International Journal of Modern Mathematical Sciences, 2023, 21(1): 12-19

Modern Scientific Press | *International Journal of Modern Mathematical Sciences* | ISSN:2166-286X

Journal homepage:www.ModernScientificPress.com/Journals/ijmms.aspx | *Florida, USA*

Article

Pore Network Model of Deactivation of Immobilized Glucose Isomerase in Packed-bed Reactors: An Analytical Approach Using the New Homotopy Perturbation Method

S. Narmatha

Department of Mathematics, Lady Doak College, Madurai, Tamil Nadu, India

Email: narmathasathyaa@gmail.com

Article history: Received 18 January 2023, Revised 14 March 2023, Accepted 15 March 2023, Published 18 April 2023.

Abstract: This paper's primary goal is to derive an approximate analytical solution to a mathematical model pertaining to a pore network model of deactivation of immobilized glucose isomerase in packed-bed reactors. To solve the previously developed mathematical model, the new approach to homotopy perturbation method is used. For all parameter values, the approximative analytical expressions for the steady-state concentration and current have been determined. The analytical solution and the numerical simulation exhibit excellent agreement. This work's findings will aid in a better understanding of the examined mathematical model.

Keywords: Mathematical modelling; Non-linear differential equation; Pore network model; New homotopy perturbation method; Numerical simulation

Mathematics Subject Classification: 34E, 35K20 and 68U20

1.Introduction

For the creation of an enzymatic conversion process, kinetic studies on enzyme deactivation is crucial. The impact of substrate protection on a commercial immobilised glucose isomerise was investigated by Jer-Yiing Houng et al. This was explored experimentally in a differential bed reactor, and a packed bed reactor theoretical study was carried out [1]. Enzymatic isomerization of glucose into fructose is carried out using a pore network model. The packed-bed reactor used for this technique contains micro - porous particles with a variety of pore diameters and is characterised by a pore size distribution. By employing enzymatic isomerization, Marshall and Kooi (1957) were able to produce glucose isomerase in quantities that were commercially viable. Glucose isomerase is an example of a highly successful application of enzyme Biotechnology to an industrial process that has no commercially viable route through conventional Chemistry. Juan-Yih and Kuo-Cheng Chen investigated how substrate protection affected enzyme deactivation. Theoretical analysis of enzyme deactivation with substrate protection offers an effective understanding which is essential for enzyme replacement and process optimization[2]. A pore-level model of the enzymatic isomerization of glucose to fructose and the resulting deactivation of the micro porous particles in which the process occurs was created by Mitra Dadvar et al. [3].

This communication's objective is to use the new homotopy perturbation method to develop expressions for the steady-state substrate concentration and current in closed form for all possible parameter values.

2. Mathematical Formulation of the Problem

The model describes the process by which glucose enzyme transforms from its intermediate complex form to fructose and then transforms back to its intermediate complex form. This can be written as

$$G + F \leftrightharpoons_{k_{-1}}^{k_1} X \leftrightharpoons_{k_{-2}}^{k_2} F + E \tag{1}$$

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:

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

where D_p is the pore diffusivity in the micro pores, a is the surface area per unit weight of the particle and $\lambda = \frac{R_M}{r}$, 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

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

$$K_m = \frac{K_{mf} K_{mr}}{K_{mr} - K_{mf}} \left[1 + \left(K_{mf}^{-1} + \frac{K}{K_{mf}} \right) \frac{G_o}{1+K} \right]$$

eqn.(2) becomes

$$D_p \frac{d^2 \overline{G}}{dx^2} - \frac{2}{r} \frac{v_m \overline{G}}{K_m + \overline{G}} = 0 \tag{3}$$

where G is the concentration of glucose, G_o is an initial concentration of glucose, R is a reaction 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

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

eqn.(3) becomes

$$\frac{d^2 C}{dz^2} - \phi^2 \left(\frac{C}{1 + \beta C} \right) = 0 \tag{4}$$

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:

$$C(z=0) = \alpha_1, \qquad C(z=1) = \alpha_2 \tag{5}$$

The dimensionless current is given by

$$J_{ij} = \left[\frac{dC}{dz} \right]_{z=1} \tag{6}$$

3. New Homotopy Perturbation Method

Many phenomena in various branches of the medical sciences can be modelled using linear and non-linear differential equations in order to illustrate their behaviours and consequences using mathematical ideas. Effective asymptotic methods [4], such as the homotopy perturbation method [5], homotopy analysis method [6], Adomian decomposition method [7], wavelet transform method [8], Akbari- Ganji'smethod [9], etc., are used to obtain analytical solutions of non-linear differential equations.

