iJRASET
International Journal For Research in
Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 2 **Issue:** XI **Month of publication:** November 2014

DOI:

International Journal for Research in Applied Science & Engineering Technology (IJRASET)

Approximate analytical solution of the steady-state concentration of mediator and current

*V. Ananthaswamy[1], P. Jeyabarathi[2], S. Anitha[3]
[1]Department of Mathematics, The Madura College, Madurai, Tamil Nadu, India.
[2]Department of Mathematics, K.L.N. Engineering College, Pottapalayam, Tamil Nadu, India

Abstract: In this research paper, we discuss the mathematical analysis for the steady-state concentration of mediator and current for the non-linear boundary value problem with Michaelis–Menten kinetics scheme. The approximate analytical expressions of the steady state concentration and the current are derived using the Homotopy analysis method. The Homotopy analysis method has the advantage of being more concise for analytical and numerical functions. This method can be easily extended to find the solution of the other strongly non-linear initial and boundary value problems in chemical and biological sciences.
Keywords: Non-linear reaction-diffusion equation; Michael-Menten kinetics; Steady state current; Homotopy analysis method; Numerical simulation.

I. INTRODUCTION

Several oxidoreductase reactions such as quinones and ferrocenes consist of electrode reactions which allow conjugating between redox enzyme reactions and electrode reactions. The redox compound-mediated and enzyme-catalyzed electrode process is called mediated bioelectrocatalysis. It is utilized for biosensors, bioreactors, and biofuel cells. Ohgaru et al. [1] have reported the analysis of mediated bioelectroanalysis mediator diffusion, Michaelis–Menten rate equation. The steady-state concentration and current have been obtained analytically for the case of very low concentrations of the mediator compared with its Michaelis constant [4–6]. Recently Rajendran et al. [2, 3] derived the steady-state analytical solution of concentration for the substrate at polymer modified electrode for all values α and k using Variational iteration method. Ohgaru et al. However, to the best of our knowledge, till date there was no analytical results corresponding to the steady-state mediator concentration and current for all values of saturation parameter α and reaction diffusion parameter k have been reported. The purpose of this communication is to derive an analytical expression for the steady state mediator concentration and the current of mediated bioelectrocatalysis based on Homotopy analysis method for values of the dimensionless parameters

II. MATHEMATICAL FORMULATION OF THE PROBLEM

We consider the following non-linear ordinary differential equation:

$$\frac{d^2u}{dx^2}-\frac{ku}{1+\alpha u}=0 \tag{1}$$

The boundary conditions are

$$u(0)=1,\ u(1)=0. \tag{2}$$

The current response is

$$\psi=-\left(\frac{du}{dx}\right)_{x=0} \tag{3}$$

There exists no small parameter in the equation. Therefore, the traditional perturbation methods cannot be applied directly. Recently, considerable attention has been directed towards analytical solutions for non-linear equations without small parameters. Many new techniques have appeared in the literature, for example, the Homotopy analysis method (HAM), the Variational iteration method.

III. SOLUTION OF THE NON-LINEAR BOUNDARY VALUE PROBLEM USING THE HOMOTOPY ANALYSIS METHOD

HAM is a non perturbative analytical method for obtaining series solutions to nonlinear equations and has been successfully applied to numerous problems in science and engineering [7-15]. In comparison with other perturbative and non-perturbative analytical methods, HAM offers the ability to adjust and control the convergence of a solution via the so-called convergence-control parameter. Because of this, HAM has proved to be the most effective method for obtaining analytical solutions to highly nonlinear differential equations. Previous applications of HAM have mainly focused on nonlinear differential equations in which the non-linearity is a polynomial in terms of the unknown function and its derivatives. As determined in (8), the nonlinearity present in the thermal stability of a reactive viscous combustible fluid flowing steadily through a channel filled with a saturated porous medium, and thus, poses a greater challenge with regard to finding approximate solutions analytically. Our results indicate that even in this case, HAM yields excellent results.

Liao [8-16] proposed a powerful analytical method for nonlinear problems, namely the Homotopy analysis method. This method offers an analytical solution in terms of an infinite power series. Nevertheless, on that point is a pragmatic need to value this solution and to obtain numerical values from the infinite power series. In order to investigate the accuracy of the Homotopy analysis method (HAM) solution in a finite number of terms, the system of differential equations was solved. The Homotopy analysis method is a good technique comparing to another perturbation method.

