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ORIGINAL

Modeling Concentration Dynamics under Michaelis-Menten Kinetics

Modelado de la dinámica de concentración según la cinética de Michaelis-Menten

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ABSTRACT

A theoretical model simulates substrate-to-fructose conversion by enzymatic reactions, described using a nonlinear reaction-diffusion equation based on Michaelis-Menten kinetics. The model's one-dimensional boundary value problem mimics processes in catalytic membranes or bioreactors, solved both analytically and numerically. Key methods include the Akbari-Ganji and hyperbolic function approaches, providing robust expressions for substrate concentration and flux dependent on pore-level Thiele modulus and kinetic parameters. Analytical and numerical results show satisfactory agreement, supporting the methods' reliability. Sensitivity analysis reveals how kinetic parameters impact substrate utilization—information valuable for optimizing industrial enzymatic processes in chemical and biochemical engineering.

Keywords: Enzymatic Reactions; Mathematical Modeling; Non-Linear Differential Equations; Akbari Ganji's Method, Hyperbolic Function Method.

RESUMEN

Un modelo teórico simula la conversión de sustrato a fructosa mediante reacciones enzimáticas, descrita mediante una ecuación de reacción-difusión no lineal basada en la cinética de Michaelis-Menten. El problema de valor límite unidimensional del modelo imita los procesos en membranas catalíticas o biorreactores, resueltos tanto analítica como numéricamente. Los métodos clave incluyen los enfoques de Akbari-Ganji y de la función hiperbólica, que proporcionan expresiones robustas para la concentración y el flujo de sustrato en función del módulo de Thiele a nivel de poro y los parámetros cinéticos. Los resultados analíticos y numéricos muestran una concordancia satisfactoria, lo que respalda la fiabilidad de los métodos. El análisis de sensibilidad revela cómo los parámetros cinéticos influyen en la utilización del sustrato, información valiosa para optimizar los procesos enzimáticos industriales en ingeniería química y bioquímica.

Palabras clave: Reacciones Enzimáticas; Modelado Matemático; Ecuaciones Diferenciales no Lineales; Método de Akbari-Ganji; Método de la Función Hiperbólica.

INTRODUCTION

Enzymatic conversion of glucose to fructose using immobilized glucose isomerase (IGI) has become a cornerstone in food processing, most efficiently conducted in packed-bed reactors

composed of microporous particles that provide substantial surface area for reaction due to their varied pore size distribution.[1,2] This process takes advantage of enzyme entrapment within reactor particle pores, allowing for continuous operation modes—such as fixed-bed and fluidized-bed reactors—with industrial-scale productivity and robust performance.[3,4,5] Modeling glucose-to-fructose conversion in packed-bed reactors requires consideration of the complex interplay between mass transport and nonlinear reaction kinetics, often approached through percolation theory and pore network model. Analytical techniques—including homotopy analysis, wavelet-based algorithms, and recent Akbari-Ganji and hyperbolic function methods—have produced reliable steady-state concentration and flux estimates, although a truly general solution applicable to all operational conditions remains elusive.[6,7,8] This work seeks to address that gap by deriving general analytical solutions for substrate concentration and current in packed-bed reactors.

Mathematical Formulation of the Problem

The reaction scheme for converting substrate to fructose by enzymatic reaction is described as follows:[3]

$$G + E \underset{k_{-1}}{\overset{k_1}{\leftrightharpoons}} X \underset{k_{-2}}{\overset{k_2}{\leftrightharpoons}} F + E \qquad (1)$$

Where G, E and F represent for substrate, enzyme, and fructose, respectively, and X stands for the intermediate complex generated, and k_1,k_2 and k_{-1},k_{-2} are the forward and backward kinetic constants, respectively.

