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Analytical solution of system of non-linear reaction-diffusion equations in a thin membrane: Homotopy perturbation approach

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ABSTRACT

This model is comprises of a system of time-independent reaction-diffusion equations describing steady state of a chemical process that involves three species: two reactions and diffusion. The system of equations coupled with the non-linear reaction terms with mixed Dirichlet and Neumann boundary conditions. A closed form of an analytical expression of concentrations for the full range of enzyme activities has been derived using Homotopy Perturbation method. A simple approximate analytical expression of concentrations in terms of dimensionless parameter λ is also reported. These analytical results are compared with numerical results (MATLAB Programme) and are found to be in good agreement.

KEYWORDS

Diffusion;
Enzyme;
Heat transfer;
Mathematical modeling;
Membranes;
Simulation.

INTRODUCTION

We consider a classical chemical reaction between two species A and B to form a product, according to the reaction mechanism $2A + B \rightarrow$ product. We model the transport inside the membrane as diffusive, thus the model will be given by a system of reaction-diffusion equations that are coupled with the non-linear reaction terms. The reaction path consists of a coupled pair of irreversible simple reaction[1].

$$\begin{aligned} &A + B \xrightarrow{\lambda} C, \\ &A + C \xrightarrow{\mu} \text{product} \end{aligned} \qquad (1)$$

where λ and μ are the binary reaction rates. The rigorous singular perturbation analysis for the steady-state problem was provided by Seidman and Kalacheve[2,3]. The corresponding time dependent system of this problem has been considered by Haario Seidman[4], for the boundary conditions of a quite different type, to describe reactions in the film model for a gas/liquid interface. Also the steady state problem has many important applications, in chemical engineering modeling. Recently, Butuzov et al.[5,6] have solved some related problems of exchange of stabilities using different techniques (upper and lower solutions). However, to the best of author's knowledge, no general analytical results of substrate concentration for all values of dimensionless parameter λ have been published. The purpose of this communication is to derive approximate analytical expressions for the steady-state concentrations for all values of λ using Homotopy Perturbation method.

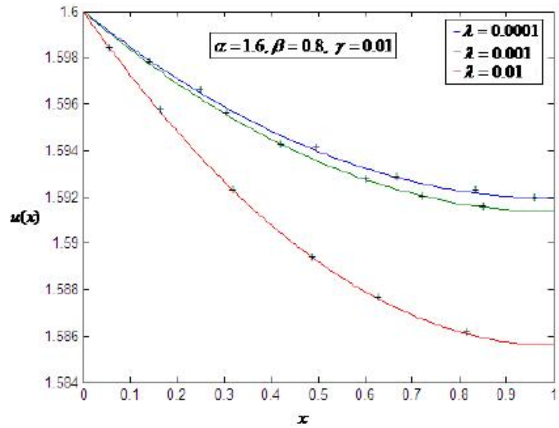

Figure 1 : Normalized steady-state concentration u. The concentrations were computed using eq.(7) for various values of the dimensionless parameter λ. (-) denotes eq. (7) and (+) denotes the numerical simulation

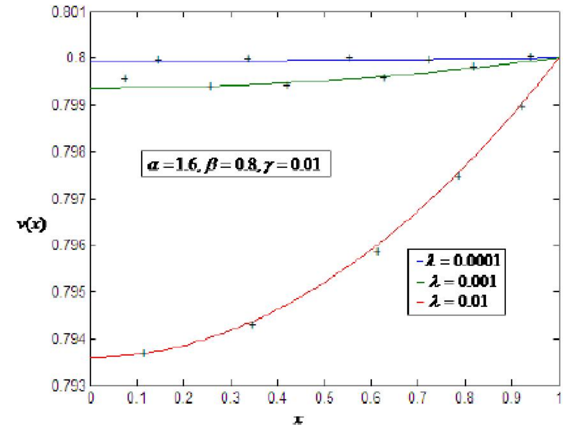

Figure 2 : Normalized steady-state concentration v. The concentrations were computed using eq. (8) for various values of the dimensionless parameter λ. (-) denotes eq. (8) and (+) denotes the numerical simulation