The Homotopy analysis method (HAM) is a powerful and easy-to-use analytic tool for nonlinear problems. The Homotopy analysis method contains the auxiliary parameter h, which provides us with a simple way to adjust and control the convergence region of solution series. Furthermore, the obtained result is of high accuracy. The approximate analytical expressions for steady state concentration and steady state current of the eqns.(1) –(3) using the Homotopy analysis method are as follows:

$$u(x)=\left(\begin{array}{l}\dfrac{\sinh\left(\sqrt{k}(1-x)\right)}{\sinh\sqrt{k}}-\dfrac{h\alpha\sinh\left(\sqrt{k}(x-1)\right)\left(1+\dfrac{\cosh\left(2\sqrt{k}\right)}{3}\right)}{2\sin^{3}h\left(\sqrt{k}\right)}\\ -\dfrac{h\alpha\cosh\left(2\sqrt{k}(1-x)\right)}{2\sin^{2}h\left(\sqrt{k}\right)(2x-3)(2x-1)}-\dfrac{h\alpha}{2\sin^{2}h\left(\sqrt{k}\right)}\end{array}\right) \tag{4}$$

$$\psi=\left\{\begin{array}{l}\dfrac{\sqrt{k}\cosh(\sqrt{k})}{\sinh(\sqrt{k})}+\dfrac{h\alpha\sqrt{k}\cosh(\sqrt{k})\left[1+\dfrac{\cosh(2\sqrt{k})}{3}\right]}{2\sinh^{3}(\sqrt{k})}\\ +\dfrac{h\alpha\left[8\cosh(2\sqrt{k})-6\sqrt{k}\sinh(2\sqrt{k})\right]}{18\sin^{2}h(\sqrt{k})}\end{array}\right\} \tag{5}$$

IV. NUMERICAL SIMULATION

The non-linear differential eqn.(1) using the boundary condition eqn.(2) is solved by numerical methods. The function pdex4 in Matlab/Scilab software which is a function of solving the initial and boundary value problems for the ordinary and partial differential equation is used to solve these equations. The Matlab/Scilab program is also given in Appendix C. The numerical results are also compared with the obtained our analytical expression (eqn.(4)).

V. RESULTS AND DISCUSSION

The concentration of substrate $u(x)$ using eqn.(4) is represented in the Figs. 1 (a)-(d). From these Figs. it is inferred that the value of concentration increase when the value k increases. Fig. 2 (a) represents the dimensionless current versus the diffusion parameter k. From this Fig. it is evident that when α increases, the current decreases and reaches the steady state value. The concentration u slowly decreases for α varies from 0.1 to 10. Fig. (3) give us the confirmation for the above discussion in 3 dimensional graph also.

International Journal for Research in Applied Science & Engineering Technology (IJRASET)

The value of the current increases when k increases and α decreases. In these Figs. our analytical results are compared with simulation results for all values of the parameter. It gives the good agreement.

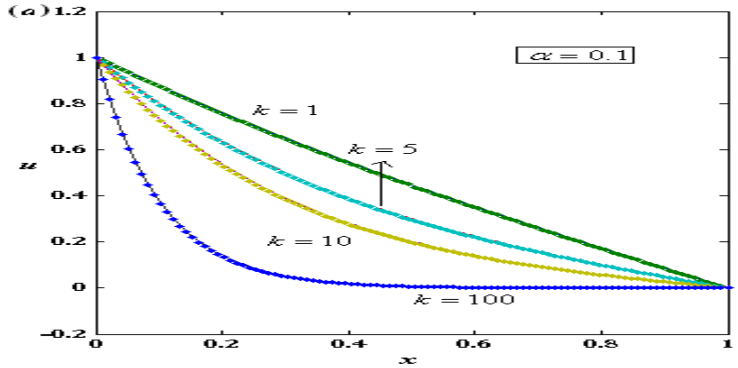


Fig. 1 (a) : Normalized steady-state mediator concentration u. The concentrations were computed using the eqn. (4) for various values of the reaction-diffusion paramter k and the saturation parameter $\alpha = 0.1$. Here (-) denotes the analytical solution and (.) denotes the numerical simulation.

