5	0.9684	0.9680	0.9654	0.04	0.3	0.9107	0.9106	0.9103	0.01	0.04	0.7722	0.7723	0.7721	0.01	0.01
0.75	0.9818	0.9823	0.9713	0.05	1.05	0.9485	0.9482	0.9385	0.03	1	0.8668	0.8667	0.8664	0.01	0.04
1	1	0.9994	0.9879	0.06	1.21	1	1	1	0	0	1	1	1	0	0
	AVG ERR %			0.04	0.781	AVG ERR %			0.022	0.482	AVG ERR %			0.012	0.04

Table 4: Examine the dimensionless concentration of nucleophile substrate with AGM and HPM with numerical results for fixed parameters $\gamma_1, \gamma_2, \alpha_1 = 0.01$ and different values of $\alpha_2 = 0.001, 0.5, 3$

X	$\alpha_2 = 0.001$					$\alpha_2 = 0.5$					$\alpha_2 = 3$				
	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM
0	0.995	0.9951	0.9948	0.01	0.02	0.9967	0.9966	0.9966	0.01	0.01	0.9988	0.9986	0.9978	0.02	0.1
0.25	0.9954	0.9953	0.9949	0.01	0.05	0.9969	0.9968	0.9967	0.01	0.02	0.9988	0.9988	0.9987	0	0.01
0.5	0.9963	0.9961	0.9970	0.02	0.07	0.9975	0.9973	0.9970	0.02	0.05	0.9991	0.9992	0.9990	0.01	0.01
0.75	0.9979	0.9980	0.9977	0.01	0.02	0.9986	0.9985	0.9980	0.01	0.06	0.9995	0.9993	0.9998	0.02	0.05
1	1	1	0.9999	0	0.01	1	1	1	0	0	1	1	0.9998	0	0.02
	AVG ERR %			0.01	0.034	AVG ERR %			0.01	0.01	AVG ERR %			0.01	0.038





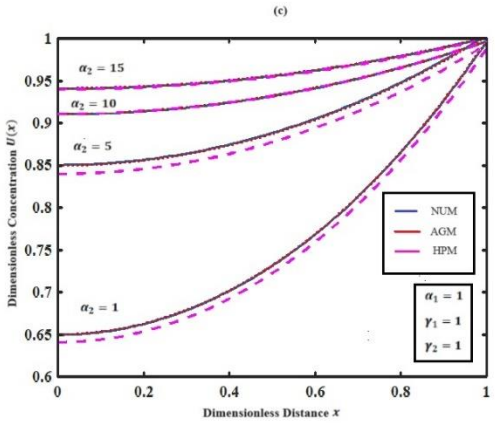


Figure 1(a-c): Graph showing dimensionless substrate concentration of acyl donor plotted against dimensionless distance x

Figure 1(a-c) shows the normalised concentration profile of the acyl donor, plotted for different values of diffusion parameters $\gamma_1, \alpha_1, \alpha_2$ using equation (3.1 and 3.3). In figure1 (a), the substrate concentration of acyl donor was calculated for various values of γ_1 while keeping α_1,α_2 fixed and it is observed that the concentration profile of the acyl donor closely approaches 1. It is evident that as the diffusion parameter γ_1 decreases, the substrate concentration of the acyl donor increases. In figure1 (b), the concentration was determined for various values of the dimensionless parameter α_1 with γ_1 and α_2 fixed and it is observed that the concentration substrate of the acyl donor increases as the parameter $\alpha_1$1 decreases. In figure (c), the concentration U(x) was calculated for different values of α_2 keeping γ_1, α_1 fixed, it can be observed that the concentration value increases with a decrease in the diffusion parameter α_2.

