New Approach of Homotopy Perturbation Method for Solving the Equations in Enzyme Biochemical Systems

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Abstract: In this paper, new homotopy perturbation method (iteration scheme) will be employed to solve the nonlinear dynamical problems that arise in thin membrane kinetics. More precisely, the method will be used to mathematically model and solve the kinetics of the thin membrane. A main property that makes the proposed method superior to other iterative methods is the way it handles boundary value problems, where both mixed Dirichlet and Neumann boundary conditions are taken into consideration, while other iterative methods only make account of the initial point and as a result, the approximate solution may deteriorate for values that are far away from the initial point and closer to the other endpoint. Our analytical results are compared with numerical solution. The method is found to be easily implemented, fast, and computationally economical and attractive.

Keywords: Mathematical Modelling, Thin Membrane, Enzyme Kinetics, Homotopy Perturbation Method

1. Introduction

Non-linear differential equations can model many phenomena in different fields of science and engineering in order to present their behaviors and effects by mathematical concepts. Most of the equations do not have analytical solution which can be handled by semi-analytical or numerical methods. In order to obtain exact solution of nonlinear differential equations, semi-analytical methods such as the Variational Iteration method (VIM) and Homotopy perturbation method (HPM) are considered. The ideas of the VIM and HPM were first pioneered by He \([1, 2]\). He \([3]\) presented application of the HPM in solving the non-linear non-homogeneous partial differential equations. They are powerful algorithms in solving various kinds of linear and nonlinear equations. The homotopy perturbation method is used by Nourazar et al. \([4-6]\) in order to obtain exact solution of nonlinear differential equations. Abzari and Abzari \([7]\) presented numerical study of Burgers–Huxley equations via reduced differential transform method. Rajendran and co-workers are solved many non-linear equation in chemical science using homotopy perturbation method and variational iteration method \([8]\). Comparative analysis of variational iteration method and Haar wavelet method for the numerical solutions of Burgers–Huxley and Huxley equations is presented by Ray and Gupta \([9]\). Soori et al. \([10, 11]\) presented application of the variational iteration method and the 2 homotopy perturbation method to the fisher type equation. Also, Soori \([12]\) presented series solution of weakly-singular kernel volterra integro-differential equations by the combined laplace-adomian method. Application of the variational iteration method for the Newell-Whitehead-Segel equation is presented by Soori \([13]\). Also recently Malini et al. \([14]\) compared variational iteration, NHPM and ADM method with numerical solution for non-linear equation in single valued carbon nanotubes. In this study we have applied NHPM to find the approximate solution of the problem of the second order non-linear differential equation in thin membrane. This method generate the analytical solutions in convergence series and it is also effective mathematical tool to handle a large class of linear and non-
linear differential equation in engineering and chemical sciences.

2. Mathematical Formulation of the Problem

In enzyme biochemical systems kinetics in thin membrane is modelled by the reaction-diffusion equations [1]:

\[ \frac{d^2 u}{dx^2} + \lambda uv - uw = 0 \]  
\[ \frac{d^2 v}{dx^2} - \lambda uv = 0 \]  
\[ \frac{d^2 w}{dx^2} - uw + \lambda uv = 0 \]

where \( u(x), v(x) \) and \( w(x) \) denote the concentrations of the chemical species, A, B and C respectively. The diffusion coefficient of three species is considered to have an equal diffusion coefficient which is equal to 1. Now the boundary conditions becomes

\[ x = 0, \quad u = \alpha, \quad \frac{dv}{dx} = 0, \quad w = \gamma \]  
\[ x = 1, \quad \frac{dv}{dx} = 0, \quad v = \beta, \quad \frac{dw}{dx} = 0, \]

NOMENCLATURE

| Symbols | Name            |
|---------|----------------|
| \( u \) | Concentrations of species A |
| \( v \) | Concentrations of species B |
| \( w \) | Concentrations of species C |
| \( \lambda \) | React ration constant |
| \( \alpha \) | Concentrations of A at \( x=0 \) |
| \( \beta \) | Concentrations of B at \( x=1 \) |
| \( \gamma \) | Concentrations of C at \( x=0 \) |