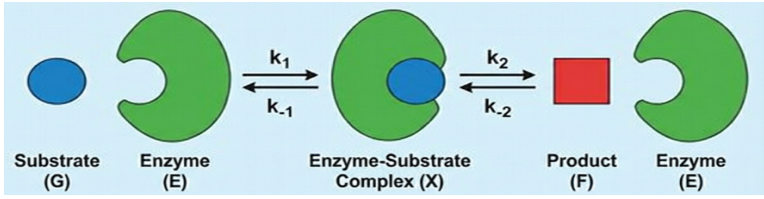


Figure 1. Schematics diagram of converting substrate to fructose by enzymatic reaction

This scheme illustrates that the enzyme is a catalyst; it participates in the reaction by forming an intermediate complex but is ultimately regenerated in its original form, ready to catalyze another reaction cycle. The reversibility indicates that under certain conditions (e.g., high product concentration), the reaction can proceed in the reverse direction, converting the product back into the substrate. The mass balance equation for the enzymatic reaction process in packed bed-reactors, as discussed by Dadvar et al.[3], can be expressed in a dimensionless form that captures the key mass transport and reaction phenomena. In general, the equation takes the form of a diffusion-reaction equation where diffusion is the primary mass transport mechanism inside the porous particles of the packed bed, and enzymatic reaction acts as a sink term. A representative form of such an equation is:

$$C(z)'' - \Phi_p^2 C(z)[1 + \beta C(z)]^{-1} = 0 \qquad (2)$$

$$C = \frac{\bar{G}}{(G_0 - G_e)}, z = \frac{x}{l}, \beta = \frac{\overline{C_0}}{K_m}, \Phi_p^2 = \frac{2\, l^2 V_m'}{r\, D_p K_m}, V_m' = \frac{v_m}{a} \qquad (3)$$

Here is the pore-level Thiele modulus and l is the pore length. The dimensionless boundary conditions are:[17]

$$C(z=0) = C_{z0} \quad (4)$$

$$C(z=1) = C_{z1} \quad (5)$$

The set of relations (2)-(5) contains four dimensionless parameters: C_{z0}, C_{z1}, β and Φp . To diminish this number up to three, we define the dimensionless concentration c(z) = $C(z)/C_{z0}$, thus leaving only three parameters $c(1) = C_{z1}/C_{z0}$, $\beta' = \beta\ C_{z0}$ and Φp. Now the equations (2)- 5) becomes.

$$\frac{d^2c(z)}{d\,z^2} - \Phi_p^2 \frac{c(z)}{1+\beta' c(z)} = 0 \quad (6)$$

The dimensionless boundary conditions are:

$$c(z=0) = 1 \quad (7)$$

$$c(z=1) = \frac{c_{z1}}{c_{z0}} = c(1) \quad (8)$$

The current becomes:

$$J_{ij} = \left(\frac{dc(z)}{dz}\right)_{z=1} \quad (9)$$

Approximate analytical expression of the concentration using Akbari-Ganji's method

A wide spectrum of asymptotic and semi-analytical techniques has been developed to tackle nonlinear differential equations. Among these, the homotopy perturbation method,[9,10,11] Akbari-Ganji's method (AGM),[12,13] the Adomian decomposition method,[14] the Taylor series method,[15] the variational iteration method. The solution obtained by AGM is close to the exact solution and has enough precision and accuracy compared to the other methods**.** The trail solution consists unknown constant coefficients. Then the unknown coefficients are computed using initial/boundary conditions and the differential equation. In contrast, other methods utilize a complicated process to achieve the solution. Using this method, we obtain the analytical expression of substrate concentration, as follows:

$$c(z) = 1 + (c(1)-1)z + \frac{c(1)\Phi_p^2}{2(1+\beta' c(1))}(z^2 - z) \quad (10)$$

It is the simplest and novel analytical expression of a substrate concentration c(z) for all dimensionless parameters c(1),β' and Φ_p. Now, from equation (10), the normalized current can be obtained as follows:-

$$J_{ij} = (c(1)-1) + \frac{c(1)\Phi_p^2}{2(1+\beta' c(1))} \quad (11)$$

Numerical Simulation

Numerically, the non-linear equation (7) in immobilised glucose in the packed-bed reactor are solved for the given boundary conditions.

Table 1. Comparison beteween numerical and analytical results for dimensionless concentration of substrate c(z) for various values of parameter Φ_p^2 when ß'=5,c(1)=0,7

