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Research Article

Approximate Analytical Solution to a Pore Network Model of Deactivation of Immobilized Glucose Isomerase in Packed-Bed Reactors Using Akbari-Ganji's Method

B. Seethalakshmi[1], V. Ananthaswamy*[1], S. Narmatha[2] and P. Felicia Shirly[2]

[1] *Research Centre and PG Department of Mathematics, The Madura College Madurai, Tamil Nadu, India*
[2] *Department of Mathematics, Lady Doak College, Madurai, Tamil Nadu, India*
***Corresponding author:** ananthu9777@gmail.com

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Abstract. The main objective of this paper is to derive an approximate analytical solution for the mathematical model pertaining to deactivation of immobilized glucose in packed-bed reactors. The Akbari-Ganji's method is applied to solve the previously developed mathematical model. The approximate analytical expressions corresponding to the concentration and current in the steady state condition have been derived for all values of parameters. Excellent agreement is obtained between the analytical solution and the numerical simulation. The analytical solution presented in this paper is presented for the first time. The results of this work will provide a better understanding of the mathematical model examined.

Keywords. Mathematical modelling, Non-linear differential equation, Pore network model, Akbari-Ganji's method, Numerical simulation

Mathematics Subject Classification (2020). 34B15, 34E05, 34E15

1. Introduction

Kinetic studies of enzyme deactivation are essential for the development of an enzymatic conversion process. Houng *et al*. [7] studied the effect of substrate protection on a commercial immobilized glucose isomerise. This was experimentally investigated in a differential bed

reactor, and a theoretical analysis was performed for a packed bed reactor. Pore network model is used for converting glucose to fructose by enzymatic isomerisation. This process takes place in a packed-bed reactor that consists of micro porous particles with a range of pore sizes, characterized by a pore size distribution. Glucose isomerase was discovered by Marshall and Kooi [11], who succeeded in producing it in commercially viable amounts using enzymatic isomerisation. Glucose isomerase is an example of the highly successful application of enzyme biotechnology to an industrial process that has no commercially viable route through conventional chemistry. Chen and Wu [3] studied the effect of substrate protection on enzyme deactivation. Theoretical analysis of enzyme deactivation with substrate protection offers an effective understanding which is essential for enzyme replacement and process optimization. Benaiges *et al*. [2] calculated the intrinsic kinetic constants of the reversible reaction Michaelis-Menten equation in operational conditions free of mass transfer effects. Dadvar and Sahimi [4] developed pore-level model of conversion of glucose to fructose by enzymatic isomerisation and the associated deactivation of the micro porous particles in which the phenomenon takes place. The purpose of this communication is to derive expressions for the steady-state substrate concentration and the current in closed form using the Akbari-Ganji's method for all values of parameters.

2. Mathematical Formulation of the Problem

The model describes the mechanism by which glucose enzyme moves from the intermediate complex form to fructose and back to the intermediate to the complex glucose enzyme. This can be written as

$$G+F \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} X \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} F+E, \tag{2.1}$$

where G, E and F represent the glucose, enzyme and fructose, X is an intermediate complex formed during the reaction and k_1, k_{-1}, k_2 and k_{-2} are kinetic constants. The non-linear differential equation for concentration of glucose is given as follows:

$$D_p(\lambda)\frac{d^2G}{dx^2}-\frac{2}{ra}R=0, \tag{2.2}$$

where D_p is the pore diffusivity in the micro pores, a is the surface area per unit weight of the particle and $\lambda=\dfrac{R_M}{r}$, where R_M is the molecular radius of the reactants and r is the radius of the micro pore. By introducing the following dimensionless variables

$$R=\frac{v_m\overline{G}}{K_m+G},\ \overline{G}=G-G_e,\ v_m=\frac{K_{mr}v_{mr}(1+K^{-1})}{K_{mr}-K_{mf}},\ K_m=\frac{K_{mf}K_{mr}}{K_{mr}-K_{mf}}\left[1+\left(K_{mf}^{-1}+\frac{K}{K_{mf}}\right)\frac{G_o}{1+K}\right].$$

The eqn. (2.2) becomes

$$D_p\frac{d^2\overline{G}}{dx^2}-\frac{2}{r}\frac{v_m\overline{G}}{K_m+\overline{G}}=0, \tag{2.3}$$

where G is the concentration of glucose, G_o is an initial concentration of glucose, R is are action rate, K_{mf} is the Michaelis-Menten constant, v_{mf} is the maximum velocity of the forward reaction and K_{mr}, v_{mr} are maximum velocities of the backward reaction.