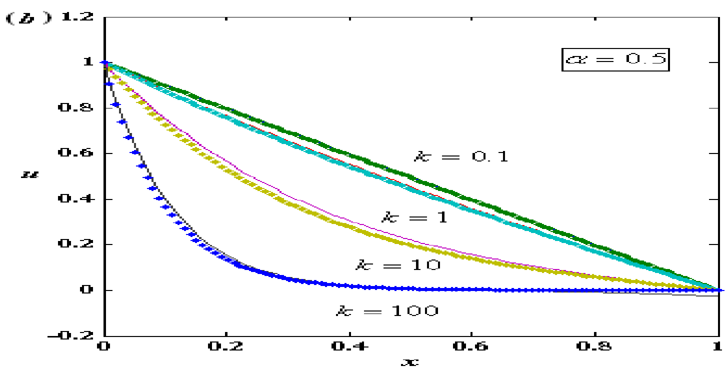


Fig. 1 (b) : Normalized steady-state mediator concentration u. The concentrations were computed using the eqn.(4) for various values of the reaction diffusion paramter k and saturation parameter $\alpha = 0.5$. Here (-) denotes the analytical solution and (.) denotes the numerical simulation.

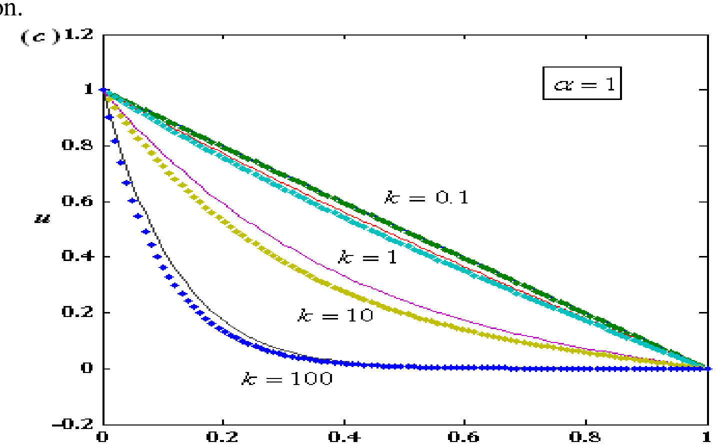


Fig.1 (c): Normalized steady-state mediator concentration u. The concentrations were computed using the eqn.(4) for various values of the reaction diffusion paramter k and saturation parameter $\alpha = 1$. Here (-) denotes the analytical solution and (.) denotes the numerical simulation.

Volume 2 Issue XI, November 2014
ISSN: 2321-9653
International Journal for Research in Applied Science & Engineering Technology (IJRASET)

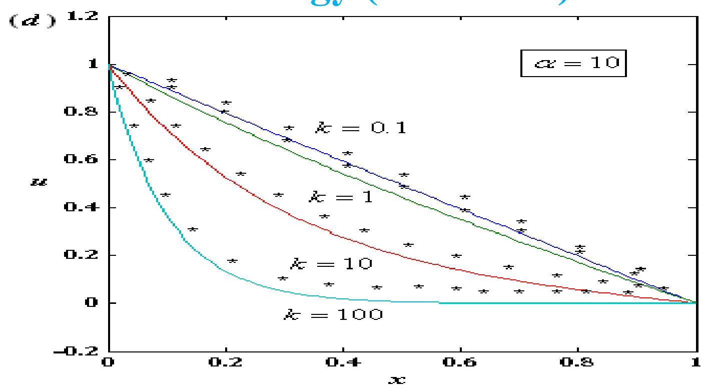


Fig. 1 (d): Normalized steady-state mediator concentration u. The concentrations were computed using the eqn.(4) for various values of the reaction diffusion paramter k and saturation parameter $\alpha = 10$. Here (-) denotes the analytical solution and (.) denotes the numerical simulation.