3. Solution of Boundary Value Problem Using HPM

Recently, many authors have applied the HPM to various problems and demonstrated the efficiency of the HPM to handle non-linear structure and solve various physics and engineering problems [5-7]. This method is a combination of homotopy in topology and classic perturbation techniques. Ji-Huan He used the HPM to solve non-linear boundary value problems [11]. These wide varieties of applications show the power of the HPM in solving functional equations. The HPM is unique in its applicability, accuracy and efficiency. The HPM [13] uses the imbedding parameter \( p \) as a small parameter and only little alteration is needed to search for an asymptotic solution. Recently, Eswari et al [15], derived the approximate analytical expressions of concentration and current in homogeneous catalytic reactions at spherical microelectrodes using the homotopy perturbation method. Thiagarajan et al. presented the approximate analytical expressions for steady-state catalytic current of mediated biocatalysis using the homotopy perturbation method. The basic concept of homotopy perturbation method is given in Appendix A. Solving the above equation (1) to (3) using new homotopy perturbation method (Appendix B) for the boundary conditions (4) and (5), we get concentration of species as follows:

\[ u(x) = \frac{\alpha}{\cosh(\sqrt{\lambda \beta} + \gamma)} \cosh(\sqrt{\lambda \beta} + \gamma)(x-1) \]  
\[ v(x) = \frac{\beta}{\cosh(\sqrt{\lambda \alpha} x)} \]  
\[ w(x) = \left[ \frac{(\gamma - \lambda \beta)}{\cosh(\sqrt{\lambda \alpha} x)} \cosh(\sqrt{\lambda \alpha}(x-1)) \right] + \lambda \beta \]

4. Numerical Simulation

The non-linear differential equations (1-3) are solved by numerical methods. The function pdex4 in SCILAB software which is a function of solving the boundary value problems for differential equation is used to solve this equation. Its numerical solution is compared with homotopy perturbation method in Figures 1-3 and it gives a satisfactory result for various values of parameter. The MATLAB program is also given in Appendix B.

5. Discussions

Fig. 1 shows the dimensionless steady-state concentration of the species A. using Eq. (6) for various values of dimensionless parameter \( \lambda \). From these figures, it is inferred that the value of the species A increases gradually when \( \lambda \) decreases. From Fig. 2, it is observed that the value of the concentration of species B is also increases when \( \lambda \) decreases. Concentration of species A and B is uniform when \( 0.001 \leq \lambda \leq 0.001 \). Fig. 3 shows the dimensionless steady-state concentrations of species C using Eq. (8). From this figure it is observed that concentration of species C decreases when \( \lambda \) increases.

6. Conclusion

A nonlinear time-independent differential equation for in thin membrane was formulated and solved using the HPM. Analytical expressions for the concentrations of species were derived using the HPM. Our approximate analytical results offer more advantages over traditional methods for an efficient operation on thin membrane. The extension of the procedure to other two-dimension and three-dimension geometrics and coupled processes of first-order chemical reactions with complex mixed-boundary conditions seems possible.
Figure 1. Normalized steady-state concentration of species A (u). The concentrations of species A are computed using eq. (6) for various values of the dimensionless parameter $\lambda$. Value of the other parameters are $\alpha = 1.6$, $\beta = 0.01$ and $\gamma = 0.8$. 

(-) represent the equation (6), and (...........) represent the numerical solution.

Figure 2. Normalized steady-state concentration of species B (v). The concentrations of species B are computed using eq. (7) for various values of the dimensionless parameter $\lambda$. Value of the other parameters are $\alpha = 1.6$, $\beta = 0.01$ and $\gamma = 0.8$.

(-) represent the equation (7), and (...........) represent the numerical solution.

Figure 3. Normalized steady-state concentration of species C (w). The concentrations of species C are computed using eq. (8) for various values of the dimensionless parameter $\lambda$. Value of the other parameters are $\alpha = 1.6$, $\beta = 0.01$ and $\gamma = 0.8$.