By introducing the following dimensionless quantities

$$C = \frac{\overline{G}}{G_o - G_e}, \quad z = \frac{x}{l_p}, \quad \beta = \frac{\overline{C_o}}{K_m}, \quad \phi^2 = \frac{2l_p^2 v'_m}{rD_p K_m}.$$

Now, the eqn. (2.3) becomes

$$\frac{d^2C}{dz^2} - \phi^2\left(\frac{C}{1+\beta C}\right) = 0, \tag{2.4}$$

where C is the dimensionless concentration, z is the dimensionless distance, l_p is pore length and ϕ is pore-level Thiele-modulus and $v'_m = \frac{v_m}{a}$.

The boundary conditions are given as follows:

$$C(z=0) = \alpha_1, \quad C(z=1) = \alpha_2. \tag{2.5}$$

The dimensionless current is given by

$$J_{ij} = \left[\frac{dC}{dz}\right]_{z=1}. \tag{2.6}$$

3. Analytical Solution of the Glucose Concentration and Current Using Akbari-Ganji's Method

A variety of powerful analytical methods such as homotopy perturbation method [1, 5, 9, 12, 13], homotopy analysis method [8], adomian decomposition method, and wavelet transform method [10], etc. are applied to solve the nonlinear problems. In this paper, Akbari-Ganji's method is applied to find the analytical expression for the concentration of the glucose [6, 14].

The approximate analytical expression for glucose concentration using Akbari-Ganji's method is given by

$$C(z) = \alpha_1 \cosh bz + \frac{(\alpha_2 - \alpha_1 \cosh b)\sinh bz}{\sinh b}. \tag{3.1}$$

The dimensionless current is given by

$$J_{ij} = \alpha_1 b \sinh b + \frac{b(\alpha_2 - \alpha_1 \cosh b)\cosh b}{\sinh b}, \tag{3.2}$$

where $b = \dfrac{\phi}{\sqrt{1+\alpha_2\beta}}$.

4. Results and Discussion

The analytical expressions for the dimensionless glucose concentration and dimensionless current have been derived using the Akbari-Ganji's method. The analytical solution derived has been compared with the numerical simulation, and is found to make an excellent fit. Further from Figures 1 to 7, we observe that the dimensionless glucose concentration varies directly with β, but inversely with ϕ. The dimensionless current varies inversely with β, but directly with ϕ. The basic concept of the Akbari-Ganji's method is given in Appendix A. The MATLAB program is given in Appendix B.