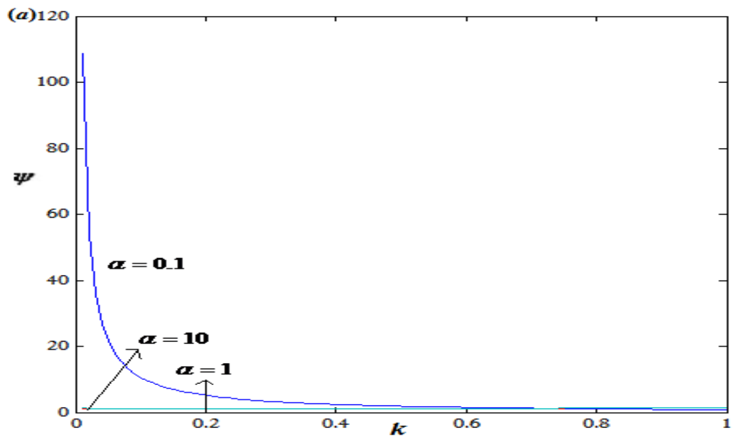


Fig. 2 (a): Variation of normalized current ψ versus parameter k using Eq. (2.5) for various values of saturation parameter α

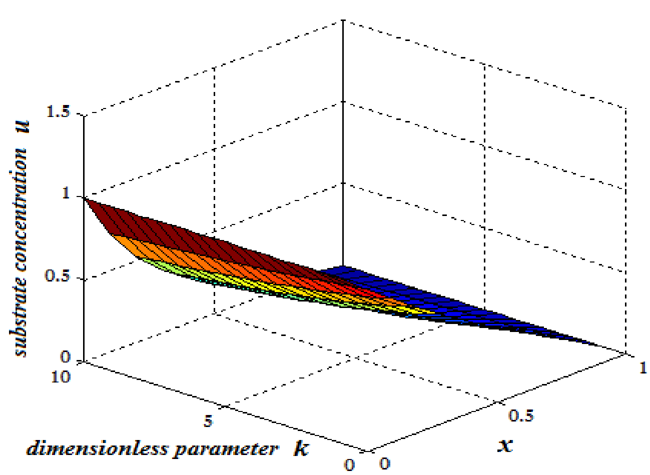


Fig. 3: The normalized numerical simulation of three dimensional concentrations u is plotted. The plot was constructed using the eqn.(5) for $\beta = 0.5$.

VI. CONCLUSION

In this work, an approximate analytical solution for non-linear reaction equations has been presented using Homotopy analysis method (HAM). Moreover, we have also presented an approximate analytical expression for the steady state current. Further, based on the outcome of this work it is possible to calculate the approximate amounts of mediator concentration and current corresponding to a non-linear Michaelis–Menten kinetics scheme. In addition, the transport and kinetics are quantified in terms of fundamental reaction/diffusion polymer parameter k and saturation parameter α.

REFERENCES

[1] T. Ohgaru, H. Tatsumi, K. Kano, T. Ikeda, Approximate and empirical expression of the steady-state catalytic current of mediated bioelectrocatalysis to evaluate enzyme kinetics, Journal of Electro Analytical Chemistry. 496 (2001), 37-43.
[2] A. Meena, L. Rajendran, Mathematical modeling of amperometric and potentiometric biosensors and system of non-linear equations – Homotopy perturbation approach J.Electroanal. Chem. 644, (2010) 50–59.
[3] P. Manimozhi, A. Subbiah, L. Rajendran, Solution of steady-state substrate concentration in the action of biosensor response at mixed enzyme kinetics, Sens. Actuators B 147, (2010), 290–297.
[4] T. Ozis, A. Yildirim, Relation of a Non-Linear Oscillator with Discontinuities, Int. J. Nonlinear Sci. Numer. Simulat. 8(2), (2007), 243–248.
[5] S.J. Li, Y.X. Liu, An improved approach to non-linear dynamical system identification using PID neural networks, Int. J. Non Linear Sci. Numer. Simulat. **7**(2), (2006), 177–182.
[6] M.M. Mousa, S.F. Ragab, Z. Naturforsch, Application of the Homotopy perturbation method to linear and non-linear schrödinger equation Zeitschrift für naturforschung, Sec. A 63, (2008), 140-144.
[7] S. J. Liao, The proposed Homotopy analysis technique for the solution of non linear Problems, Ph.D. Thesis, Shanghai Jiao Tong University, (1992).
[8] S. J. Liao, An approximate solution technique which does not depend upon small parameters: a special example, Int. J. Non-Linear Mech. 30, (1995) 371-380.
[9] S. J. Liao, Beyond perturbation introduction to the Homotopy analysis method, 1st edn., Chapman and Hall, CRC press, Boca Raton (2003) 336.
[10] S. J. Liao, On the Homotopy analysis method for non-linear problems, Appl. Math. Comput.147, (2004) 499-513.
[11] S. J. Liao, An optimal Homotopy-analysis approach for strongly non-linear differential equations, Commun. Nonlinear Sci. Numer. Simulat. 15, (2010) 2003-2016.
[12] S. J. Liao, The Homotopy analysis method in non-linear differential equations, Springer and Higher education press, (2012).
[13] S. J. Liao, An explicit totally analytic approximation of blasius viscous flow problems, Int J Nonlinear Mech, 34, (1999)759–778.
[14] S.J. Liao, On the analytic solution of magnetohydrodynamic flows non-Newtonian fluids over a stretching sheet, J Fluid Mech 488, (2003) 189–212.
[15] S. J. Liao, A new branch of boundary layer flows over a permeable stretching plate, Int J Nonlinear Mech;42 (2007) 819–830.