(-) represent the equation (8), and (...........) represented the numerical solution.

Appendix-A: Basic Idea of Homotopy Perturbation Method for Initial Value Problem

We outline the basic idea of Homotopy perturbation method. This method has eliminated the limitations of the traditional perturbation methods. On the other hand, it can take full advantage of the traditional perturbation techniques, so there has been a considerable deal of research in applying homotopy technique for solving various strongly non-linear equations. To explain this method, let us consider the following function

$$A(u) - f(t) = 0, \quad t \in \Omega$$  \hspace{1cm} (A1)

With the boundary conditions of

$$B \left( u, \frac{\partial u}{\partial n} \right) = 0, \quad t \in \Gamma$$  \hspace{1cm} (A2)

where $A, B, f(t)$ and $\Gamma$ denote a general differential operator, a boundary operator, a known analytical function on the domain $\Omega$, respectively. Generally speaking, the operator $A$ can be divided into a linear part $L$ and a non-linear part $N$:

$$L(u) + N(u) - f(t) = 0$$  \hspace{1cm} (A3)

By the homotopy technique, we construct a homotopy $v(t, p): \Omega \times [0,1] \rightarrow \mathbb{R}$, which satisfies:

$$H(v, p) = (1 - p)[L(v) - L(u_0)] + p[A(v) - f(t)] = 0$$  \hspace{1cm} (A4)

or

$$H(v, p) = L(v) - L(u_0) + p[N(v) - f(t)] = 0$$  \hspace{1cm} (A5)

where $p \in [0,1]$ is an embedding parameter, and $u_0$ is an initial approximation of Eq. A1, which satisfies the boundary conditions. Obviously from Eqs. A4 and A5, we will have

$$H(v, 0) = L(v) - L(u_0) = 0$$  \hspace{1cm} (A6)

When $p = 0$ Eq. A4 or A5 becomes a linear Equation; when $p = 1$ it becomes a non-linear Equation. So the changing process of $p$ from zero to unity is just that of

$$L(v) - L(u_0) = 0 \Rightarrow A(v) - f(t) = 0.$$  \hspace{1cm} (A7)

We can first use the embedding parameter $p$ as a “small parameter”, and assume that the solutions of Eqs. A4 and A5 can be written as a power series in $p$

$$v = v_0 + p^1v_1 + p^2v_2 + \cdots$$  \hspace{1cm} (A8)

Setting $p = 1$, results in the approximate solution of Eq. (A1)
\[ u = \lim_{p \to 1} v = v_0 + v_1 + v_2 + \cdots \quad (A9) \]

The combination of the perturbation method and the Homotopy method is called the Homotopy perturbation method.

**Appendix B: Analytical Solutions of Non-Linear Equations (1)-(3) Using HPM**

In this Appendix, we indicate how the solutions of the equations B1 to B3 are derived:

\[
\frac{d^2 u}{dx^2} - \lambda uv - uw = 0 \quad (B1)
\]

\[
\frac{d^2 v}{dx^2} - \lambda uv = 0 \quad (B2)
\]

\[
\frac{d^2 w}{dx^2} - uw + \lambda uv = 0 \quad (B3)
\]

We construct the Homotopy for the above equations as follows:

\[
(1-p) \frac{d^2 u}{dx^2} - \lambda u(1) - au(x = 0) + p \left[ \frac{d^2 u}{dx^2} - \lambda uv - uw \right] = 0 \quad (B4)
\]

\[
(1-p) \frac{d^2 v}{dx^2} - \lambda (0) + p \left[ \frac{d^2 v}{dx^2} - \lambda uv \right] = 0 \quad (B5)
\]

\[
(1-p) \frac{d^2 w}{dx^2} - \lambda (0) + p \left[ \frac{d^2 w}{dx^2} + \lambda uv - uw \right] = 0 \quad (B6)
\]