z	Φ_p^2=0,01					Φ_p^2=4					Φ_p^2=9				
	Concentration			Error (%)		Concentration			Error (%)		Concentration			Error (%)	
	Num.	AGM Eq. ()	HFM Eq. ()	AGM Eq. ()	HFM Eq. ()	Num.	AGM Eq. ()	HFM Eq. ()	AGM Eq. ()	HFM Eq. ()	Num.	AGM Eq. ()	HFM Eq. ()	AGM Eq. ()	HFM Eq. ()
0	1,0000	1,0000	1,0000	0,0000	0,0000	1,0000	1,0000	1,0000	0,0000	0,0000	1,0000	1,0000	1,0000	0,0000	0,0000
0,2	0,9393	0,9393	0,9393	0,0000	0,0000	0,8876	0,8892	0,8812	0,1803	0,7210	0,8253	0,8265	0,8199	0,1454	0,6543
0,4	0,8786	0,8786	0,8786	0,0000	0,0000	0,8019	0,8039	0,7945	0,2494	0,9228	0,7097	0,7102	0,7071	0,0704	0,3663
0,6	0,8180	0,8180	0,8180	0,0000	0,0000	0,7424	0,7439	0,7367	0,2020	0,7677	0,6516	0,6511	0,6525	0,0767	0,1381
0,8	0,7575	0,7575	0,7574	0,0000	0,0132	0,7085	0,7093	0,7057	0,1129	0,3952	0,6497	0,6490	0,6514	0,1077	0,2617
1	0,7000	0,7000	0,7000	0,0000	0,0000	0,7000	0,7000	0,7000	0,0000	0,0000	0,7000	0,7000	0,7000	0,0000	0,0000
	Average error (%)			0,0000	0,0022	Average error (%)			0,1241	0,4678	Average error (%)			0,0667	0,2367

Table 2. Comparison beteween numerical and analytical results for dimensionless concentration of substrate c(z) for various values of parameter ß' when ,Φ_p^2=4,c(1)=0,7

z	ß'=1					ß'=5					ß'=10				
	Concentration			Error (%)		Concentration			Error (%)		Concentration			Error (%)	
	Num.	AGM Eq. ()	HFM Eq. ()	AGM Eq. ()	HFM Eq. ()	Num.	AGM Eq. ()	HFM Eq. ()	AGM Eq. ()	HFM Eq. ()	Num.	AGM Eq. ()	HFM Eq. ()	AGM Eq. ()	HFM Eq. ()
0	1,0000	1,0000	1,0000	0,0000	0,0000	1,0000	1,0000	1,0000	0,0000	0,0000	1,0000	1,0000	1,0000	0,0000	0,0000
0,2	0,8047	0,8066	0,8025	0,2361	0,2733	0,8876	0,8892	0,8812	0,1803	0,7210	0,9106	0,9112	0,9055	0,0659	0,5600
0,4	0,6824	0,6805	0,6827	0,2784	0,0440	0,8019	0,8039	0,7945	0,2494	0,9228	0,8359	0,8366	0,8296	0,0837	0,7537
0,6	0,6266	0,6216	0,6290	0,7980	0,3830	0,7424	0,7439	0,7367	0,2020	0,7678	0,7757	0,7764	0,7706	0,0902	0,6575
0,8	0,6340	0,6299	0,6362	0,6467	0,3470	0,7085	0,7093	0,7057	0,1129	0,3952	0,7301	0,7304	0,7273	0,0411	0,3835
1	0,7000	0,7000	0,7000	0,0000	0,0000	0,7000	0,7000	0,7000	0,0000	0,0000	0,7000	0,7000	0,7000	0,0000	0,0000
	Average error (%)			0,3265	0,1745	Average error (%)			0,1241	0,4678	Average error (%)			0,0468	0,3924

We have used the function pdex1 in Scilab/ Matlab software to solve the initial-boundary value problems numerically. This numerical solution is compared with the present AGM and HFM. Tables 1-2 show the comparison of analytical and simulation results for the concentration. Upon comparison, it gives a satisfactory agreement when all values of the other parameters. The maximum average error between numerical and our AGM and HFM are 0,33 % and 0,47 %.

Approximate analytical expression of the concentration using hyperbolic function method

The hyperbolic function method is also a special case of Akbari-Ganji's method. Analytical expressions for the substrate concentration and normalized current are obtained using the hyperbolic function method as follows:

$$c(z) = \frac{\sinh\left(A(1-z)\right)+c(1)\sinh(Az)}{\sinh(A)} \qquad (12)$$

$$A = \frac{\Phi_p}{\sqrt{1+\beta' c(1)}}$$

$$J_{ij} = A[\, c(1)\coth(A) - \mathrm{cosech}(A)] \qquad (13)$$

When ß›=0, the concentration of substrate from the equation (12) reduces to:

$$c(z) = \frac{\sinh\left(\Phi_p(1-z)\right)}{\sinh(\Phi_p)} + \frac{c(1)\sinh(\Phi_p z)}{\sinh(\Phi_p)} \qquad (14)$$

This is the exact solution of the equation (6) when ß'=0.

