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Analytical Solutions of Nonlinear Equation in Immobilized Enzyme In A Spherical Porous Matrix: New Homotopy Perturbation Approach

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ABSTRACT
Mathematical modeling of immobilized enzyme in a spherical porous matrix is discussed. This analysis was performed by using an analytical method called new Homotopy perturbation method, and the results were compared with numerical solution. Our analytical solution has a satisfactory agreement with numerical solution.
***Keywords**: New Homotopy Perturbation Method, Mathematical Modeling, Nonlinear Equation, Immobilized Enzyme Substrate Concentration.*

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I. INTRODUCTION

The Homotopy perturbation method (HPM) was proposed by He [1,2] in 1998. This method has been used by many mathematicians and scientist to solve various linear/ nonlinear differential equations. In this method the solution is considered as the summation of an infinite series which usually converges rapidly to the exact solution. This simple method has been applied to solve linear and nonlinear heat equations [3,4], fluid mechanics [5], non-linear Schrodinger equations [6], some boundary value problems [7-10] and physical sciences problems [11-13]. Since He's Homotopy perturbation method (HPM) is a new technique, attempts have been conducted to apply this method for solving Blasius equation [5, 14]. In this paper, a new approach Homotopy perturbation method [10] is applied which has not been used in previous works. The analytical result are compared with simulation result and satisfactory agreement is noted.

Nomenclature

Symbols	Name
D_e	Effective Diffusivity of Substrate
D_e^D	Effective Diffusivity of Dextrin
D_e^s	Effective Diffusivity of Soluble Starch
K_m	Michael's Constant
K_m^D	Michael's Constant For Dextrin
K_m^s	Michael's Constant For Soluble Starch
r	Radius
R	Radius of Support
$\bar{r}$	Dimensionless Radius
s	Substrate Concentration
s_0	Initial Substrate Concentration
$\bar{s}$	Dimensionless Substrate Concentration
V_m	Maximum Reaction Rate

$V_m{}^D$	Maximum Reaction Rate of Dextrin
$V_m{}^s$	Maximum Reaction Rate of Soluble Starch
$W(x)$	Weight Function
SBR	Stirred Batch Reactor
RDBR	Recycling Differential Batch Reactor
Greek Symbols	
φ	Thiele modulus
β	Dimensionless Michael's constant

Mathematical Formulation of The Problem

Enzymes are used on porous supports in order to contain the enzyme, and allow continued catalytic activity [15]. When enzymes are immobilized on the internal surface of a porous spherical support, the substrate diffuses thorough the pathway among the pores, and reacts with the immobilized enzyme [15]. Assume that enzymes are uniformly distributed in a spherical porous matrix. The mass balanced equation for steady-state diffusion of substrate in porous spherical matrix under Michaelis-Menden kinetics is given as follows:

$$D_e\left(\frac{d^2s}{dr^2}+\frac{2}{r}\frac{ds}{dr}\right)=\frac{V_m}{K_m+s} \qquad (1)$$

The dimensionless steady state diffusion equation in spherical coordinate can be reduces to the following form:

$$\frac{d^2\bar{s}}{d\bar{r}^2}+\frac{2}{\bar{r}}\frac{d\bar{s}}{d\bar{r}}=\frac{\phi^2\bar{s}}{1+\dfrac{\bar{s}}{\beta}} \qquad (2)$$

Where the dimensionless parameter are

$$\bar{s}=\frac{s}{s_0},\ \bar{r}=\frac{r}{R},\ \beta=\frac{K_m}{S_0},\ \phi=R\sqrt{\frac{V_m}{D_eK_m}}$$

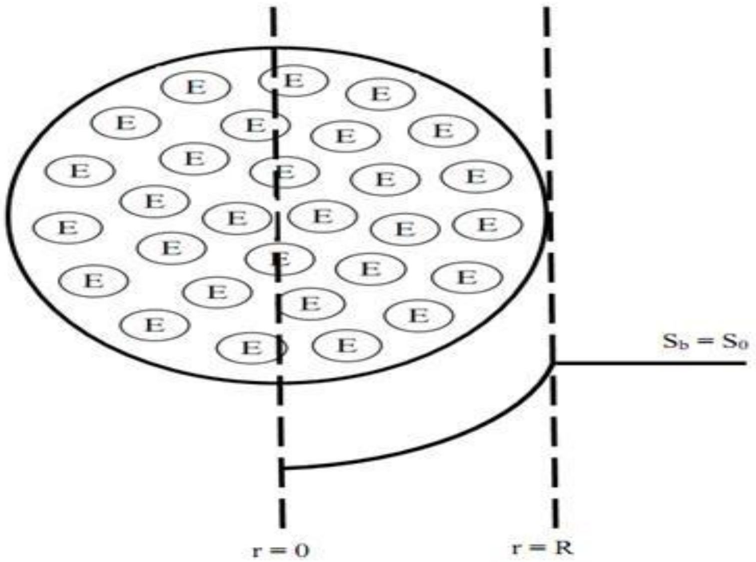

Figure 1. Schematic of the problem (substrate concentration profile in immobilized enzyme in a spherical porous matrix) [15].