Using the boundary conditions (4) and (5) the above equations becomes as follows:

\[
(1-p) \left[ \frac{d^2 u}{dx^2} - u(\lambda \beta + \gamma) + p \left[ \frac{d^2 u}{dx^2} - \lambda uv - uw \right] \right] = 0 \quad (B7)
\]

\[
(1-p) \left[ \frac{d^2 v}{dx^2} - \lambda \alpha v \right] + p \left[ \frac{d^2 v}{dx^2} - \lambda uv \right] = 0 \quad (B8)
\]

\[
(1-p) \left[ \frac{d^2 w}{dx^2} - \lambda \alpha \beta w \right] + p \left[ \frac{d^2 w}{dx^2} + \lambda uv - uw \right] = 0 \quad (B9)
\]

The approximate solution of (B1- B3) are,

\[ u = u_0 + pu_1 + p^2 u_2 + \cdots \quad (B10) \]

\[ v = v_0 + pv_1 + p^2 v_2 + \cdots \quad (B11) \]

\[ w = w_0 + pw_1 + p^2 w_2 + \cdots \quad (B12) \]

Substituting Eq. (B10) to Eq. (B12) into Eq. (B7) to Eq. (B9) we have

\[
\begin{align*}
(1-p) & \left[ \frac{d^2 (u_0 + pu_1 + p^2 u_2 + \cdots)}{dx^2} - \lambda (u_0 + pu_1 + p^2 u_2 + \cdots)\right] + p \left[ \frac{d^2 (u_0 + pu_1 + p^2 u_2 + \cdots)}{dx^2} - \lambda (u_0 + pu_1 + p^2 u_2 + \cdots)\right] \\
& = 0
\end{align*} \quad (B13)
\]

Comparing the coefficients of like powers of \( p \) in Eq. (B13) we get

\[
\begin{align*}
p^0 : & \frac{d^2 u_0}{dx^2} - u_0(\gamma - \lambda u_0) = 0 \\
p^1 : & \frac{d^2 u_1}{dx^2} - \lambda u_1 = 0 \quad (B16)
\end{align*}
\]

Comparing the coefficients of like powers of \( p \) in Eq. (B14) we get

\[
\begin{align*}
p^0 : & \frac{d^2 v_0}{dx^2} - \lambda \alpha v_0 = 0 \\
p^1 : & \frac{d^2 v_1}{dx^2} - \lambda \alpha v_1 = 0 \quad (B18)
\end{align*}
\]

Comparing the coefficients of like powers of \( p \) in Eq. (B15) we get

\[
\begin{align*}
p^0 : & \frac{d^2 w_0}{dx^2} - \alpha w_0 + \lambda \alpha \beta = 0 \\
p^1 : & \frac{d^2 w_1}{dx^2} - \alpha w_1 + \lambda w_0 = 0 \quad (B20)
\end{align*}
\]

The initial and boundary conditions are as follows:
\[ u_0(0) = \alpha \text{ and } u_{0,x}(l) = 0 \]  
(B22)

\[ u_i(0) = \alpha \text{ and } u_{i,x}(l) = 0, \quad i = 1, 2, \ldots \]  
(B23)

\[ v_0(0) = \beta \text{ and } v_{0,x}(0) = 0 \]  
(B24)

\[ v_i(1) = 0 \text{ and } v_{i,x}(0) = 0, \quad i = 1, 2, \ldots \]  
(B25)

\[ w_0(0) = \gamma \text{ and } w_{0,x}(l) = 0 \]  
(B26)

\[ w_i(0) = 0 \text{ and } w_{i,x}(l) = 0 \]  
(B27)

Solving the Eq. (B16) to (B21) and using the boundary conditions (B20) to (B27). We can find the following results:

\[ u_0 = \frac{\alpha}{\cosh(\sqrt{\lambda \beta + \gamma})} \cosh(\sqrt{\lambda \beta + \gamma})(x - 1) \]  
(B28)

\[ v_0 = \frac{\beta}{\cosh(\sqrt{\lambda \alpha}(x - 1))} \cosh(\sqrt{\lambda \alpha}(x - 1)) \]  
(B29)

\[ w_0 = \frac{(\gamma - \lambda \beta)}{\cosh(\sqrt{\lambda \alpha}(x - 1))} + \lambda \beta \]  
(B30)

Considering the first iteration only we conclude that Next iteration (2nd or 3rd) will improve the accuracy of the result.