RESULTS AND DISCUSSION

Equations (10) and (12) represents the closed and simple approximate analytical expression of substrate concentration for all values of the parameters. Equations (11) and (13) is a new simple analytical flux expression. The values of the parameters c(1),ß' and Φp determine the substrate concentration. Also, from the equation (A1), the concentration of substrate is minimum when:

$$z = \frac{-C_1}{2C_2} \qquad (15)$$

Where:

$$c_1 = c(1) - 1 - \frac{\Phi_p^2\, c(1)}{2\left(1+\beta' c(1)\right)}, c_2 = \frac{\Phi_p^2 c(1)}{2(1+\beta' c(1))} \qquad (16)$$

The minimum value is:

$$c(z)_{min} = 1 - \frac{C_1^2}{4C_2} \qquad (17)$$

When:

$$c(1) = 0.7, \beta' = 5, \Phi_p^2 = 9,$$

Using the equation (15) to (17), we get the minimum $c(z)_{min}$=0,64 when z=0,7. This result is confirmed in figure 1 (b).

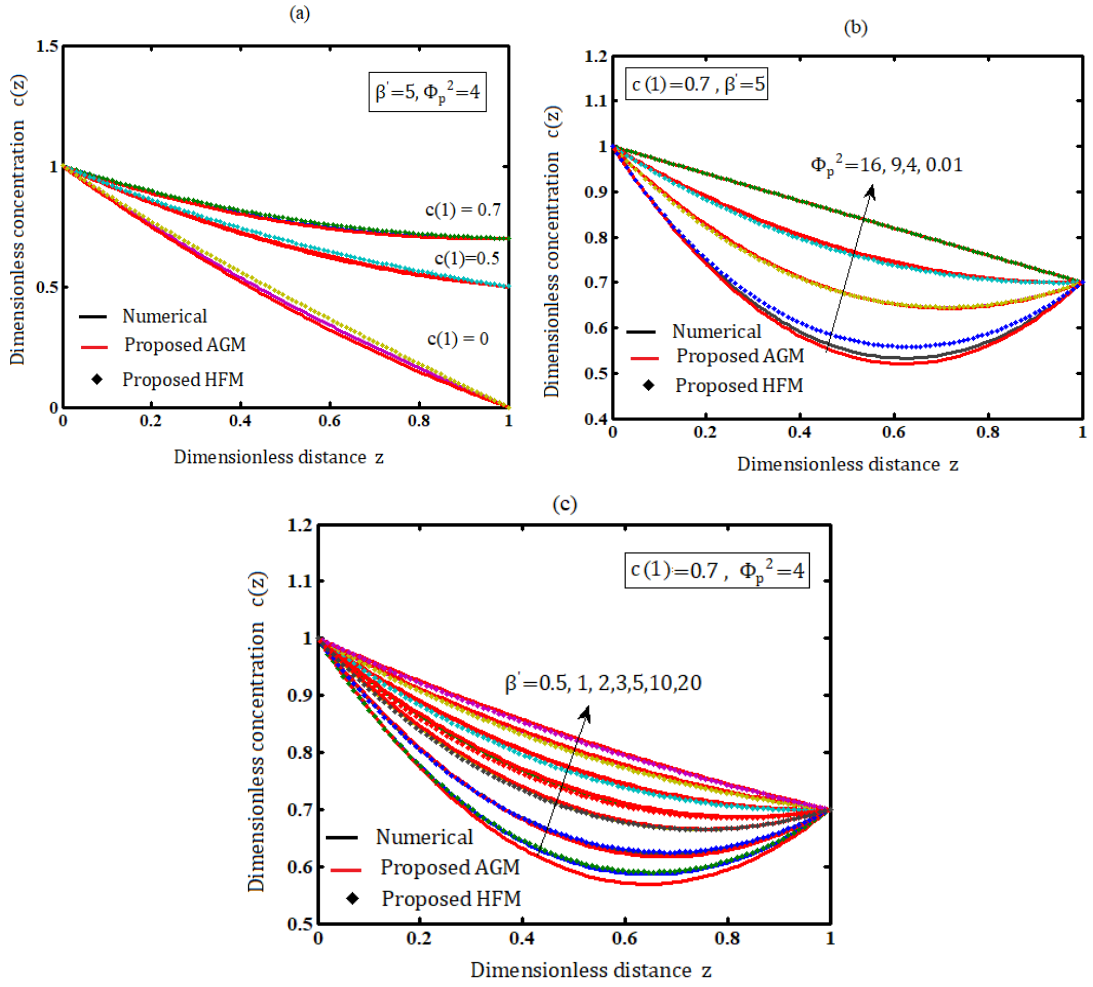
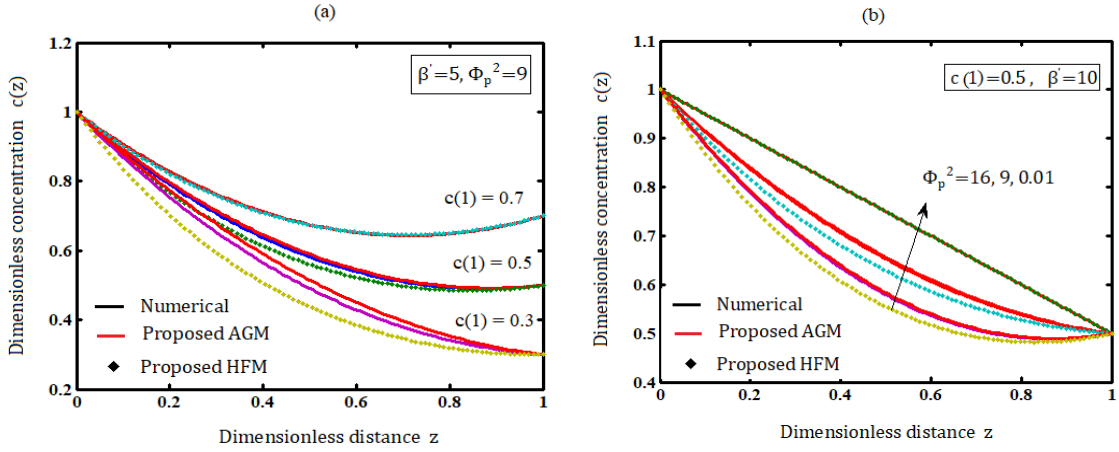