where, $\bar{s}$ is the dimensionless substrate concentration, s_0 is the bulk substrate concentration, $\bar{r}$ is the dimensionless radius, K_m is the Michael's constant, V_m is maximum reaction rate, and D_e is effectiveness diffusion coefficient. The appropriate boundary conditions are:

$$\bar{r}=1 \quad : \ \bar{s}=1 \tag{4}$$

$$\bar{r}=0 \quad : \frac{d\,\bar{s}}{d\,\bar{r}}=0 \tag{5}$$

Recently Ali Izadi et al. [15] solved the above problem using least square method [16]. In this paper a new approach of Homotopy perturbation method is used to solve the nonlinear equation (2).

II. BASIC IDEA OF HOMOTOPY PERTURBATION METHOD

To illustrate the basic ideas of this method, we consider the following non-linear functional equation:

$$A(U)-f(r)=0, \quad r\in\Omega \tag{6}$$

With the following boundary condition:

$$B\left(u,\frac{\partial u}{\partial n}\right)=0, \quad r\in\Gamma, \tag{7}$$

Where A is a general functional operator, B a boundary operator, $f(r)$ is a known analytical function and Γ is the boundary of the domain Ω. The operator A can be decomposed into two operators L and N, where L is linear, and N is nonlinear operator. Eqn. (6) can be, therefore, written as follows:

$$L(U)+N(U)-f(r)=0. \tag{8}$$

Using the Homotopy technique, we construct a Homotopy $U(r,p):\Omega\times[0,1]\to R$, which satisfies:

$$H(U,p)=(1-p)[L(U)-L(U_0)]+p[A(U)-f(r)]=0, \ \ p\in[0,1], \ r\in\Omega, \tag{9}$$

or

$$H(U,p)=L(U)-L(U_0)+pL(U_0)+p[N(U)-f(r)]=0, \tag{10}$$

where $p\in[0,1]$ is an embedding parameter, u_0 is an initial approximation for the solution of Eqn. (6),which satisfies the boundary conditions. Obviously, from Eqns. (9) and (10) we will have:

$$H(U,0)=L(U)-L(U_0)=0, \tag{11}$$

$$H(U,1)=A(U)-f(r)=0. \tag{12}$$

The changing values of p from zero to unity are just that of $U(r,p)$ from $u_0(r)$ to $u(r)$.In topology, this is called Homotopy. According to HPM, we can first use the embedding parameter $p$as a small parameter, and assume that the solution of Eqns. (9) and (10) as a power series in p:

$$V=U_0+pU_1+p^2U_2+\ldots \tag{13}$$

Setting p = 1, results in the approximation to the solution of Eqn. (13)

$$U=\lim_{p\to 1}V=U_0+U_1+U_2+\ldots \tag{14}$$

The combination of the perturbation method and the Homotopy method is called the Homotopy perturbation method (HPM), which has eliminated limitations of the traditional perturbation techniques. The series Eqn. (14) is convergent for more cases.

3.1. Analytical Expression Substrate Concentration Using Nhpm

The dimensionless nonlinear Eqn. (2) defines the boundary value problem. New Homotopy perturbation method used to give the approximate solutions of the nonlinear Eqn. (2).
The analytical expression substrate concentration using NHPM is,

$$\bar{s}(\bar{r})=\left(\frac{1}{e^{-\sqrt{b}}-e^{\sqrt{b}}}\right)\frac{e^{-\sqrt{b}\,\bar{r}}}{\bar{r}}-\left(\frac{1}{e^{-\sqrt{b}}-e^{\sqrt{b}}}\right)\frac{e^{\sqrt{b}\,\bar{r}}}{\bar{r}} \tag{14}$$

where $b=\dfrac{\phi^2}{1+\alpha}, \alpha=\dfrac{1}{\beta}$ (15)

III. NUMERICAL SIMULATION

The NHPM provides an analytical solution in terms of an infinite power series. However, there is a practical need to evaluate this solution and to obtain numerical values from the infinite power series. In order to investigate the accuracy of the NHPM solution with a finite number of terms, the differential equation is solved. To show the efficiency of the present method our analytical solution in compared with numerical solution in Figs.2 and 3, and table 1-4 satisfactory agreement is noted. The SCILAB program is also given in appendix (B).