The homotopy perturbation approach, which can transform non-linear differential equations into some straightforward linear differential equations, is a potent and effective tool for addressing non-linear problems. Ji-Huan He first suggested using this approach in 2003.

This method has the notable advantage of offering an approximative analytical solution to a variety of non-linear problems in Applied Sciences without the need for a small parameter in the equation. In most circumstances, the homotopy perturbation approach produces a very quick convergence of the solution series; typically, a small number of iterations results in very precise solutions. Recently, a new method of solving non-linear differential equations using the Homotopy perturbation method[10,11] has been developed.

4. Analytical Expressions for the Glucose Concentration and Current Using New Homotopy Perturbation Method

Construct the homotopy for eqn. (4) as follows

$$(1-p)\left[\frac{d^2C}{dz^2}-\phi^2\left(\frac{C}{1+\beta\alpha_1}\right)\right]+p\left[\frac{d^2C}{dz^2}-\phi^2\left(\frac{C}{1+\beta C}\right)\right]=0 \tag{7}$$

Let the approximate solution of eqn. (7) be

$$C=C_0+pC_1+p^2C_2+... \tag{8}$$

Substituting eqn. (8) in eqn. (7) and equating the coefficients of p^0, we get

$$\frac{d^2C_0}{dz^2}-\phi^2\left(\frac{C_0}{1+\beta\alpha_1}\right) \tag{9}$$

The boundary conditions for the above equation becomes

$$z=0,\ C_0=\alpha_1 \tag{10}$$

$$z=1,\ C_0=\alpha_2 \tag{11}$$

Solving eqns. (9) to (11), we get the approximate analytical expression for glucose concentration as

$$C(z)=\frac{\left(\alpha_2-\alpha_1e^{-\sqrt{k}}\right)e^{\sqrt{k}x}+\left(\alpha_1e^{\sqrt{k}}-\alpha_2\right)e^{-\sqrt{k}x}}{e^{\sqrt{k}}-e^{-\sqrt{k}}} \tag{12}$$

The dimensionless current is given by

$$J_{ij} = \frac{\sqrt{k}\left(\alpha_2 e^{2\sqrt{k}} + \alpha_2 - 2\alpha_1 e^{\sqrt{k}}\right)}{e^{2\sqrt{k}} - 1} \tag{13}$$