Figure 1 Comparison of analytical expressions (equations (10) and (12)) of concentration of substrate c(z) with simulation result for various value parameters c(1),β' and Φp



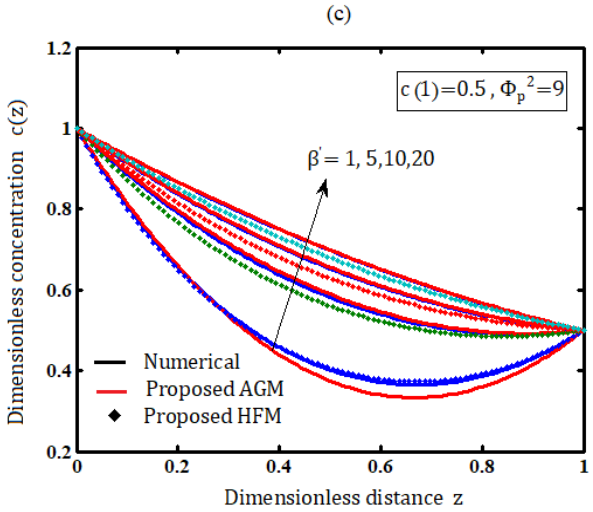
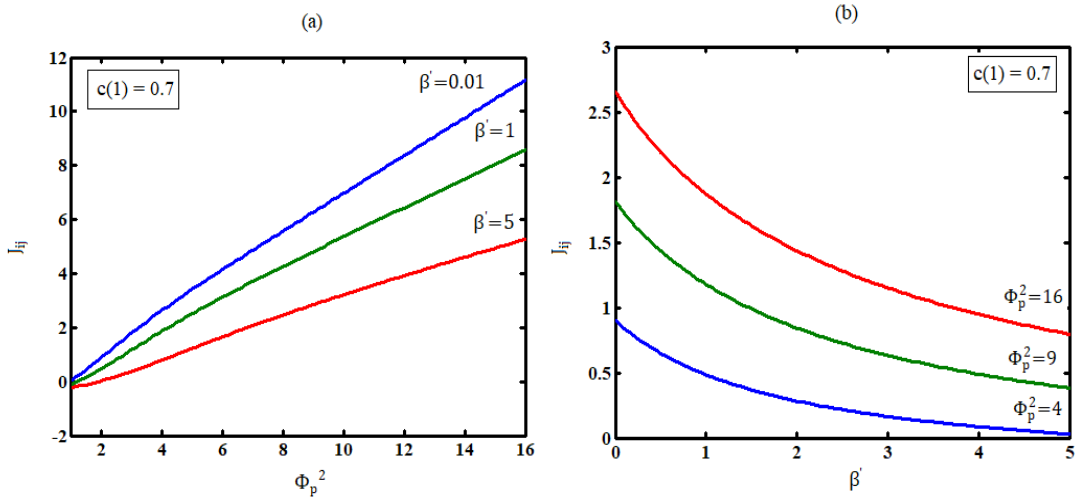