IV. RESULTS AND DISCUSSION

Equations (10) represent the new the analytical expression of the concentration of substrate. The Thiele modulus ϕ can be varied by changing either the particle radius or the amount of concentration of substrate. This parameter describes the relative importance of diffusion and reaction in the particle radius. When ϕ is small, the kinetics are the dominant resistance; the overall uptake of substrate in the enzyme matrix is kinetically controlled. Under these conditions, the substrate concentration profile across the membrane is essentially uniform. In contrast, when the Thiele modulus ϕ is large, diffusion limitations are the principal determining factor. Figs. 2-3 shows the dimensionless steady-state substrate concentration for the different values of β calculated using Eq. (14). From these figures, we can see that the value of the concentration increases when α increases.

V. CONCLUSIONS

In this paper we have studied a well-known Michaelis-Menten equation. We have applied new Homotopy perturbation method to solve this nonlinear differential equation. Simple and closed form analytical expression of concentration of substrate is obtained. Analytical results are compared with numerical result and satisfactory agreement is noted.

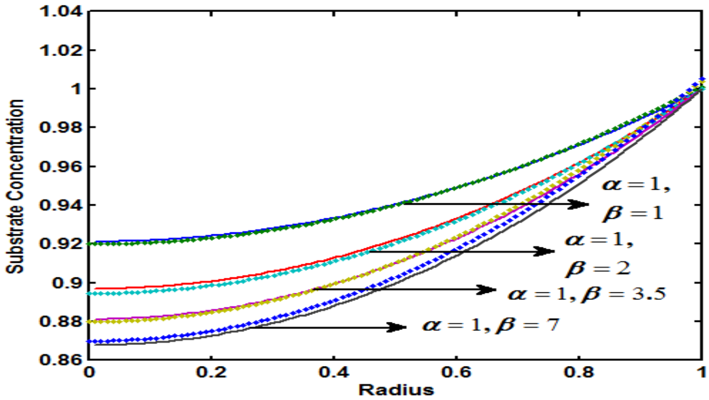

Figure 2. Plot of dimensionless substrate concentration $\bar{s}(\bar{r})$ versus dimensionless radius $\bar{r}$ for various values of the parameter, α and β using eqn. (2).

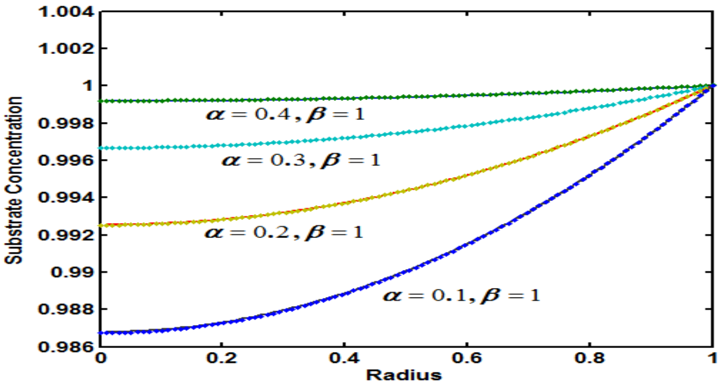

Figure 3. Plot of dimensionless substrate concentration $\bar{s}(\bar{r})$versus dimensionless radius $\bar{r}$ for various values of the parameter, α and β . Solid lines represent eqn. (2) and dotted line represents numerical solution.

Table 1. Comparison of analytical results with numerical results for substrate concentration $\bar{s}(\bar{r})$

	$\alpha=1,\ \beta=1$			$\alpha=1,\ \beta=2$		
$\bar{r}$	Numerical simulation	Analytical Eqn. (14)	Error(%)	Numerical simulation	Analytical Eqn. (14)	Error(%)
0	0.9992	0.9992	0.00	0.8945	0.8970	0.0028
0.1	0.9992	0.9992	0.00	0.8956	0.8980	0.0027
0.2	0.9992	0.9992	0.00	0.8988	0.9010	0.0025
0.3	0.9993	0.9992	0.00	0.9040	0.9061	0.0023
0.4	0.9993	0.9993	0.00	0.9114	0.9133	0.0021
0.5	0.9994	0.9994	0.00	0.9210	0.9226	0.0017
0.6	0.9995	0.9995	0.00	0.9327	0.9340	0.0014
0.7	0.9996	0.9996	0.00	0.9467	0.9476	0.0009
0.8	0.9997	0.9997	0.00	0.9629	0.9365	0.0282
0.9	0.9999	0.9999	0.00	0.9814	0.9816	0.0002
1	1	1	0.00	1	1	0
		Average error (%)	0.00	Average error (%)	0.0012	