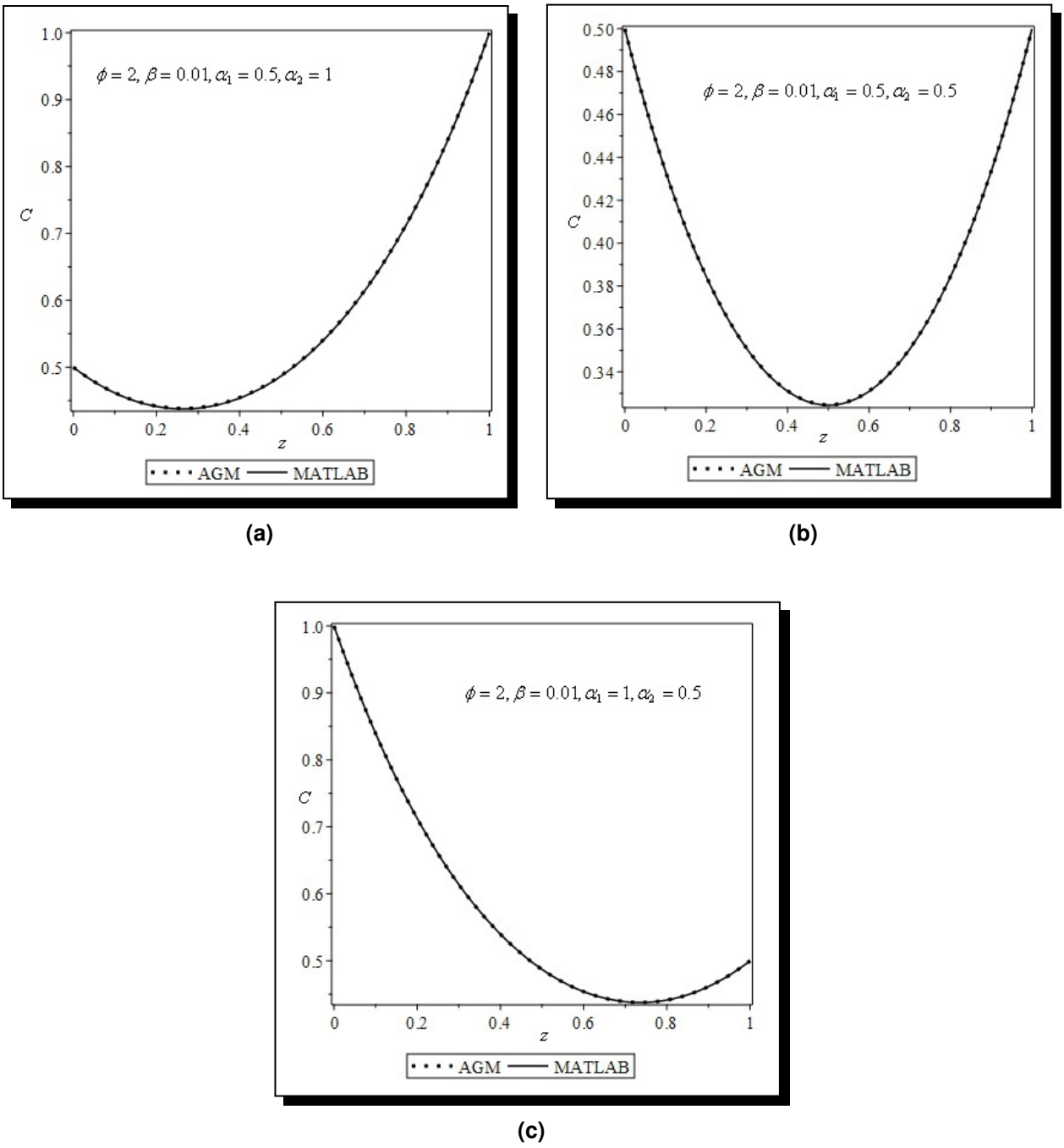


Figure 1. Dimensionless glucose concentration C versus dimensionless distance z. The dotted lines represent the analytical solution and the solid lines represent the numerical solution