Figure 2. Comparison of analytical expressions (Equations. (10) and (12)) of concentration of substrate c(z) with simulation result for various value parameters c(1), Φp and ß'

The parameter Thiele modulus Φ_p can be varied by changing either the pore length or the amount of glucose immobilized in the matrix. This parameter describes the relative importance of diffusion and reaction in the pore. Figures 1(a-e) represent the dimensionless steady- state concentration of glucose C for different values of the Thiele modulus Φp. From the figure it is inferred that the concentration of glucose C(z) is decreased when Thiele modulus Φp increases. Also, the concentration is uniform when $\Phi_p \ll 0{,}01$ for all values of other parameters. $\Phi_p=0$ implies no chemical reaction, and hence $C(z)= C_{z0}$ for all z when $C_{z1}= C_z0$. But the maximum or minimum value of the concentration of glucose depends upon the value of C_{z1} and C_{z0}.

Figures 2 represent the dimensionless steady- state concentration for different values of the dimensionless kinetic parameter ß. From figure (2), it is observed that, when dimensionless kinetic parameter ß increases, the corresponding substrate concentration also increases for some fixed values of the other dimensionless parameters. When $ß \gg 100$ and $C_{z1}= C_{z0}$ the concentration of glucose $C(z)= C_{z0}$ for all z.



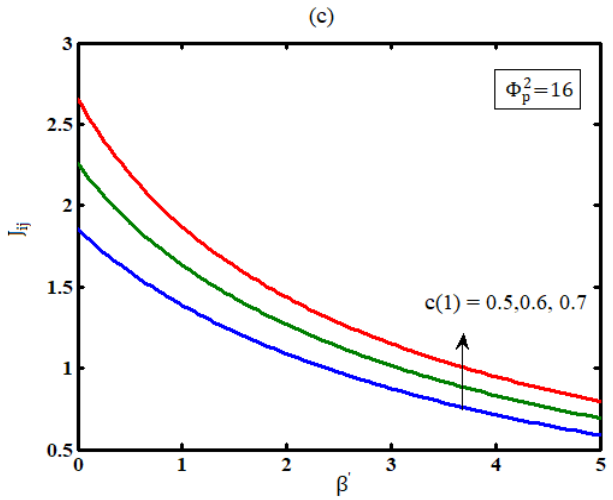


Figure 3. Effect of the parameters Φ_p^2,ß',and c(1) on the flux J_{ij} using equation ()

Figure 3 (a-d) represent the dimensionless flux J_{ij} versus dimensionless kinetic parameter ß for various values of Thiele modulus Φ_p. From this figure, it is evident that the flux value increases as the kinetic parameter ß and Thiele modulus Φ_p increases.

Sensitivity analysis of the parameters

The sensitivity analysis yields the influence of each parameter on the current. By evaluating the slope of the current with respect to the desired parameters, their influence on current can be ascertained. Figure 4 depicts the sensitivity analysis of the steady-state current. The percentage of change in current with respect to the parameters C_{z0}, C_{z1}, Φ_p and ß are 42, 47, 10 and 1 respectively. It is inferred that the concentration at the boundaries, C_{z0} and C_{z1} has a significant influence in dictating the current density, followed by the Thiele modulus Φ_p and rate constant ß.