Table 2. Comparison of analytical results with numerical results for substrate concentration $\bar{s}(\bar{r})$

	$\alpha=1,\ \beta=3.5$			$\alpha=1,\ \beta=7$		
$\bar{r}$	Numerical simulation	Analytical Eqn. (14)	Error(%)	Numerical simulation	Analytical Eqn. (14)	Error(%)
0	0.8800	0.8813	0.0015	0.87	0.8679	0.0024
0.1	0.8812	0.8824	0.0014	0.8713	0.8691	0.0025
0.2	0.8849	0.8859	0.0012	0.8753	0.8730	0.0026
0.3	0.8911	0.8918	0.0008	0.8820	0.8795	0.0028
0.4	0.8997	0.9000	0.0003	0.8914	0.8886	0.0031
0.5	0.9109	0.9107	0.0002	0.9035	0.9004	0.0034
0.6	0.9246	0.9238	0.0009	0.9185	0.9150	0.0038
0.7	0.9410	0.9395	0.0016	0.9363	0.9325	0.0041
0.8	0.9600	0.9578	0.0023	0.9571	0.9528	0.0045
0.9	0.9818	0.9787	0.0032	0.9810	0.9762	0.0049
1	1	1	0.00	1	1	0
		Average error (%)	0.0004	Average error (%)	0.0034	

Table 3. Comparison of analytical results with numerical results for substrate concentration $\bar{s}(\bar{r})$

	$\alpha=0.1,\ \beta=1$			$\alpha=0.2,\ \beta=1$		
$\bar{r}$	Numerical simulation	Analytical Eqn. (14)	Error(%)	Numerical simulation	Analytical Eqn. (14)	Error(%)
0	0.9992	0.9992	0.00	0.9967	0.9967	0.00
0.1	0.9992	0.9992	0.00	0.9967	0.9967	0.00
0.2	0.9992	0.9992	0.00	0.9968	0.9968	0.00
0.3	0.9993	0.9992	0.0001	0.997	0.9970	0.00
0.4	0.9993	0.9993	0.00	0.9972	0.9972	0.00
0.5	0.9994	0.9994	0.00	0.9975	0.9975	0.00
0.6	0.9995	0.9995	0.00	0.9979	0.9979	0.00
0.7	0.9996	0.9996	0.00	0.9983	0.9983	0.00
0.8	0.9997	0.9997	0.00	0.9988	0.9988	0.00
0.9	0.9999	0.9999	0.00	0.9994	0.9994	0.00
1	1	1	0.00	1	1	0.00
		Average error (%)	0.00	Average error (%)	0.00	

Table 4. Comparison of analytical results with numerical results for substrate concentration $\bar{s}(\bar{r})$

	$\alpha = 0.3,\ \beta = 1$			$\alpha = 0.4,\ \beta = 1$		
$\bar{r}$	Numerical simulation	Analytical Eqn. (14)	Error(%)	Numerical simulation	Analytical Eqn. (14)	Error(%)
0	0.9925	0.9925	0.00	0.9867	0.9867	0.00
0.1	0.9926	0.9926	0.00	0.9869	0.9869	0.00
0.2	0.9928	0.9928	0.00	0.9873	0.9873	0.00
0.3	0.9932	0.9932	0.00	0.9879	0.9879	0.00
0.4	0.9937	0.9937	0.00	0.9889	0.9889	0.00
0.5	0.9944	0.9944	0.00	0.9901	0.9901	0.00
0.6	0.9953	0.9953	0.00	0.9916	0.9916	0.00
0.7	0.9963	0.9963	0.00	0.9934	0.9934	0.00
0.8	0.9974	0.9974	0.00	0.9954	0.9954	0.00
0.9	0.9987	0.9987	0.00	0.9977	0.9977	0.00
1	1	1	0.00	1	1	0.00
		Average error (%)	0.00	Average error (%)	0.00	

Appendix A : Analytical Solution On Nonlinear Eqn. (2) Using New Homotopy Perturbation Method (Nhpm)

The nonlinear Eqn. (2) can be written as

$$\frac{d^2\bar{s}}{d\bar{r}^2} + \frac{2}{\bar{r}}\frac{d\bar{s}}{d\bar{r}} = \frac{\varphi^2\bar{s}}{1+\alpha\bar{s}} \quad \text{where } \alpha = \frac{1}{\beta} \tag{A1}$$