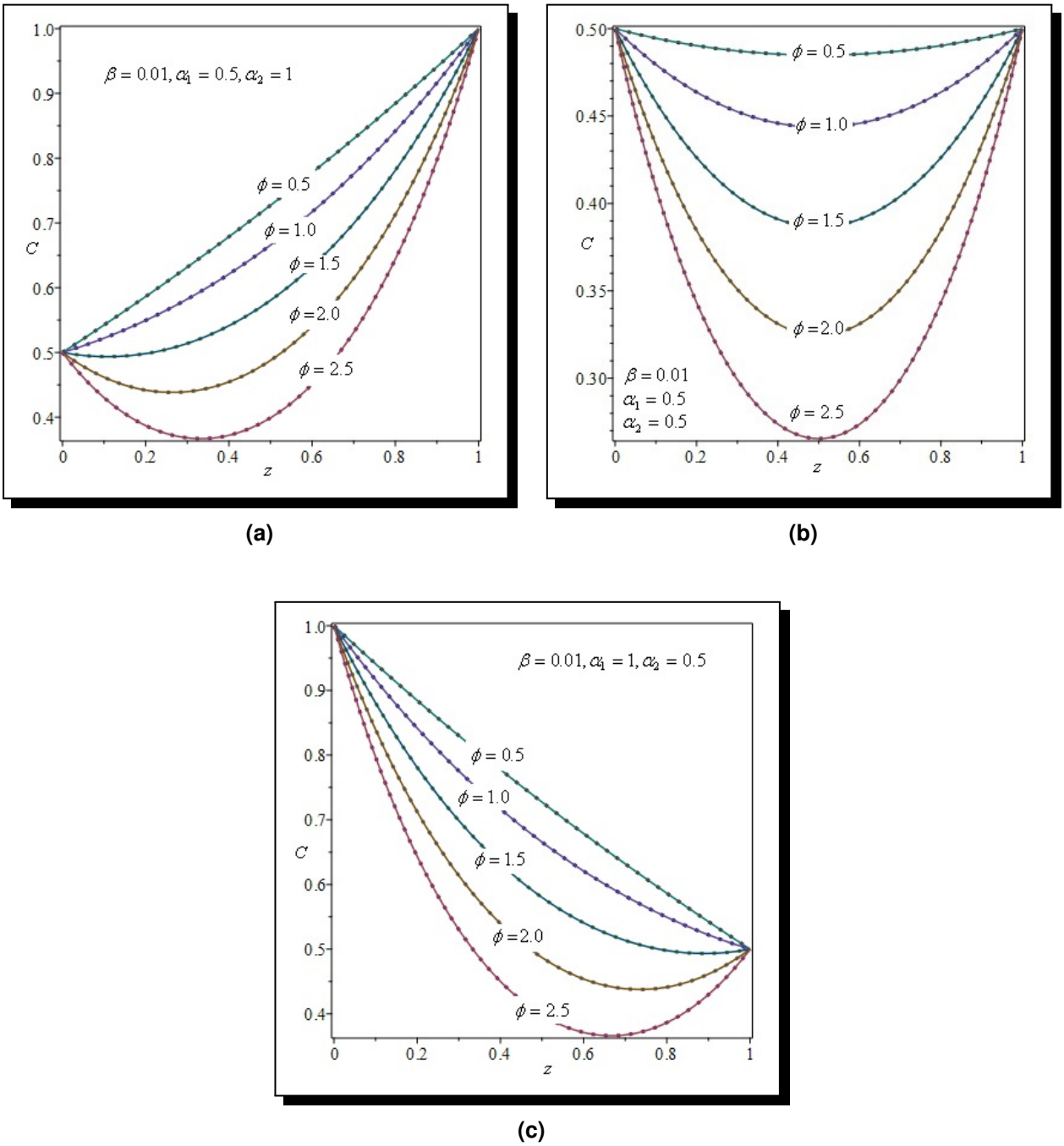


Figure 2. Dimensionless glucose concentration C versus dimensionless distance z for various values of ϕ. The dotted lines represent the analytical solution and the solid lines represent the numerical simulation