After putting the equations (B31) to (B33) in the equation (B28) to (B30) we obtain the equations (6) – (8) in the text.

### Appendix C: Matlab Program to Find the Numerical Solution of Non-linear Equations (1)-(3)

```matlab
function ananthu
m = 0;
x = linspace(0, 1);
t = linspace(0, 100000);
sol = pdepe(m, @pdex4pde, @pdex4ic, @pdex4bc, x, t);
u1 = sol(:,:,1);
u2 = sol(:,:,2);
u3 = sol(:,:,3);
figure
%title('u1(x, t)')
%sxlabel('Distance x')
%ylabel('u2(x, 2)')

function [c, f, s] = pdex4pde(x, t, u, DuDx)
c = [1; 1; 1];
f = [1; 1; 1] * DuDx;
% y = u(1) * u(2);
% y1 = u(1) * u(3);
% alpha = 1.6;
% beta = 0.01;
% gamma = 0.8;
lamta = 1;
F = (-lamta * u(1) * u(2)) - (u(1) * u(3));
F1 = (-lamta * u(1) * u(2));
F2 = (lamta * u(1) * u(2)) - (u(1) * u(3));
s = [F; F1; F2];
figure
%title('u2(x, t)')
%ylabel('Distance x')
%ylabel('u3(x, 2)')

function [pl, ql, pr, qr] = pdex4bc(xl, u1, xr, ur, t)
pl = [u1(1) - 1.6; 0; u1(3) - 0.01];
ql = [0; 1; 0];
pr = [0; ur(2) - 0.8; 0];
qr = [1; 0; 1];
end

function u0 = pdex4ic(x)
create an initial conditions
u0 = [0; 1; 0];
end

function [c, f, s] = pdex4pde(x, t, u, DuDx)
c = [1; 1; 1];
f = [1; 1; 1] * DuDx;
% y = u(1) * u(2);
% y1 = u(1) * u(3);
% alpha = 1.6;
% beta = 0.01;
% gamma = 0.8;
lamta = 1;
F = (-lamta * u(1) * u(2)) - (u(1) * u(3));
F1 = (-lamta * u(1) * u(2));
F2 = (lamta * u(1) * u(2)) - (u(1) * u(3));
s = [F; F1; F2];
figure
%title('u2(x, t)')
%ylabel('Distance x')
%ylabel('u3(x, 2)')

function [pl, ql, pr, qr] = pdex4bc(xl, u1, xr, ur, t)
pl = [u1(1) - 1.6; 0; u1(3) - 0.01];
ql = [0; 1; 0];
pr = [0; ur(2) - 0.8; 0];
qr = [1; 0; 1];
end

function u0 = pdex4ic(x)
create an initial conditions
u0 = [0; 1; 0];
end

function [c, f, s] = pdex4pde(x, t, u, DuDx)
c = [1; 1; 1];
f = [1; 1; 1] * DuDx;
% y = u(1) * u(2);
% y1 = u(1) * u(3);
% alpha = 1.6;
% beta = 0.01;
% gamma = 0.8;
lamta = 1;
F = (-lamta * u(1) * u(2)) - (u(1) * u(3));
F1 = (-lamta * u(1) * u(2));
F2 = (lamta * u(1) * u(2)) - (u(1) * u(3));
s = [F; F1; F2];
figure
%title('u2(x, t)')
%ylabel('Distance x')
%ylabel('u3(x, 2)')

function [pl, ql, pr, qr] = pdex4bc(xl, u1, xr, ur, t)
pl = [u1(1) - 1.6; 0; u1(3) - 0.01];
ql = [0; 1; 0];
pr = [0; ur(2) - 0.8; 0];
qr = [1; 0; 1];
end

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