Now the boundary conditions becomes

$$\bar{r} = 1, \qquad \bar{S} = 1 \tag{A2}$$

$$\bar{r} = 0, \qquad \frac{d\bar{S}}{d\bar{r}} = 0 \tag{A3}$$

We construct the Homotopy for the Eqn. (A1) as follows:

$$(1-p)\left(\frac{d^2\bar{s}}{d\bar{r}^2} + \frac{2}{\bar{r}}\frac{d\bar{s}}{d\bar{r}} - \frac{\varphi^2\bar{s}}{1+\alpha}\right)_{\bar{s}(\bar{r})=1} + p\left((1+\alpha\bar{s})\left(\frac{d^2\bar{s}}{d\bar{r}^2} + \frac{2}{r}\frac{d\bar{s}}{d\bar{r}}\right) - \phi^2\bar{s}\right) = 0 \tag{A4}$$

where p is the embedding parameter and $p \in [0,1]$

The approximate solution of (A1) is

$$\bar{s} = \bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots\ldots. \tag{A5}$$

The initial approximation are as follows

$$\bar{s}_0(1) = 1; \bar{s}_{0,\bar{r}}(0) = 0$$

$$\bar{s}_i(1) = 0; \bar{s}_{i,\bar{r}}(0) = 0; i = 1,2,3\ldots\ldots \tag{A6}$$

Substituting Eqns. (A5) in (A4), we have

$$(1-p)\left[\frac{d^2(\bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots)}{d\bar{r}^2} + \frac{2}{r}\frac{d(\bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots)}{d\bar{r}} - \frac{\varphi^2(\bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots)}{1+\alpha}\right]$$

$$+ p\left[\begin{array}{r}(1+\alpha(\bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots))\left(\dfrac{d^2(\bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots)}{d\bar{r}^2} + \dfrac{2}{r}\dfrac{d(\bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots)}{d\bar{r}}\right) \\ -\varphi^2(\bar{s}_0 + p\bar{s}_1 + p^2\bar{s}_2 + \ldots)\end{array}\right] = 0$$

(A7)

Comparing the coefficients of like powers of p in Eqn. (A7), we get

$$p^0 : \frac{d^2\bar{s}_0}{d\bar{r}^2} + \frac{2}{\bar{r}}\frac{d\bar{s}_0}{d\bar{r}} - \frac{\varphi^2\bar{s}_0}{1+\alpha} = 0 \tag{A8}$$

$$p^1 : \frac{d^2\bar{s}_1}{d\bar{r}^2} + \frac{2}{\bar{r}}\frac{d\bar{s}_1}{d\bar{r}} - \frac{\varphi^2\bar{s}_1}{1+\alpha} + \left(\frac{\bar{s}_0}{\beta}\right)\left(\frac{d^2\bar{s}_0}{d\bar{r}^2} + \frac{2}{\bar{r}}\frac{d\bar{s}_0}{d\bar{r}}\right) - \varphi^2\bar{s}_0\left(\frac{\alpha}{1+\alpha}\right) = 0 \tag{A9}$$

Solving the Eqn. (A8) and using the boundary condition (A5), we can obtain the following results:

$$\bar{s}(\bar{r}) = \left(\frac{1}{e^{-\sqrt{b}} - e^{\sqrt{b}}}\right)\frac{e^{-\sqrt{b}\,\bar{r}}}{\bar{r}} - \left(\frac{1}{e^{-\sqrt{b}} - e^{\sqrt{b}}}\right)\frac{e^{\sqrt{b}\,\bar{r}}}{\bar{r}} \tag{A10}$$

where $b = \frac{\phi^2}{1+\alpha}$, and $\alpha = \frac{1}{\beta}$ (A11)

According to the HPM, we can conclude that

$$\bar{s} = \lim_{p\to 1} \bar{s}(\bar{r}) = \bar{s}_0 \tag{A12}$$

After putting Eqns. (A10) and (A11) into Eqn. (A12), we can obtain the Eqn. (15) in the text.

Appendix B: Matlab/Scilab Program Is To Find The Numerical Solution Of The Eqn. (2)

```
function pdex1
m = 2;
x = linspace(0,1);
t = linspace(0,100000);
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
% Extract the first solution component as u.
u = sol(:,:,1);
% A solution profile can also be illuminating.
figure
plot(x,u(end,:))
title('Solution at t = 2')
xlabel('Distance x')
ylabel('u(x,2)')
% --------------------------------------------------------------
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = pi^2;
f = DuDx;
phi=1;
alpha=.2;
s = -(9*phi^2*u)/(1+alpha*u);
% -------------------------------------------------------------
function u0 = pdex1ic(x)
u0 = 0;
% --------------------------------------------------------------
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = ur-1;
qr = 0;
```

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