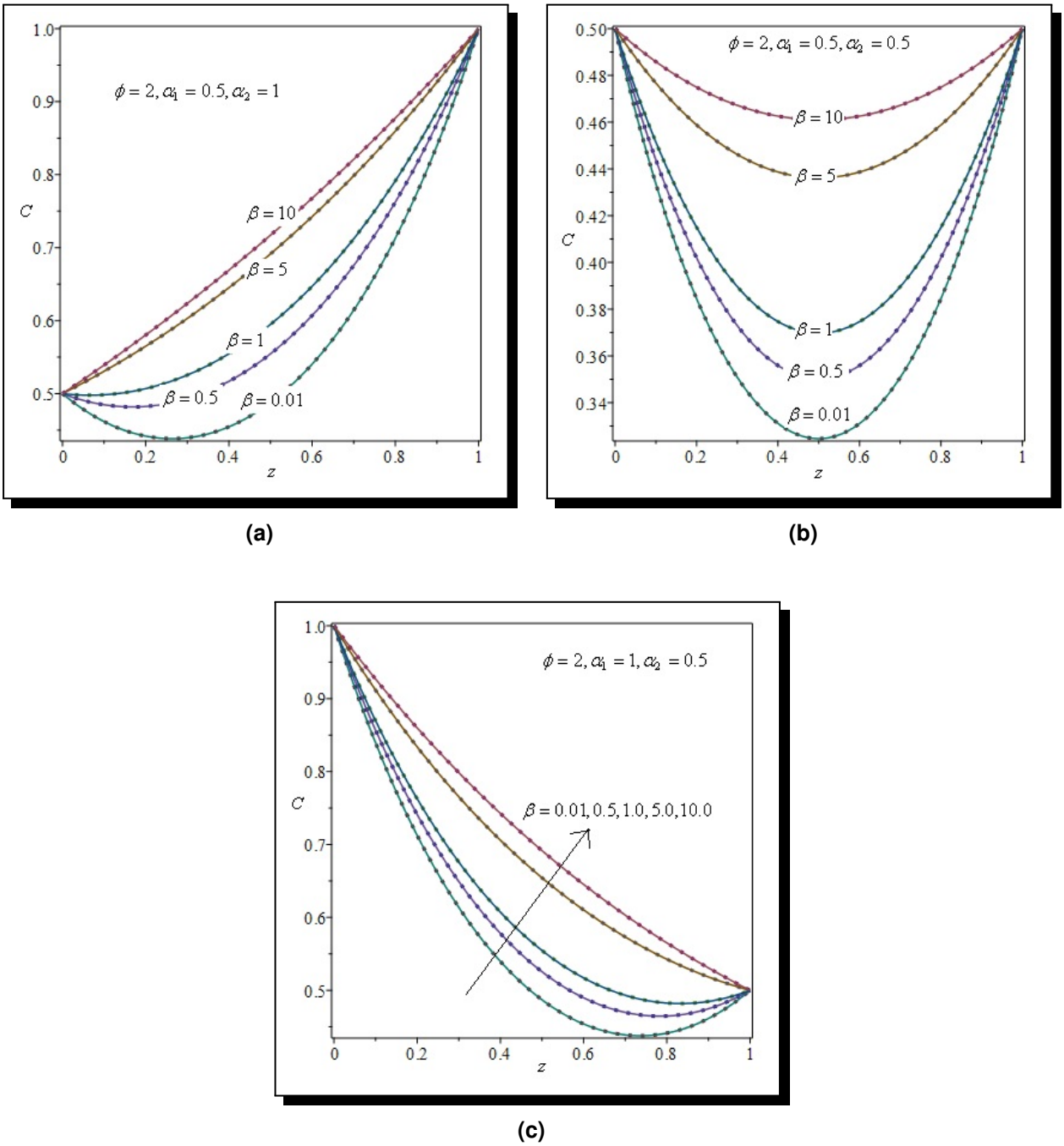
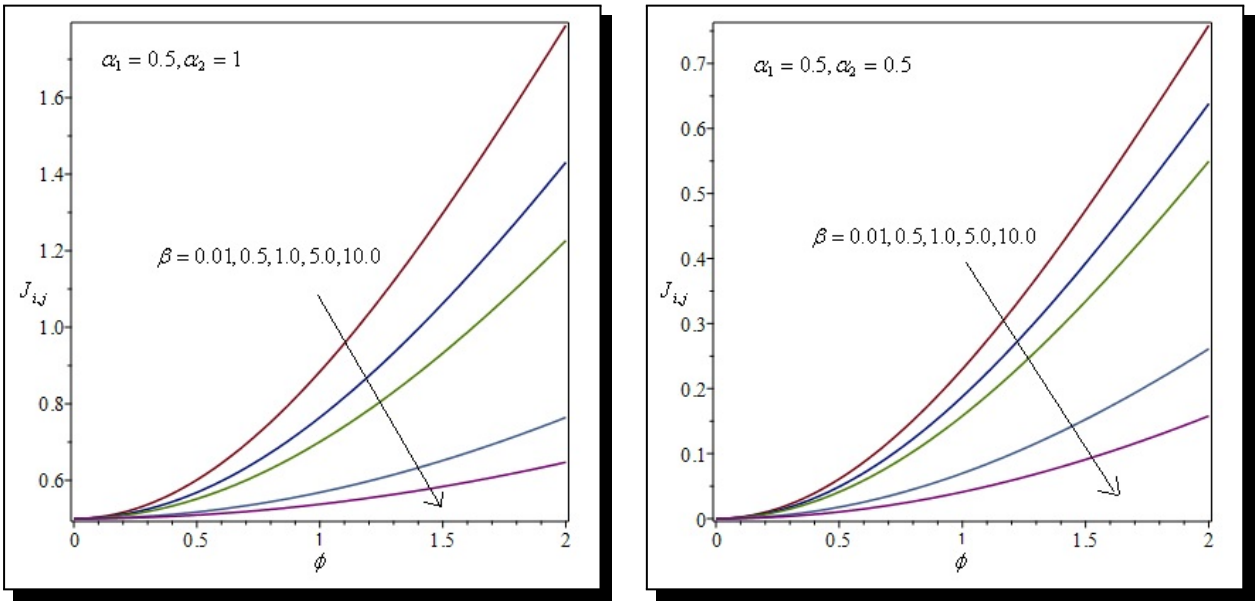