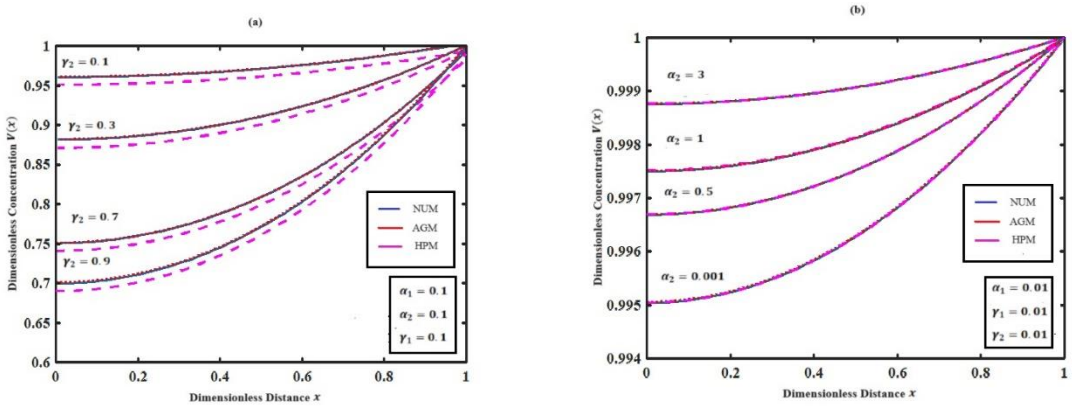


Figure 2(a-b): Graph showing dimensionless substrate concentration of nucleophile plotted against dimensionless distance x

Figure 2(a-b) shows that the normalised concentration profile for nucleophile substrate V for different values of parameter γ_2 and α_2 using equation (3.2 and 3.4). In Figure 2(a) the value of concentration of nucleophile increases when the diffusion parameter γ_2 decreases while holdingγ_1,α_1, α_2 constant the substrate concentration of nucleophile was computed for various values of γ_2. In Figure 2(b) the concentration of nucleophile substrate concentration was determined for various values of α_2

maintaining constant values of $\gamma_1, \gamma_2, \alpha_1$, the concentration value of nucleophile substrate V increases the diffusion parameter α_2 increases.

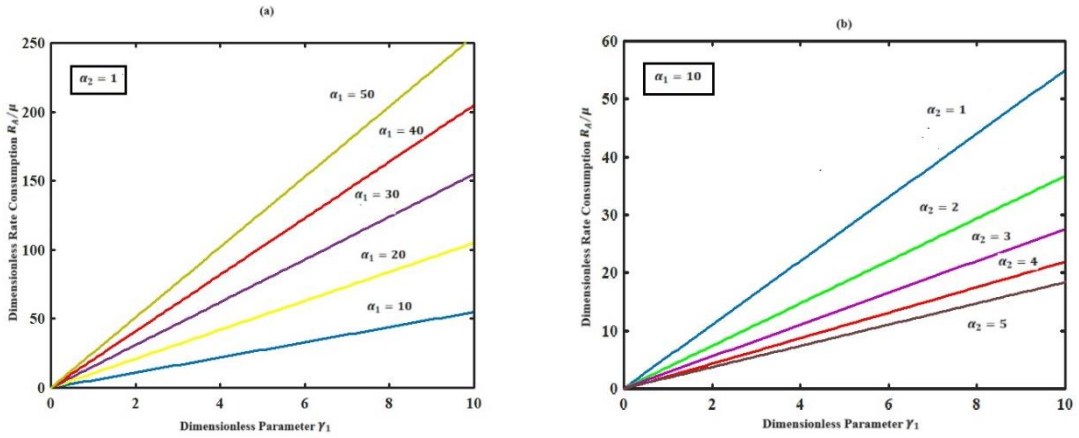


Figure 3(a-b): Graph showing the dimensionless rate consumption R_A/μ versus dimensionless parameter γ_1.

γ_1 is plotted using equation (3.5) for acyl donor substrate U. From Figure 3 (a) It is evident with varying values of α_1 the rate of consumption R_A/μ increases, for some fixed value of α_2.Figure 3 (b) It is noted that the rate of consumption R_A/μ decreases for different values of α_2 and for fixed parameter α_1.