where $k = \dfrac{\phi^2}{1+\alpha_1\beta}$

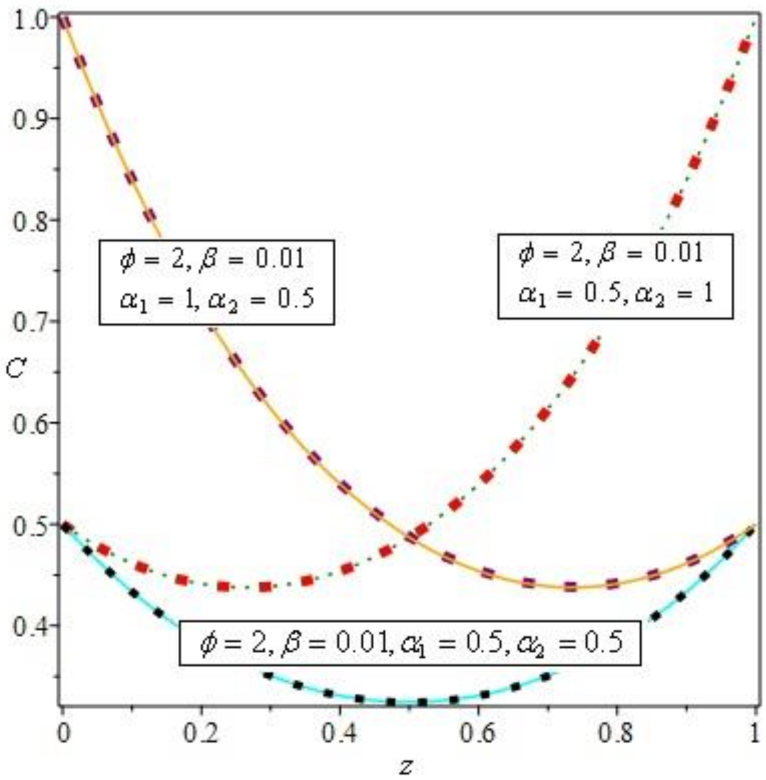

Fig. 1: Dimensionless glucose concentration *C* versus dimensionless distance *z*. The dotted lines reflect the numerical simulation, whereas the solid lines indicate the analytical solution.

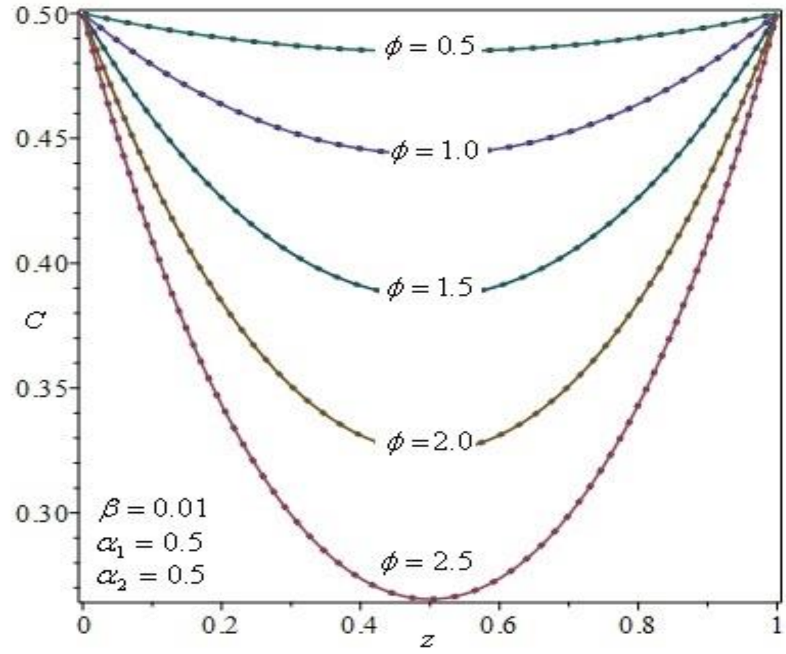

Fig. 2: Dimensionless glucose concentration *C* versus dimensionless distance *z* for various values of ϕ. The dotted lines reflect the numerical simulation, whereas the solid lines indicate the analytical solution.

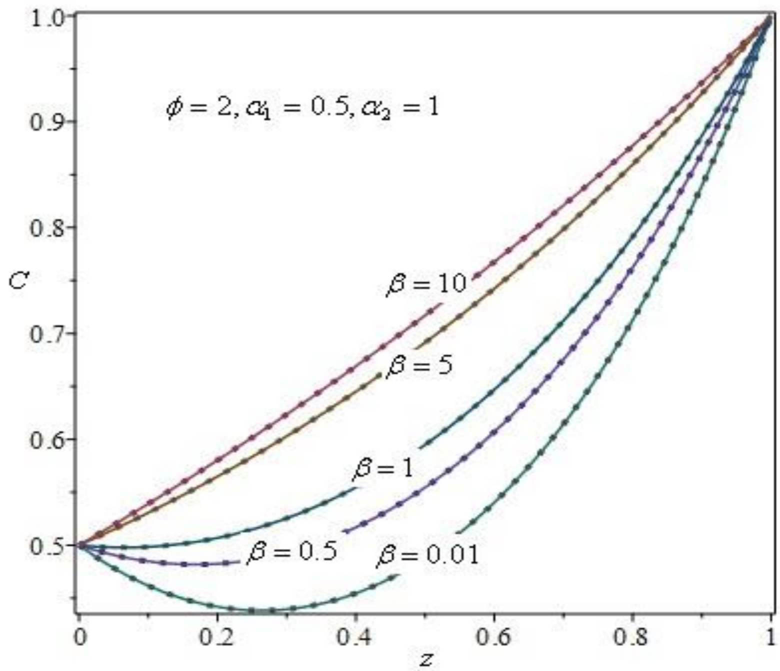

Fig. 3: Dimensionless glucose concentration *C* versus dimensionless distance *z* for various values of β. The dotted lines reflect the numerical simulation, whereas the solid lines indicate the analytical solution.