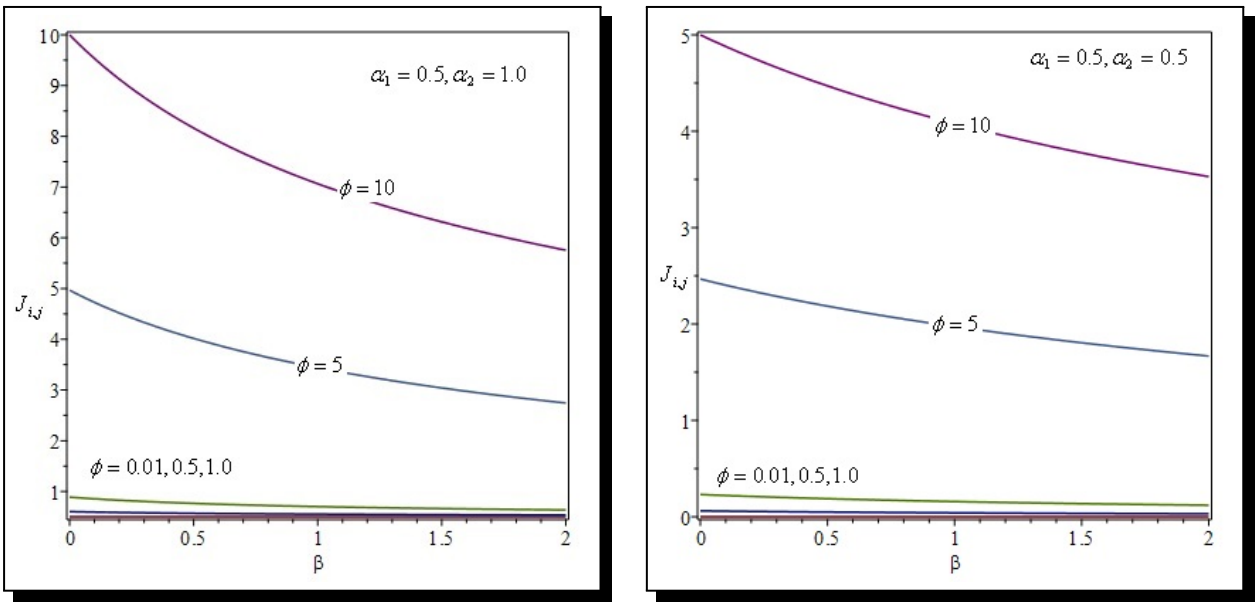