Appendix A

Basic concept of the Liao's Homotopy Analysis Method (HAM)

Consider the following nonlinear differential equation

$$N[u(x)] = 0 \qquad \text{(A.1)}$$

where N is a nonlinear operator, t denotes an independent variable, $u(t)$ is an unknown function. For simplicity, we ignore all boundary or initial conditions, which can be treated in the similar way. By means of generalizing the conventional Homotopy method, Liao constructed the so-called zero-order deformation equation as:

$$(1-p)L[\varphi(x;p)-u_0(x)] = phH(x)N[\varphi(x;p)] \qquad \text{(A.2)}$$

where $p\in$ [0,1] is the embedding parameter, $h \neq 0$ is a nonzero auxiliary parameter, $H(x) \neq 0$ is an auxiliary function, L is an auxiliary linear operator, $u_0(x)$ is an initial guess of $u(x)$, $\varphi(x:p)$ is an unknown function. It is important, that one has great freedom to choose auxiliary unknowns in HAM. Obviously, when $p = 0$ and $p = 1$, it holds:

$$\varphi(x;0) = u_0(x) \text{ and } \varphi(x;1) = u(x) \qquad \text{(A.3)}$$

respectively. Thus, as p increases from 0 to 1, the solution $\varphi(x;p)$ varies from the initial guess $u_0(x)$ to the solution $u(t)$. Expanding $\varphi(x;p)$ in Taylor series with respect to p, we have:

$$\varphi(x;p) = u_0(x) + \sum_{m=1}^{+\infty} u_m(x)p^m \qquad \text{(A.4)}$$

where

$$u_m(x) = \frac{1}{m!}\frac{\partial^m \varphi(x;p)}{\partial p^m}|_{p=0} \qquad (A.5)$$

If the auxiliary linear operator, the initial guess, the auxiliary parameter *h,* and the auxiliary function are so properly chosen, the series (A.4) converges at $p=1$ then we have:

$$u(t) = u_0(x) + \sum_{m=1}^{+\infty} u_m(x). \qquad A.6)$$

Define the vector

$$\vec{u} = \{u_0, u_1, ..., u_n\} \qquad (A.7)$$

Differentiating the eqn.(A.2) for *m* times with respect to the embedding parameter *p*, and then setting *p* = 0 and finally dividing them by *m*!, we will have the so-called mth-order deformation equation as:

$$L[u_m - \chi_m u_{m-1}] = hH(x)\Re_m(\vec{u}_{m-1}) \qquad (A.8)$$

where

$$\Re_m(\vec{u}_{m-1}) = \frac{1}{(m-1)!}\frac{\partial^{m-1} N[\varphi(x;p)]}{\partial p^{m-1}} \qquad (A.9)$$

and

$$\chi_m = \begin{cases} 0, & m \le 1, \\ 1, & m > 1. \end{cases} \qquad (A.10)$$