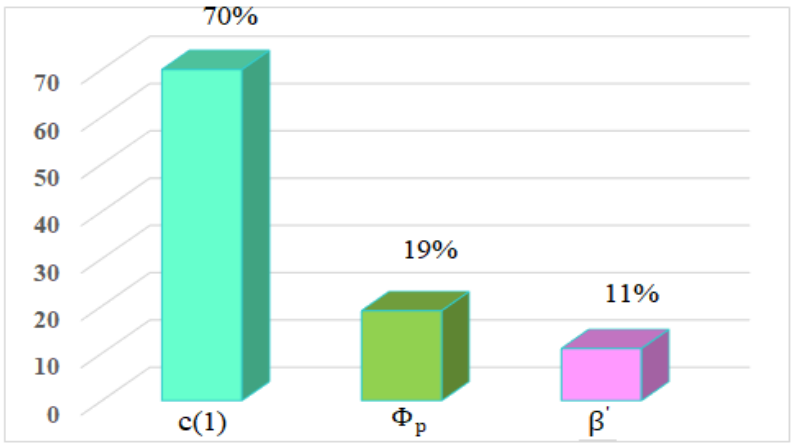


Figure 4. Sensitivity analysis of the parameters: Percentage change in dimensionless current density when c(1)=0,5,Φ_p^2=9 and ß'=0,5

CONCLUSIONS

The steady-state concentration and flux of immobilized glucose isomerase in packed-bed reactors governed by Michaelis–Menten kinetics are analyzed. Approximate closed-form analytical solutions for both concentration and flux are derived using the Akbari–Ganji method and the hyperbolic function method. These expressions provide a straightforward way to estimate glucose concentration and flux over a broad range of parameter values. A sensitivity analysis is also performed to illustrate how key parameters influence the flux. The approach presented here is flexible and can be extended to solve other nonlinear reaction–diffusion equations in immobilized enzyme reactors with complex boundary conditions.

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FINANCING

None.

CONFLICT OF INTEREST

None.

AUTHORSHIP CONTRIBUTION

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Drafting - original draft: P. Jeyabarathi, L. Rajendran.
Writing - proofreading and editing: P. Jeyabarathi, L. Rajendran.

ANNEXES

Appendix-A. Models of transport and reaction

The rate equation of enzyme for a pseudo-steady state condition can be written as follows:

$$\frac{d\,X}{d\,t} = k_1 E\,G - (k_{-1} + k_2)X + k_{-2}\,EF \simeq 0, \qquad \text{(A1)}$$

Where E,G, and F is the concentration of enzyme, glucose and fructose, respectively. The reaction rate is given by:

$$R = \frac{v_m\,\bar{G}}{K_m + \bar{G}} \qquad \text{(a1)}$$

Where:

$$v_m = \frac{K_{mr} v_{mf}(1+K^{-1})}{K_{mr} - K_{mf}}, K_m = \frac{K_{mf}\,K_{mr}\left[1+(K_{mf}^{-1}+KK_{mr}^{-1})G_0(1+K)^{-1}\right]}{K_{mr}-K_{mf}},$$
$$K = \frac{F_e}{G_e} = \frac{v_{mf}}{v_{mr}}\frac{K_{mr}}{K_{mf}} \qquad \text{(A2)}$$

The non-linear mass balance reaction- diffusion equation is written as follows:(17)

$$D_p(\lambda)\frac{d^2G}{d\,z^2} - \frac{2}{ra}R = 0 \qquad \text{(A3)}$$

Where $\lambda = R_{M/r}$, R_M is the molecular radius and r is the pore radius, and a is the surface area per unit weight of the particle. D_p is the pore diffusivity. Equation (A3) can be rewritten in the following way.

$$D_p\frac{d^2\bar{G}}{d\,z^2} - \frac{2}{ra}\frac{V_m\bar{G}}{(K_m+\bar{G})} = 0 \qquad \text{(A4)}$$

This equation is transformed in the dimensionless form of equation (2), which is given in the text.

Appendix B: Approximate analytical expression of the concentration using Akbari-Ganji's method

We can assume that the trail solution of the equation (6) is:

$$c(z) = \sum_{i=0}^{2} c_i\,z^i = c_0 + c_1 z + c_2 z^2 \qquad \text{(B1)}$$

Where c_0, c_1 and c_2 are constants. Using the boundary conditions (7) and (8) we get

$$c_0 = 1, c_1 + c_2 = c(1) - 1 \qquad \text{(B2)}$$

Now define the function H by

$$H(z) = \frac{d^2c(z)}{d\,z^2} - \Phi_p^2 \frac{c(z)}{1+\beta' c(z)} = 0 \qquad \text{(B3)}$$