Figure 3. Dimensionless glucose concentration C versus dimensionless distance z for various values of β. The dotted lines represent the analytical solution and the solid lines represent the numerical simulation



(a) **(b)**

Figure 4. Plot of dimensionless current versus ϕ for various values of β



(a) **(b)**

Figure 5. Plot of dimensionless current versusβ for various values of ϕ

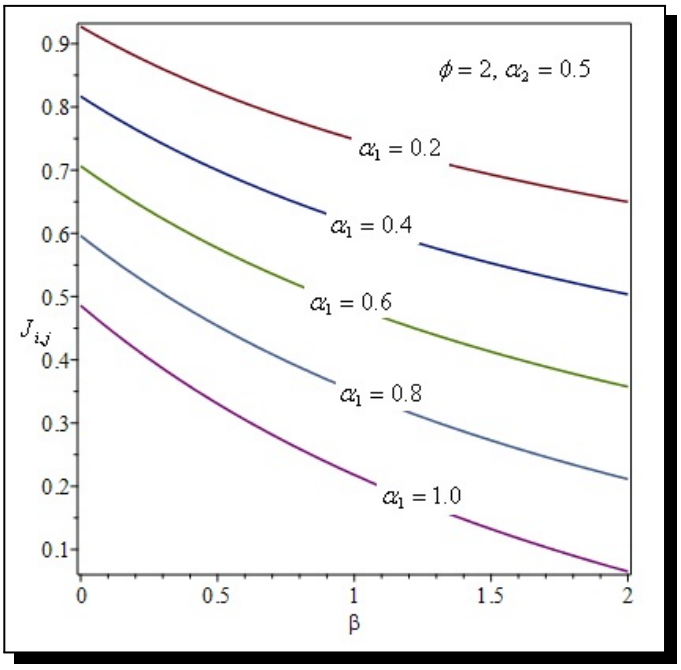


Figure 6. Plot of dimensionless current versus β for various values of α_1

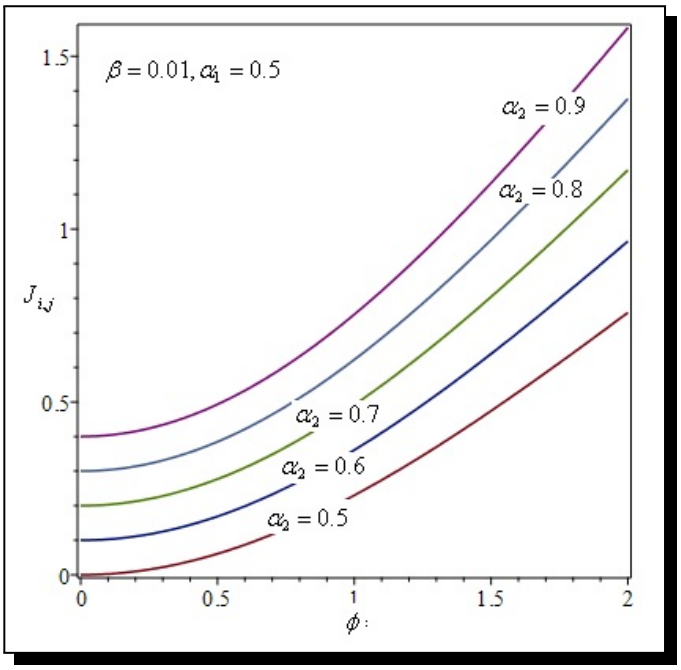


Figure 7. Plot of dimensionless current versus ϕ for various values of α_2

5. Conclusion

A pore network model of deactivation of immobilized glucose isomerase in packed-bed reactors is solved using the Akbari-Ganji's method to obtain approximate analytical expressions for dimensionless glucose concentration and dimensionless current. The result obtained in this paper may be used to make prediction in future experiments.

Appendices

A. Basic Concept of Akbari-Ganji's Method

Consider the following nonlinear differential equation and boundary conditions

$$f(u'', u', u, F_o(\sin \omega t)) = 0, \tag{A.1}$$

$$u(0) = A, \quad u'(0) = B. \tag{A.2}$$

Choose an initial guess which satisfies eqn. (A.2), as follows

$$u(x) = e^{-at}\{b\cos(\omega t + \phi)\}, \tag{A.3}$$

where $\{a, b, \omega, \phi\}$ are constant coefficients.
Using the initial conditions of eqn. (A.2) the following two cases arises:

$$\text{(a)} \quad u(t) = u(IC), \tag{A.4}$$

$$\text{(b)} \quad u(t) = g(t). \tag{A.5}$$

Substituting eqn. (A.5) in eqn. (A.1), we get

$$f(t) = f(g''(t), g'(t), g(t), F_o(\sin \omega t)) = 0. \tag{A.6}$$

Substituting eqn. (A.4) in eqn. (A.6) and its derivatives, the following is obtained

$$f(IC) = f(g''(IC), g'(IC), g(IC), \ldots) = 0, \tag{A.7}$$

$$f'(IC) = f(g''(IC), g'(IC), g(IC), \ldots) = 0, \tag{A.8}$$

$$f''(IC) = f(g''(IC), g'(IC), g(IC), \ldots) = 0. \tag{A.9}$$

From the eqn. (A.7), the set of n-algebraic equations with n-unknowns can be determined. From these equations, the constant coefficients $\{a, b, \omega, \phi\}$ can be obtained.

B. MATLAB Program to Find the Numerical Solution of eqns. (2.4) and (2.5)

```
function pdex4
m=0;
x=linspace(0,1);
t=linspace(0,100000);
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=DuDx;
```

```
q=2;
B=0.01;
F=-q^2*u(1)/(1+B*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
pl=[ul(1)-1];
ql=[0];
pr=[ur(1)-0.5];
qr=[0];
```

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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