Mathematical formulation of the problem and analysis

The covering nonlinear reaction diffusion equation in the membrane is expressed in the following non-dimensional format[1]:

$$u_{xx} = \lambda uv + uw \quad (2)$$

$$v_{xx} = \lambda uv \quad (3)$$

$$w_{xx} = uw - \lambda uv \quad (4)$$

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. We assume that the specie *A* is supplied with a given fixed concentration α>0 at x = 0, and the specie *B* with β>0 at x = 1. Boundary conditions are

$$u=\alpha;\ v_x=0;\ w=\gamma \text{ at } x=0 \quad (5)$$

$$u_x = 0;\ v=\beta;\ w_x=0 \text{ at } x=1 \quad (6)$$

Due to the appearance of the large factor λ>>1 is one of the terms in each reaction-diffusion equation. The equations have features of singularly perturbed problems[1].

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 hand non-linear structure and solve various physics and engineering problems[7-10]. This method is a combination of Homotopy in topology and classic perturbation techniques. Ji-Huan He used the HPM to solve Lighthill equation[11], Duffing equation[12], then the idea goes through and has been used to solve non-linear boundary value problems[13], Emden-Flower type equations[14] and many other problems. 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[15] 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.[16] derived the approximate analytical expressions for the substrate hydrogen peroxide concentrations and current for the non-linear Michaelis-Menten kinetic scheme in a system of coupled non-linear reaction-diffusion equations using the Homotopy Perturbation method. Meena et al.[17] presented the approximate analytical expressions for the substrate and mediator concentrations for the non-linear reaction-diffusion processes of conducting the polymer modified ultra microelectrodes exhibits the spillover using the Homotopy Perturbation method. Using this method[18], we can obtain the following solution to the equations (2) to (4) (Appendix A).

$$u(x) = \alpha + \frac{1}{2}\alpha x^2\lambda\beta + \frac{1}{2}\alpha\gamma x^2 - \lambda\alpha\beta x - \alpha\gamma x \quad (7)$$

$$v(x) = \beta + \frac{1}{2}\alpha x^2\lambda\beta - \frac{1}{2}\lambda\alpha\beta \quad (8)$$

and

$$w(x) = \gamma - \frac{1}{2}\alpha x^2\lambda\beta + \frac{1}{2}\alpha x^2\gamma + \lambda\alpha\beta x - \alpha\gamma x \quad (9)$$

The eq. (7) to (9) represent the new analytical expression of concentration of species for all values of

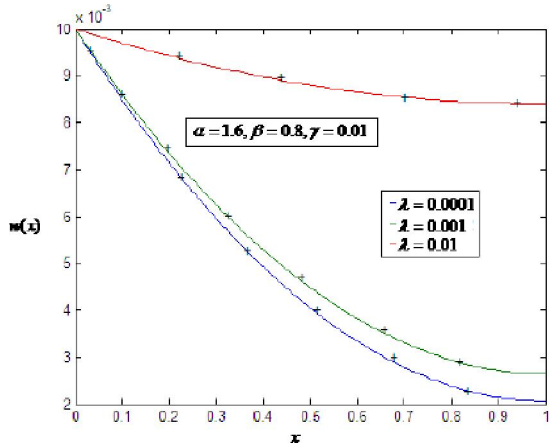

Figure 3 : Normalized steady-state concentration w. The concentrations were computed using eq. (9) for various values of the dimensionless parameter λ. (-) denotes eq. (9) and (+) denotes the numerical simulation

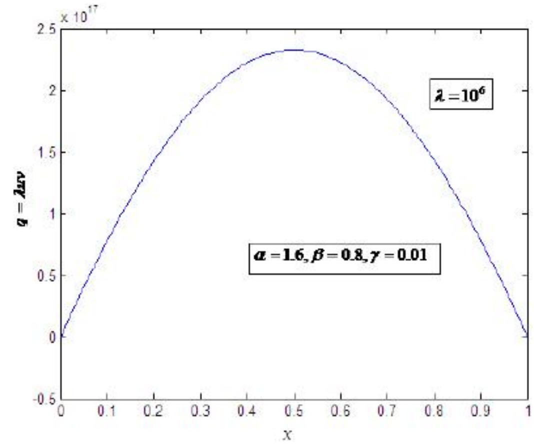

Figure 4 : Dimensionless reaction rate q versus the dimensionless distance x for the value of dimensionless parameter $\lambda = 10^3$, when $\alpha = 1.6$, $\beta = 0.8$, $\gamma = 0.01$

dimensionless parameter. The reaction rate q is given by

$$\mathbf{q = \lambda uv}$$

$$= \lambda\left(\alpha+\frac{1}{2}\alpha x^2\lambda\beta+\frac{1}{2}\alpha\gamma x^2-\lambda\alpha\beta x-\alpha\gamma x\right)\left(\beta+\frac{1}{2}\alpha x^2\lambda\beta-\frac{1}{2}\lambda\alpha\beta\right) \quad (10)$$

Numerical simulation

The nonlinear differential eq. (2-4) are also solved by numerical methods. The function bvp4c in MATLAB software which is a function of solving two-point boundary value problems (BVPs) for ordinary differential equations are used to solve these equations. Its numerical solution is compared with Homotopy Perturbation method and it gives a satisfactory agreement (Figure 1-6). The MATLAB program is also given in appendix B.

DISCUSSION

Figure 1 represents the normalized steady-state concentration u(x) for different values of dimensionless parameter $\lambda = 0.0001, 0.001, 0.01$. From this figure, it is evident that the values of the concentration decreases when dimensionless parameter λ increases for $\alpha = 1.6$, $\beta = 0.8$ and $\gamma = 0.01$. Figure 2 shows the normalized steady-state concentration v(x) versus the dimensionless distance x for various values of dimensionless parameter λ. From this figure, it is obvious that the values of the concentration increases when dimensionless parameter λ decreases for $\alpha = 1.6$, $\beta = 0.8$ and $\gamma = 0.01$. The normalized steady-state concentration w(x) versus the dimensionless distance x for various values of dimensionless parameter λ is plotted in figuer 3. In this figure, it is inferred that the value of the concentration decreases when the diffusion parameter λ decreases. Figure 4, 5 and 6 show the dimensionless reaction rate q using eq. (10) for all values of λ. Thus, it is concluded that there is a simultaneous increase in the values of the reaction rate as well as in λ for the fixed value of $\alpha = 1.6$, $\beta = 0.8$ and $\gamma = 0.01$.

CONCLUSIONS

The time independent non-linear reaction-diffusion equation in membrane has been formulated and solved analytically and numerically. Analytical expressions for the concentrations are derived by using the HPM. The primary result of this work is simple approximate calculations of concentration for all values of dimensionless parameter λ. The HPM is an extremely simple method and it is also a promising method to solve other non-linear equations. This method can be easily extended to find the solution of all other non-linear equations.

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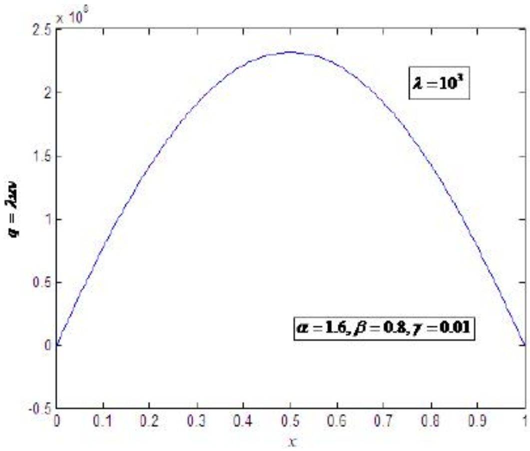

Figure 5 : Dimensionless reaction rate q versus the dimensionless distance x for the value of dimensionless parameter $\lambda = 10^6$, when $\alpha = 1.6$, $\beta = 0.8$, $\gamma = 0.01$

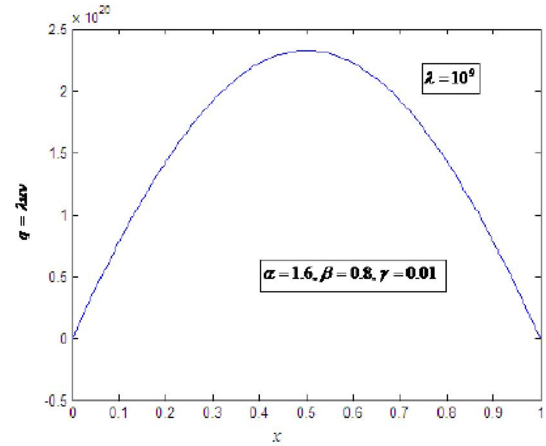

Figure 6 : Dimensionless reaction rate q versus the dimensionless distance x for the value of dimensionless parameter $\lambda = 10^9$, when $\alpha = 1.6$, $\beta = 0.8$, $\gamma = 0.01$

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APPENDIXES

Appendix A

In this Appendix, we indicate how eqns. (7), (8) and (9) in this paper are derived. To find the solution of eqns. (2), (3) and (4), it can be simplified to (Ariel, 2010)

$$\frac{d^2u}{dx^2} - \lambda uv - uw = 0 \qquad \text{(A1)}$$

$$\frac{d^2v}{dx^2} - \lambda uv = 0 \qquad \text{(A2)}$$

$$\frac{d^2w}{dx^2} - uw + \lambda uv = 0 \qquad \text{(A3)}$$

Now the boundary conditions becomes

$$x = 0,\ u = \alpha,\ \frac{dv}{dx} = 0,\ w = \gamma \qquad \text{(A4)}$$

$$x = 1,\ \frac{du}{dx} = 0,\ v = \beta,\ \frac{dw}{dx} = 0 \qquad \text{(A5)}$$

We construct the Homotopy as follows

$$(1-p)\left[\frac{d^2u}{dx^2}\right] + p\left[\frac{d^2u}{dx^2} - \lambda uv - uw\right] = 0 \qquad \text{(A6)}$$

$$(1-p)\left[\frac{d^2v}{dx^2}\right] + p\left[\frac{d^2v}{dx^2} - \lambda uv\right] = 0 \qquad \text{(A7)}$$

$$(1-p)\left[\frac{d^2w}{dx^2}\right] + p\left[\frac{d^2w}{dx^2} + \lambda uv - uw\right] = 0 \qquad \text{(A8)}$$

The approximate solution of (A1) and (A2) and (A3) is,

$$u = u_0 + pu_1 + p^2u_2 + \ldots.. \qquad \text{(A9)}$$

$$v = v_0 + pv_1 + p^2v_2 + \ldots.. \qquad \text{(A10)}$$

$$w = w_0 + pw_1 + p^2w_2 + \ldots.. \qquad \text{(A11)}$$

The initial approximations are as follows

$$u_0(0) = \alpha \text{ and } u_{0,x}(1) = 0 \qquad \text{(A12)}$$

$$u_i(0) = 0 \text{ and } u_{i,x}(1) = 0,\ i = 1,2\ldots \qquad \text{(A13)}$$

$$v_0(0) = \beta \text{ and } v_{0,x}(0) = 0 \qquad \text{(A14)}$$

$$v_i(1) = 0 \text{ and } v_{1,x}(0) = 0,\ i = 1,2\ldots \qquad \text{(A15)}$$

$$w_0(0) = \gamma \text{ and } w_{0,x}(0) = 0 \qquad \text{(A16)}$$

$$w_i(0) = 0 \text{ and } w_{i,x}(1) = 0 \qquad \text{(A17)}$$

Substituting eq. (A9) to (A11) into eq. (A6) to (A8) we have

$$(1-p)\left[\frac{d^2(u_0 + pu_1 + \ldots)}{dr^2}\right] + p\left[\begin{array}{l}\dfrac{d^2(u_0 + pu_1 + \ldots)}{dx^2} - \\ \lambda(u_0 + pu_1 + \ldots..)(v_0 + pv_1 + \ldots..) \\ -(U_0 + pU_1 + \ldots.)(W_0 + pW_1 + \ldots.)\end{array}\right] = 0 \qquad \text{(A18)}$$

$$(1-p)\left[\frac{d^2(v_0 + pv_1 + ..)}{dx^2}\right] + p\left[\begin{array}{l}\dfrac{d^2(v_0 + pv_1 + ..)}{dx^2} - \lambda(u_0 + pu_1 + \ldots.) \\ (v_0 + pv_1 + \ldots\ldots.)\end{array}\right] = 0 \qquad \text{(A19)}$$

$$(1-p)\left[\frac{d^2(w_0+pw_1+....)}{dx^2}\right]+ p\left[\begin{array}{l}\frac{d^2(w_0+pw_1+....)}{dx^2}+\\ \lambda(u_0+pu_1+...)(v_0+pv_1+...)-\\ (u_0+pu_1+....)(w_0+pw_1+....)\end{array}\right]=0 \quad (A20)$$

Comparing the coefficients of like powers of p in eq. (A18) we get

$$p^0:\frac{d^2u_0}{dx^2}=0 \quad (A21)$$

$$p^1:\frac{d^2u_1}{dx^2}-\lambda u_0v_0-u_0w_0=0 \quad (A22)$$

Comparing the coefficients of like powers of p in eq. (A19) we obtain

$$p^0:\frac{d^2v_0}{dx^2}=0 \quad (A23)$$

$$p^1:\frac{d^2v_1}{dx^2}-\lambda u_0v_0=0 \quad (A24)$$

comparing the coefficients of like poser of p in eqn. (A20) we have

$$p^0:\frac{d^2w_0}{dx^2}=0 \quad (A25)$$

$$p^1:\frac{d^2w_1}{dx^2}-\lambda u_0v_0-u_0w_0=0 \quad (A26)$$

Solving the eq. (A21)-(A26) and using the boundary conditions (A12)-(A17), we can find the following results:

$$u_0=\alpha \quad (A27)$$

$$u_1=\frac{1}{2}\alpha\lambda\beta x^2+\frac{1}{2}\alpha\gamma x^2-\lambda\alpha\beta x-\alpha\gamma x \quad (A28)$$

$$v_0=\beta \quad (A29)$$

$$v_1=\frac{1}{2}\alpha\lambda\beta x^2-\frac{1}{2}\lambda\alpha\beta \quad (A30)$$

$$w_0=\gamma \quad (A31)$$

$$w_1=-\frac{1}{2}\alpha\lambda\beta x^2+\frac{1}{2}\alpha\gamma x^2+\lambda\alpha\beta x-\alpha\gamma x \quad (A32)$$

According to the HPM, we can conclude that

$$u=\lim_{p\to1}u(x)=u_0+u_1 \quad (A33)$$

$$v=\lim_{p\to1}v(x)=v_0+v_1 \quad (A34)$$

$$w=\lim_{p\to1}w(x)=w_0+w_1 \quad (A35)$$

After putting eq. (A27) and (A28) into eq. (A33) and eq. (A29) and (A30) into eq. (A34) and eq. (A31) and (A32) into eq. (A35), we obtain the equations (7), (8) and (9) in the text.

Appendix B

```
function pdex4
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
plot(x, u1(end,:))
title('u1(x, t)')
xlabel('Distance x')
ylabel('u1(x, 2)')
%
Figure
plot(x, u2(end,:))
title('u2(x, t)')
xlabel('Distance x'')
ylabel('u2(x, 2)')
%
Figure
plot(x, u3(end,:))
title('Solution at t = 2')
xlabel('Distance x')
ylabel('u3(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);
α=1.6;
γ=0.01;
β=0.8;
lamta=0.0001; % parameters
F =(-lamta*y-y1);
F1=(-lamta*y); % non linear terms
F2=(lamta*y-y1);
s=[F; F1; F2];
%
```

Full Paper

function u_0 = pdex4ic(x);
%create a initial conditions
u_0 = [0; 1; 0];
%
Function [pl, ql, pr, qr] =pdex4bc(x_l, u_l, x_r, u_r, t)
%create a boundary conditions
p_l = [u_l(1)-1.6; 0; u_l(3)-0.01];
q_l =[0; 1; 0];
p_r = [0; u_r(2)-0.8; 0];
q_r = [1; 0; 1];

Appendix C

Nomenclature

Symbol	Meaning
u	Concentration of the chemical species A
V	Concentration of the chemical species B
w	Concentration of the chemical species C
λ	Dimensionless parameter
X	Dimensionless distance
α	Fixed concentration of the specie A
β	Fixed concentration of the specie B
γ	Fixed concentration of the specie C
q	Dimensionless reaction rate

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