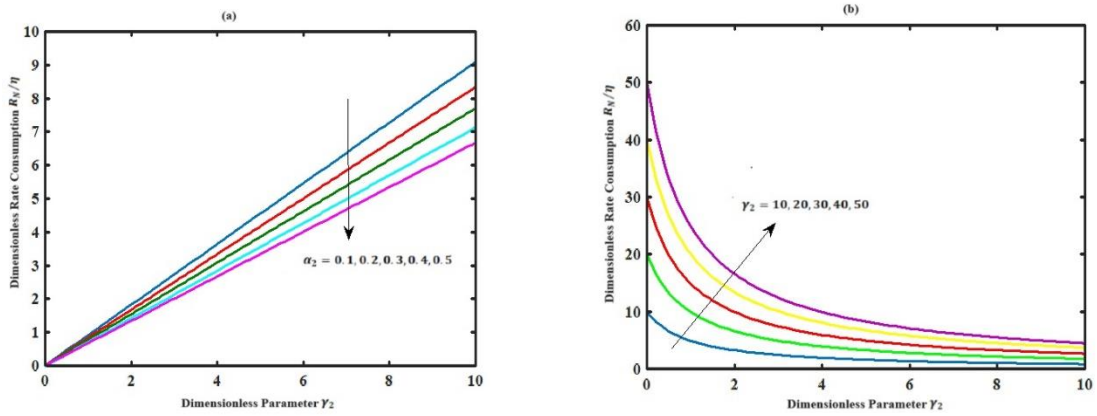


Figure 4(a-b): Graph shows the dimensionless rate of consumption R_N/η versus dimensionless parameter γ_2

γ_2 Plotted using the equation (3.6) for substrate concentration of nucleophile. From Figure 4(a) it is noticed that the rate of consumption R_N/η decreases for different values of α_2 and from figure 4(b) it is clear that the rate of consumption R_N/η increases for different values of γ_2 .

5. Conclusion

The nonlinear reaction-diffusion equation for immobilised alpha-chymotrypsin in acetonitrile solvent has been adequately explored mathematically in this article. We derived approximate analytical formulas for the concentrations of the acyl donor and nucleophile substrates across all ranges of dimensionless parameters. We solved nonlinear reaction equations using the AGM and HPM,

achieving closed-form expressions for these concentrations. Our analytical results closely match the numerical simulations, indicating strong agreement. The AGM offers the most direct and precise convergent solution series for nonlinear cases when contrasted with HPM .The insights from this theoretical model can significantly aid in analysing experimental kinetics and predicting product distributions. Additionally, the suggested methods' accessibility, dependability, and simplicity would make them useful for estimating the approximate substrate concentrations of acyl donor and nucleophile and reaction rates for immobilised biocatalysts.

Nomenclature

Parameter	Meaning	Units
D_{Aeff}	acyl donor Effective diffusion coefficient	cm^2/s
D_{Neff}	nucleophile Effective diffusion coefficient	cm^2/s
[AcD]	acyl donor concentration	mM
[Nuc]	nucleophile concentration	mM
[Hyp]	Hydrolysis product concentration	mM
[Pep]	Peptide product concentration	mM
k_{Hydr}	Kinetic constant	$\mu\ mol\ min^{-1}\ mg\ \ CT^{-1}$
k_N	Kinetic constant	mM
k_{Synth}	Kinetic constant	ml $min^{-1} mg\ CT^{-1}$
E_0	Enzyme Amount	mg min^{-1}
LG	Leaving Group (Ethanol or Methanol)	None
$[AcD]_B$	acyl donor molar concentration	mM
$[Nuc]_B$	nucleophile molar concentration	mM
D	Distance from the particle's centre	Cm
R	Radius of the particle	Cm