Using the equation (B1), equation (B3) at z=0 becomes

$$H(z=1) = 2\,c_2 - \frac{\Phi_p^2\, c(1)}{1+\beta' c(1)} = 0 \qquad \text{(B4)}$$

Using equation (B2) in equation (B4), gives:

$$c_2 = \frac{\Phi_p^2 c(1)}{2(1+\beta' c(1))}\,,\; c_1 = c(1) - 1 - \frac{\Phi_p^2\, c(1)}{2(1+\beta' c(1))} \qquad \text{(B5)}$$

Equation (B5) and (B2) into Eq. (B1) gives the closed form of analytical expression of a substrate concentration c(z) for all dimensionless parameters c(1),Φ_p and ß'.

$$c(z) = 1 + (c(1)-1)z + \frac{\Phi_p^2\, c(1)}{2(1+\beta' c(1))}(z^2 - z) \qquad \text{(B6)}$$

The current becomes:

$$J_{ij} = (c(1)-1) + \frac{\Phi_p^2\, c(1)}{2(1+\beta' c(1))} \qquad \text{(B7)}$$

Appendix C: Approximate analytical expression of the concentration using Hyperbolic function method:

Assume that the solution to equation (6) is of the following hyperbolic form:

$$c(z) = A_0 \cosh(m\,z) + B_0 \sinh(m\,z) \qquad \text{(C1)}$$

where A_0, B_0 and m are constant. From boundary conditions (7) and (8), the values of A_0 and B_0 are readily obtained, that is:

$$A_0 = 1,\; B_0 = \frac{c(1) - \cosh(m)}{\sinh(m)} \qquad \text{(C2)}$$

Now the equation (C1) becomes:

$$c(z) = \frac{\sinh\big(m(1-z)\big)}{\sinh(m)} + \frac{c(1)\sinh(mz)}{\sinh(m)} \qquad \text{(C3)}$$

To determine the constant m in equation (C3), we consider the functional form of equation (6)

$$F(z) = \big(1+\beta' c(z)\big)\frac{d^2\,C(z)}{d\,z^2} - \Phi_p^2 c(z) = 0 \qquad \text{(C4)}$$

By substituting Eq. (C4) into Eq. (C3), we obtain:

$$F(z)|_{z=0} = (1+\beta' c(1))\, m^2 = \Phi_p^2 \qquad \text{(C5)}$$

From the above equation we get:

$$m = \frac{\Phi_p}{\sqrt{1+\beta' c(1)}} \qquad \text{(C6)}$$

Substitute equation (C6) into Eq. (C3) gives the following closed form of analytical expression of a substrate concentration c(z) for all dimensionless parameters c_{z1}/c_{z0} ,Φ_p and βc_{z0}.

$$c(z) = \frac{\sinh\left(\frac{\Phi_p}{\sqrt{1+\beta' c(1)}}(1-z)\right)}{\sinh\left(\frac{\Phi_p}{\sqrt{1+\beta' c(1)}}\right)} + \frac{c(1)\sinh\left(\frac{\Phi_p}{\sqrt{1+\beta' c(1)}}z\right)}{\sinh\left(\frac{\Phi_p}{\sqrt{1+\beta' c(1)}}\right)} \qquad \text{(C7)}$$

The current becomes:

$$J_{ij} = \frac{\Phi_p}{\sqrt{1+\beta' c(1)}}\left[c(1)\coth\left(\frac{\Phi_p}{\sqrt{1+\beta' c(1)}}\right) - \operatorname{cosech}\left(\frac{\Phi_p}{\sqrt{1+\beta' c(1)}}\right)\right] \qquad \text{(C8)}$$

Appendix D

MATLAB code for numerical solution of the non-linear Eq. (6)

```
function pdex4
m = 0;
x = linspace(0,1);
t = linspace(0,1000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,2)')
%------------------------------------------------------------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1];
f = [1] .* DuDx;
alpha=1;
beta=0,01;
F=-((alpha^2)*u(1))/(1+beta*u(1));
s=[F];
% ------------------------------------------------------------
function u0 = pdex4ic(x)
```

```
%create a initial conditions
u0 = [1];
% --------------------------------------------------------------
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
%create a boundary conditions
a=1;b=1;
pl = [ul(1)-a];
ql = [0];
pr = [ur(1)-b];
qr = [0];
```