Applying L^{-1} on both side of equation (A.8), we get

$$u_m(x) = \chi_m u_{m-1}(x) + hL^{-1}[H(x)\Re_m(\vec{u}_{m-1})] \qquad (A.11)$$

In this way, it is easily to obtain u_m for $m \ge 1$, at M^{th} order, we have

$$u(x) = \sum_{m=0}^{M} u_m(x) \qquad (A.12)$$

When $M \to +\infty$, we get an accurate approximation of the original equation (A.1). For the convergence of the above method we refer the reader to Liao. If equation (A.1) admits unique solution, then this method will produce the unique solution. If equation (A.1) does not possess unique solution, the HAM will give a solution among many other (possible) solutions

Appendix B

Solution of the non-linear differential eqns. (1) and (2) using the Homotopy analysis method

In this Appendix, we indicate how the eqn. (4) is derived using Homotopy analysis method .

The given differential equations are of the form as:

$$\frac{d^2u}{dx^2} - \frac{ku}{1+\alpha u} = 0 \qquad (B.1)$$

In order to solve the (B.1) by means of the HAM, we construct the Homotopy as follows:

$$(1-p)\left(\frac{d^2u}{dx^2} - ku\right) = ph\left[\frac{d^2u}{dx^2} + \alpha u\frac{d^2u}{dx^2} - ku\right] \qquad (B.2)$$

The approximate solution of the eqn.(B.4) is

International Journal for Research in Applied Science & Engineering Technology (IJRASET)

$$u = u_0 + pu_1 + p^2 u_2 + ...\qquad (B.3)$$

Substituting the eqn.(B.3) into an eqn.(B.2), we get

$$(1-p)\left(\frac{d^2(u_0 + pu_1 + p^2u_2 + ...)}{dx^2} - k\,u_0 + pu_1 + p^2u_2 + ...)\right)$$

$$= ph\left[\begin{array}{l}\dfrac{d^2(u_0 + pu_1 + p^2u_2 + ...)}{dx^2} \\ + \alpha\,(u_0 + pu_1 + p^2u_2 + ...)\left(\dfrac{d^2(u_0 + pu_1 + p^2u_2 + ...)}{dx^2}\right) \\ - k(u_0 + pu_1 + p^2u_2 + ...)\end{array}\right]\qquad (B.4)$$

Now comparing the coefficients of like powers of p, we get

$$p^0 : \frac{d^2u_0}{dx^2} - ku_0 = 0\qquad (B.5)$$

$$p^1 : \frac{d^2u_1}{dx^2} - ku_1 - h\alpha u_0 \frac{d^2u_0}{dx^2} = 0\qquad (B.6)$$

The initial approximations are as follows:

$$u_0(0) = 1,\ u_0(1) = 0.\qquad (B.7)$$

$$u_i(0) = 0,\ u_i(1) = 0, i = 1,2,3......\qquad (B.8)$$

Solving the eqns. (B.5) and (B.6) and using the initial conditions the eqns. (B.7) and (B.8), we obtain the following results:

$$u_0(x) = \frac{\sinh\left(\sqrt{k}(1-x)\right)}{\sinh\left(\sqrt{k}\right)}\qquad (B.9)$$

$$u_1(x) = \left\{\begin{array}{l}\dfrac{-h\alpha\sinh\left[\sqrt{k}(x-1)\right]\left[1 + \dfrac{\cosh\left(2\sqrt{k}\right)}{3}\right]}{2\sin^3 h(\sqrt{k})} - \dfrac{h\alpha\cosh\left[2\sqrt{k}(1-x)\right]}{2\sin^2 h(\sqrt{k})(2x-3)(2x-1)} \\ -\dfrac{h\alpha}{2\sin^2 h(\sqrt{k})}\end{array}\right\}\qquad (B.10)$$