Appendix A

Approximate Analytical solution using Akbari Ganji Method

Approximate trial solution for equation (2.7) and (2.8) is

$$U(x) = A\cosh(mx) + B\ \sinh\ (mx) \quad \text{(A1)}$$
$$V(x) = C\cosh(nx) + B\ sinh(nx) \quad \text{(A2)}$$

where A, B, C, D are constant. Applying the boundary condition equation (2.9) and (2.10) in equation (A1), (A2), we obtain,

$$A = \frac{1}{\cosh(m)}\ \ , B = 0\ , C = \frac{1}{\cosh(n)}, D = 0 \quad \text{(A3)}$$

Substituting equation (A3) in Equation (A1) and (A2)

$$U(x) = \frac{\cosh\ (mx)}{\cosh\ (m)} \quad \text{(A4)}$$
$$V(x) = \frac{\cosh\ (nx)}{\cosh\ (n)} \quad \text{(A5)}$$

Where m and n are constant coefficient. The equation (2.7) and (2.8) can be arranged in the following manner to get the values of m and n.

$$\frac{d^2U(x)}{dx^2} - \frac{\gamma_1 U(x)(1+\alpha_1 V(x))}{1+\alpha_2 V(x)} = 0 \quad \text{(A6)}$$

$\frac{d^2V(x)}{dx^2} - \frac{\gamma_2 U(x)V(x)}{1+\alpha_2 V(x)} = 0$ (A7)

The above two equations can be expressed by substituting equation (A4) an (A5) by substituting the boundary conditions $x = 1$

$$m^2 \frac{\cosh(mx)}{\cosh(m)} = \frac{\gamma_1 \frac{\cosh(mx)}{\cosh(m)}\left[1+\alpha_1 \frac{\cosh(nx)}{\cosh(n)}\right]}{\left[1+\alpha_2\left[\frac{\cosh(nx)}{\cosh(n)}\right]\right]} \quad \text{(A8)}$$

$$m^2 = \frac{\gamma_1(1+\alpha_1)}{1+\alpha_2}$$

$$m = \sqrt{\frac{\gamma_1(1+\alpha_1)}{1+\alpha_2}}, m = -\sqrt{\frac{\gamma_1(1+\alpha_1)}{1+\alpha_2}} \quad \text{(A9)}$$

Appendix B

Approximate Analytical solution using Homotopy perturbation method

$(1-P)\left(\frac{d^2U(x)}{dx^2}\right) + P\left(\frac{d^2U(x)}{dx^2} - \frac{\gamma_1(U(x))(1+\alpha_1(V(x))}{1+\alpha_2 V(x)}\right) = 0$ (B1)

Analytical solution of equation (B1) is

$U = U_0 + PU_1 + P^2U_2 + \cdots$ (B2)

By employing the same power of P terms, the results obtained from substituting equation (B1) into equation (B2) can be expressed as

$P^0: \frac{d^2U_0(x)}{dx^2} = 0$ (B3)

$\frac{dU_0(1)}{dx} = 0 \qquad U_0(1) = 1$ (B4)

$P^1 = \frac{d^2U_1(x)}{dx^2} - \frac{\gamma_1(U(x))(1+\alpha_1(V(x))}{1+\alpha_2 V(x)} = 0$ (B5)

$\frac{dU_1(0)}{dx} = 0 \qquad U_1(1) = 0$ (B6)

By solving equation (B3) and (B4)

We get the following results

$U_0 = 1$ (B7)

$U_1 = \frac{\gamma_1(1+\alpha_1)}{2(1+\alpha_2)}(x^2-1)$ (B8)

HPM can therefore be utilized to represent the solution in the following manner

$U = \lim_{P\to 1} U = U_0 + U_1 = 1 + \frac{\gamma_1(1+\alpha_1)}{2(1+\alpha_2)}(x^2-1)$ (B9)

Similarly we can find V=$\lim_{P\to 1} V = V_0 + V_1 = 1 + \frac{\gamma_2}{2(1+\alpha_2)}(x^2-1)$ (B10)

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