Fig. 4: Sensitivity analysis for the rate of change of current J_{ij} with respect to the various parameters.

5. Results and Discussion

Using the new homotopy perturbation method, analytical expressions for the dimensionless glucose concentration and dimensionless current have been developed. The numerical simulation and the analytical solution that was developed are found to fit very well. Further, from figures 2 and 3, we observe that the dimensionless glucose concentration varies directly with β, but inversely with ϕ. From figure 4, we see that the dimensionless current varies inversely with β, but directly with ϕ.

6. Conclusion

In this study, the new homotopy perturbation method is used to solve a pore network model of deactivation of immobilized glucose isomerase in packed-bed reactors, in order to establish approximative analytical expressions for dimensionless glucose concentration and dimensionless current. The findings in this paper may be applied to future experiments to make predictions.

References

[1] Jer-Yiing Houng, Hong-Yang Yu, and Kuo-Cheng Chen, Analysis of Substrate Protection of an Immobilized Glucose lsomerase. *Reactor Biotechnology and Bioengineering*, 41(193): 451 -458.

[2] K. C. Chen, & J. Y. Wu, Substrate protection of immobilized glucose isomerase. *Biotechnology and Bioengineering*, 30(1987): 817.-824.

[3] Mitra Dadvara, Muhammad Sahimib, Pore network model of deactivation of immobilized glucose isomerase inpacked-bed reactors Part III: Multiscale modelling, *Chemical Engineering Science*, 58(2003): 4935–4951.

[4] V. Ananthaswamy, S. Narmatha, A comparison among the homotopy based methods in solving a system of cubic autocatalytic reaction-diffusion equations, *Journal of Information and Computational Science* , 9(12)(2019): 1130-1141.

[5] P. Felicia Shirly, S. Narmatha, L. Rajendran, Analytical solution of boundary value problem in reactive gas absorption, *International Journal of Mathematical Archive*, 4(6)(2013): 228-242.

[6] V. Ananthaswamy, S. Narmatha, Mathematical analysis of reversible inhibitor biosensor systems in dynamic mode, *Singapore Journal of Scientific Research*, 10(3)(2020): 229-265.

[7] P. Felicia Shirly, S. Narmatha and L. Rajendran, Analytical solution of nonlinear dynamics of a self-igniting reaction diffusion system using modified Adomian decomposition method, *International Journal of Chemical Engineering*, Art ID: 825797(2014).

[8] M. Mahalakshmi, G. Hariharan, K. Kannan, The wavelet methods to linear and nonlinear reaction-diffusion model arising in mathematical chemistry, *Journal of Mathematical Chemistry*, 51(9)(2013): 2361-2385.

[9] B. Seethalakshmi, V. Ananthaswamy, S. Narmatha, P. Felicia Shirly, Approximate Analytical Solution to a Pore Network Model of Deactivation of Immobilized Glucose Isomerase in Packed-Bed Reactors Using Akbari-Ganji's Method. *Communications in Mathematics and Applications*, 13(3)(2022): 865–875.

[10] S. Narmatha, V. Ananthaswamy, M. Subha, Seenith Sivasundaram, Semi-analytical solution to a system of non-linear differential equations involving non-Michaelis-Menten parameters using a new approach to Homotopy perturbation method, *Nonlinear Studies*, 29(3): 841-850.

[11] S. Narmatha, V. Ananthaswamy, Seenith Sivasundaram, M. Subha, Semi analytical solution to an SIR model using new approach to Homotopy perturbation method, *Mathematics in Engineering, Science and Aerospace*, 13(4)(2022):1053-1069.