According to HAM we conclude that

$$u = \lim_{p\to 1} u(x) = u_0(x) + u_1(x)\qquad (B.11)$$

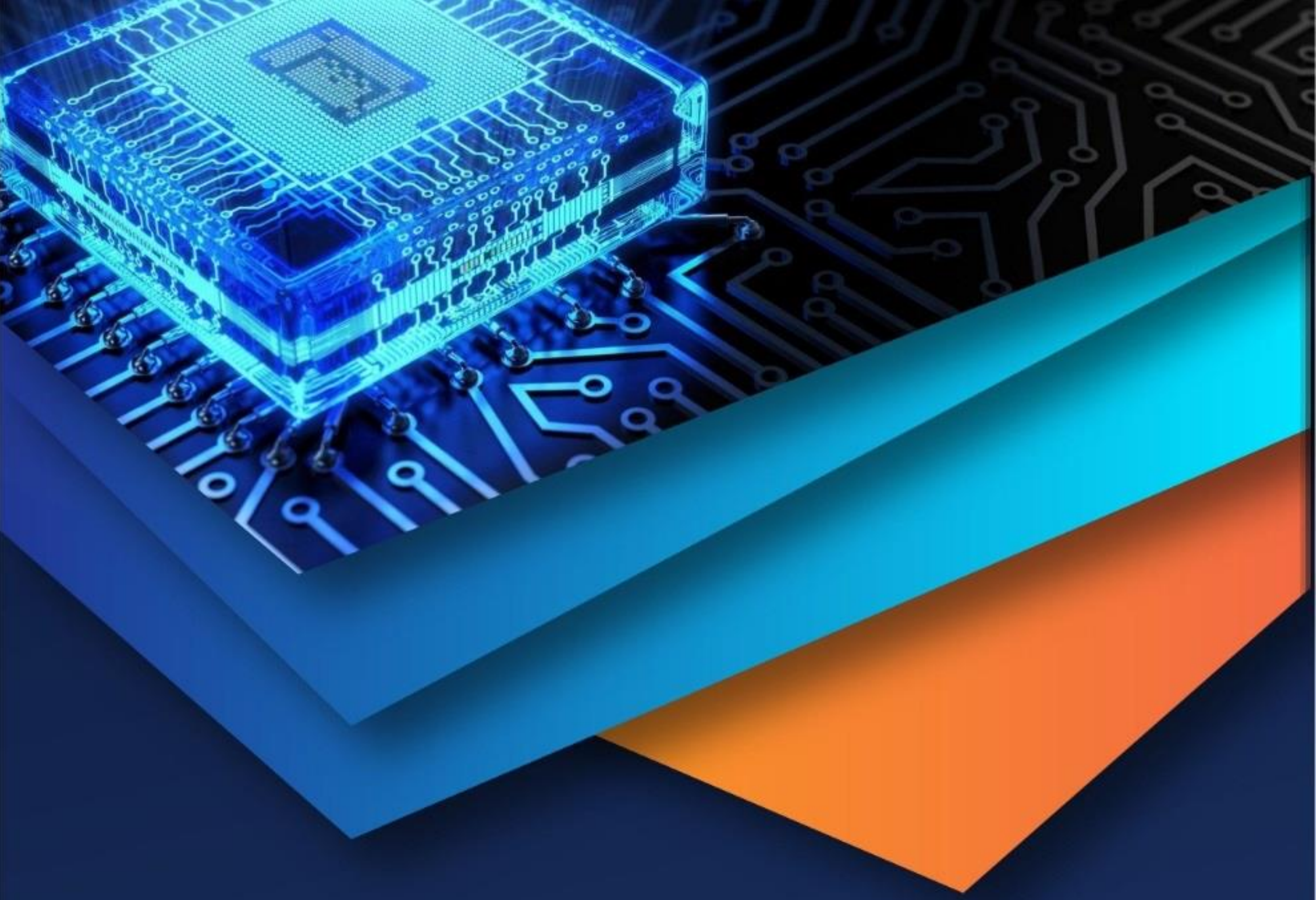
After putting the eqns.(B.9) and (B.10) into an eqn. (B.11), we obtain the solution in the text eqn.(4)

Appendix C

Matlab/Scilab program to find the numerical solution of the eqns. (1) and (2)

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

```
t = linspace(0,1000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u = sol(:,:,1);
figure
plot(x,u(end,:))
title('u(x,t)')
% --------------------------------------------------------------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = 1.*DuDx;
k=0.01;
a=0.1;
F =-(k*u)/(1+(u*a));
s=F;
% --------------------------------------------------------------
function u0 = pdex4ic(x);
 u0 = [1];
% --------------------------------------------------------------
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = ul(1)-1;
ql = 0;
pr = ur(1) ;
qr = 0;
```



10.22214/IJRASET

45.98

IMPACT FACTOR: 7.129

IMPACT FACTOR: 7.429

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY