# Theoretical Analysis of Nonlinear Equation in Reaction-Diffusion System: Hyperbolic Function Method

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***Abstract*** **- The nonlinear reactions-diffusion process describes a chemical reaction that involves three species, two reactions, and diffusion. The system of equations coupled with the nonlinear reaction terms with mixed Dirichlet and Neumann boundary conditions is solved analytically. The hyperbolic function method is used an approximate analytical expression of species concentrations. These analytical results are compared with numerical and previous available analytical results and are in good agreement.**

***Keywords*** **- Mathematical model, Reaction diffusion equations, Hyperbolic function method, Numerical simulation.**

## I. Introduction

The chemical reaction $2A+B \rightarrow$ product which we decompose as a pair of simultaneous binary reactions involving an intermediate species $C$.

$$A + B \xrightarrow{\lambda} C \tag{1}$$
$$A + C \xrightarrow{\mu} product \tag{2}$$

where $\lambda$ and $\mu$ denotes the binary reaction rates. To characterize reactions in the film model for a gas/liquid interface, [1] thought about the equivalent time-dependent system of this problem for boundary conditions of a very different type. Reference [2]-[4] have recently used a variety of techniques to solve several problems related to the exchange of stabilities (upper and lower solutions). Reference [5] discusses the presence of solutions but also the existence, uniqueness, and characterization of a limit when the rate of the fast reaction approaches infinite. Reference [6] derived the analytical expression of concentrations for the full range of enzyme activities using the homotopy perturbation method.

In this paper, a new and innovative semi-analytical technique, namely hyperbolic function method (HFM), is employed for solving three nonlinear reaction diffusion equation. The differential equation and its derivatives are needed to solve the trial solution of the equation. The approach's usefulness and effectiveness are shown by comparing the analytical results with the numerical method.

## II. Mathematical Formulation of the Problem

The steady-state nonlinear reaction-diffusion equations for a three-component chemical system [5] are given as follows:

$$\frac{d^2u(x)}{d\,x^2} - \lambda\, u(x)v(x) - u(x)w(x) = 0 \tag{3}$$
$$\frac{d^2v(x)}{d\,x^2} - \lambda\, u(x)v(x) = 0 \tag{4}$$
$$\frac{d^2w(x)}{d\,x^2} + \lambda\, u(x)v(x) - u(x)w(x) = 0 \tag{5}$$

where $u(x), v(x)$ and $w(x)$ denotes the dimensionless concentrations of the chemical species $A, B$ and $C$ respectively. The boundary conditions are

Published on January 31, 2023
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$$\text{At } x = 0,\ u = \alpha > 0,\ \frac{d\,v}{d\,x} = 0,\ w = \gamma \tag{6}$$

$$\text{At } x = 1,\ \frac{d\,u}{d\,x} = 0,\quad v = \beta,\ \frac{d\,w}{d\,x} = 0 \tag{7}$$

The reaction rate $q$ is given by

$$q = \lambda\, u(x) v(x) \tag{8}$$

## III. Results

### A. Approximate Analytical Expression of the Concentrations Using Hyperbolic Function Method.

Many asymptotic methods for solving nonlinear reaction-diffusion equations have been developed. Recently the homotopy perturbation method [7]-[10], Adomian decomposition method [11], [12], Variational iteration method [13], [14], Pade approximations [15], [16], and hyperbolic function method [17]-[19], Rajendran-Joy method [20] are applied to solve the nonlinear equations in physical and chemical sciences.

The hyperbolic function method assumes that a solution function with unknown constant coefficients will satisfy both the initial conditions and the differential equation. Then, the unknown coefficients are calculated using algebraic equations concerning the initial condition and their derivatives. The analytical expression of the concentration of species $u(x), v(x)$ and $w(x)$ for all dimensionless parameters is obtained (Appendix-A) as follows:

$$u(x) = \frac{\alpha \cosh\, m\,(1-x)}{\cosh m} \tag{9}$$

$$v(x) = \frac{\beta\, \cosh(\sqrt{\lambda\,\alpha}\,x)}{\cosh(\sqrt{\lambda\,\alpha})} \tag{10}$$

$$w(x) = \frac{\gamma \cosh\, p\,(1-x)}{\cosh p} \tag{11}$$

where $m$ and $p$ is obtained by solving below (12) and (13) using wolfram alpha.com (online free software) for the given values of the parameters $\alpha, \beta, \gamma$ and $\lambda$.

$$m^2 - \lambda\beta\, \operatorname{sech}\sqrt{\lambda\,\alpha)} - \gamma = 0 \tag{12}$$

$$p^2\gamma + \alpha\beta\lambda\, \operatorname{sech}\sqrt{\lambda\,\alpha)} - \alpha\gamma = 0 \tag{13}$$

Using (8) the reaction rate $q$ is given by

$$q(x) = \frac{\alpha\,\beta\lambda \cosh\, m\,(1-x) \cosh(\sqrt{\lambda\,\alpha}\,x)}{\cosh m \cosh(\sqrt{\lambda\,\alpha})} \tag{14}$$

### B. Previous Analytical Results

Reference [6] solved (3)-(5) with boundary conditions (6) and (7) using the Homotopy perturbation method. They derived the concentrations of species as follows:

$$u(x) = \alpha + \frac{1}{2}x^2\,\alpha\,\beta\lambda + \frac{1}{2}x^2\,\alpha\,\gamma - x\,\alpha\,\beta\lambda - \alpha\,\gamma\,x \tag{15}$$

$$v(x) = \beta + \frac{1}{2}\,\alpha\,\beta\lambda(x^2 - 1) \tag{16}$$

$$w(x) = \gamma - \frac{1}{2}x^2\,\alpha\,\beta\lambda + \frac{1}{2}x^2\,\alpha\,\gamma + x\,\alpha\,\beta\lambda - \alpha\,\gamma\,x \tag{17}$$

The reaction rate $q$ is given by

$$q = \lambda\left(\alpha + \frac{1}{2}x^2\,\alpha\,\beta\lambda + \frac{1}{2}x^2\,\alpha\,\gamma - x\,\alpha\,\beta\lambda - \alpha\,\gamma\,x\right)\left(\beta + \frac{1}{2}\,\alpha\,\beta\lambda(x^2 - 1)\right) \tag{18}$$

### C. Numerical Simulation

Numerical methods are used to solve the nonlinear (3)-(5) for the mixed Dirichlet and Neumann boundary conditions (6) and (7). The initial boundary value problems for the ordinary partial differential equation were solved using the MATLAB function. The Matlab program is also given in Appendix B. The numerical results are compared with our analytical and previous results in Tables I-III. The average error deviation between our result (HFM method) and the numerical result is less than the average error deviation between the previous result (HPM method) and the numerical result for all values of parameters.

TABLE I: COMPARISON OF DIMENSIONLESS CONCENTRATION OF SPECIES $u(x)$ WITH SIMULATION RESULTS AND PREVIOUS ANALYTICAL RESULTS FOR $\alpha = 0.1$,$\beta$=2, and $\gamma$=0.1

| $x$ | $\lambda = 0.1$ | | | | | $\lambda = 0.5$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Numerical | HFM (9) This work | HPM [6] (15) | Error % HFM (9) This work | Error % HPM [6] (15) | Numerical | HFM (9) This work | HPM [6] (15) | Error % HFM (9) This work | Error % HPM [6] (15) |
| 0 | 0.1000 | 0.1000 | 0.1000 | 0.0000 | 0.0000 | 0.1000 | 0.1000 | 0.1000 | 0.0000 | 0.0000 |
| 0.2 | 0.0950 | 0.0951 | 0.0945 | 0.1053 | 0.5263 | 0.0855 | 0.0855 | 0.0800 | 0.0000 | 6.4327 |
| 0.4 | 0.0913 | 0.0914 | 0.0903 | 0.1095 | 1.0953 | 0.0748 | 0.0754 | 0.0645 | 0.8021 | 13.770 |
| 0.6 | 0.0886 | 0.0887 | 0.0873 | 0.1129 | 1.4673 | 0.0676 | 0.0683 | 0.0535 | 1.0355 | 20.858 |
| 0.8 | 0.0870 | 0.0872 | 0.0855 | 0.2299 | 1.7241 | 0.0634 | 0.0642 | 0.0470 | 1.2618 | 25.867 |
| 1 | 0.0865 | 0.0867 | 0.0850 | 0.2312 | 1.7341 | 0.0621 | 0.0625 | 0.0450 | 0.6441 | 27.536 |
| Average error (%) | | | | 0.1315 | 1.0908 | Average error (%) | | | 0.6239 | 15.744 |

TABLE II: COMPARISON OF DIMENSIONLESS CONCENTRATION OF SPECIES $v(x)$ WITH SIMULATION RESULTS AND PREVIOUS ANALYTICAL RESULTS FOR $\alpha = 0.1$ and $\beta$=0.1

| $x$ | $\lambda = 0.1$ | | | | | $\lambda = 5$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Numerical | HFM (10) This work | HPM [6] (16) | Error % HFM (10) This work | Error % HPM [6] (16) | Numerical | HFM (10) This work | HPM [6] (16) | Error % HFM (10) This work | Error % HPM [6] (16) |
| 0 | 0.0995 | 0.0995 | 0.0995 | 0.0000 | 0.0000 | 0.0811 | 0.0793 | 0.0750 | 2.2195 | 7.5216 |
| 0.2 | 0.0995 | 0.0995 | 0.0995 | 0.0000 | 0.0000 | 0.0819 | 0.0801 | 0.0760 | 2.1978 | 7.2039 |
| 0.4 | 0.0996 | 0.0996 | 0.0996 | 0.0000 | 0.0000 | 0.0842 | 0.0826 | 0.0791 | 1.9002 | 6.0570 |
| 0.6 | 0.0997 | 0.0997 | 0.0998 | 0.0000 | 0.1003 | 0.0881 | 0.0867 | 0.0842 | 1.5891 | 4.4268 |
| 0.8 | 0.0998 | 0.0998 | 0.0999 | 0.0000 | 0.1002 | 0.0935 | 0.0926 | 0.0913 | 0.9627 | 2.3529 |
| 1 | 0.1000 | 0.1000 | 0.1000 | 0.0000 | 0.0000 | 0.1000 | 0.1000 | 0.1000 | 0.0000 | 0.0000 |
| Average error (%) | | | | 0.0000 | 0.3341 | Average error (%) | | | 1.4782 | 4.5937 |

TABLE III: COMPARISON OF DIMENSIONLESS CONCENTRATION OF SPECIES $w(x)$ WITH SIMULATION RESULTS AND PREVIOUS ANALYTICAL RESULTS FOR $\alpha = 0.1$,$\beta$=0.01, and $\gamma$=0.1

| $x$ | $\lambda = 0.1$ | | | | | $\lambda = 5$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Numerical | HFM (11) This work | HPM [6] (17) | Error % HFM (11) This work | Error % HPM [6] (17) | Numerical | HFM (11) This work | HPM [6] (17) | Error % HFM (11) This work | Error % HPM [6] Eq. (17) |
| 0 | 0.1000 | 0.1000 | 0.1000 | 0.0000 | 0.0000 | 0.1000 | 0.1000 | 0.1000 | 0.0000 | 0.0000 |
| 0.2 | 0.0983 | 0.0983 | 0.0982 | 0.0000 | 0.1017 | 0.0991 | 0.0991 | 0.0991 | 0.0000 | 0.0000 |
| 0.4 | 0.0970 | 0.0969 | 0.0968 | 0.1031 | 0.2062 | 0.0983 | 0.0982 | 0.0984 | 0.1017 | 0.1017 |
| 0.6 | 0.0961 | 0.0960 | 0.0958 | 0.1041 | 0.3122 | 0.0979 | 0.0978 | 0.0977 | 0.1021 | 0.2043 |
| 0.8 | 0.0956 | 0.0954 | 0.0952 | 0.2092 | 0.4184 | 0.0976 | 0.0976 | 0.0976 | 0.0000 | 0.0000 |
| 1 | 0.0954 | 0.0952 | 0.0950 | 0.2096 | 0.4193 | 0.0975 | 0.0971 | 0.0970 | 0.4103 | 0.5128 |
| Average error (%) | | | | 0.1043 | 0.2430 | Average error (%) | | | 0.1023 | 0.1365 |

## IV. DISCUSSION

Equations (9)-(11) are the new, closed and simple approximate analytical expressions concentrations of species A, B and C, which depend on the dimensionless parameters $\alpha, \beta, \gamma$ and $\lambda$.

The effects the various parameter $\alpha$, $\beta$, $\gamma$ and $\lambda$ on species concentration profiles $u(x)$ are shown in Fig. 1 (a-d). From Fig-1(a) it is observed that the concentration of species A ( $i.e\ u(x)$) increases when the parameter $\alpha$ increases. Additionally, as the reaction parameters $\beta, \gamma$ and $\lambda$ decreases, species A's concentration $u(x)$ rises.

Fig. 2 (a-c) represents the concentration of species B ( $i, e\ v(x)$) for all values of parameters. It is noticed that decrease in the parameters $\alpha$, $\lambda$ leads to a decrease in the value of concentration. Moreover, as $\beta$ raises, the concentration increases.

The effect of the parameters on the concentration of species C is represented in Fig. 3 (a-c). From the figure, it is observed that the concentration of species increases when $\alpha$ decreases. It shows an increasing concentration profile as other parameter values $\beta$, $\gamma$ and $\lambda$ increase.

Fig. 4 illustrates the reaction rate vs the distance for all possible parameter values. From the figure, it can be seen that the reaction rate increases when $\alpha$, $\beta$, and $\lambda$ increases or b decreases.

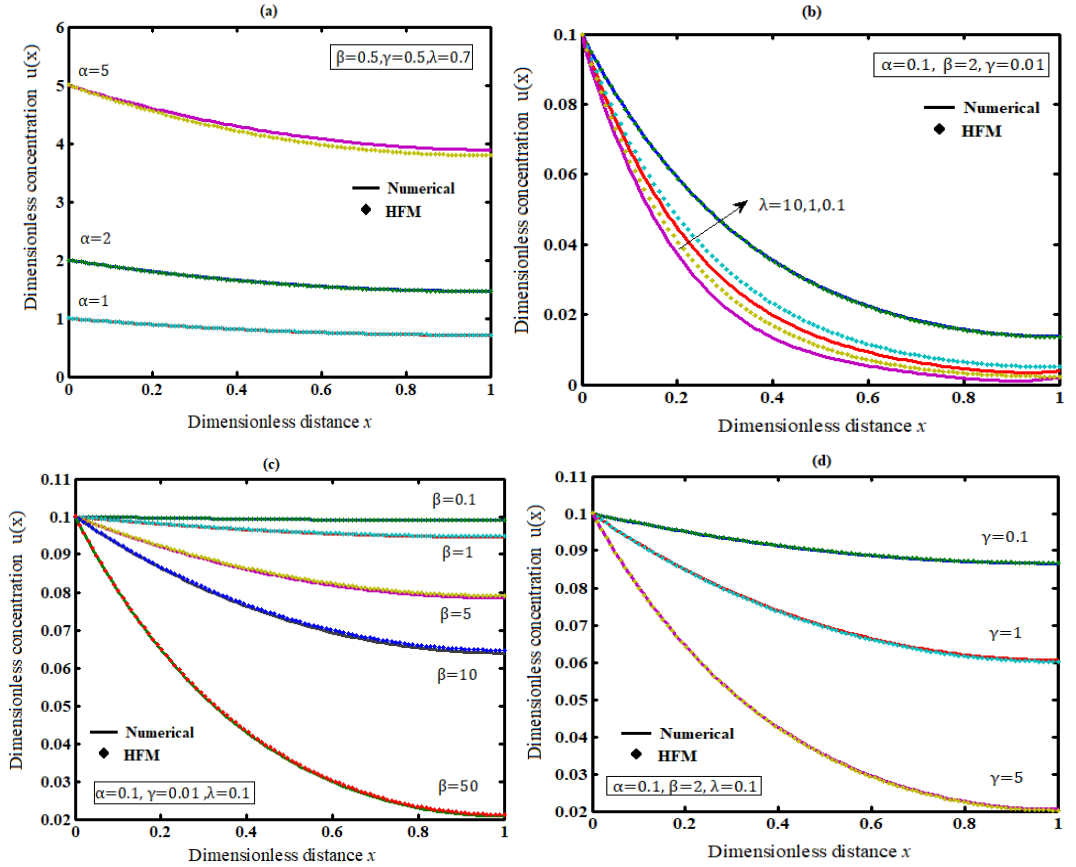


Fig. 1. Comparison of analytical expression (Eq. (9)) of concentration of species $u(x)$ with simulation result for all value of parameters α, β, γ and λ.

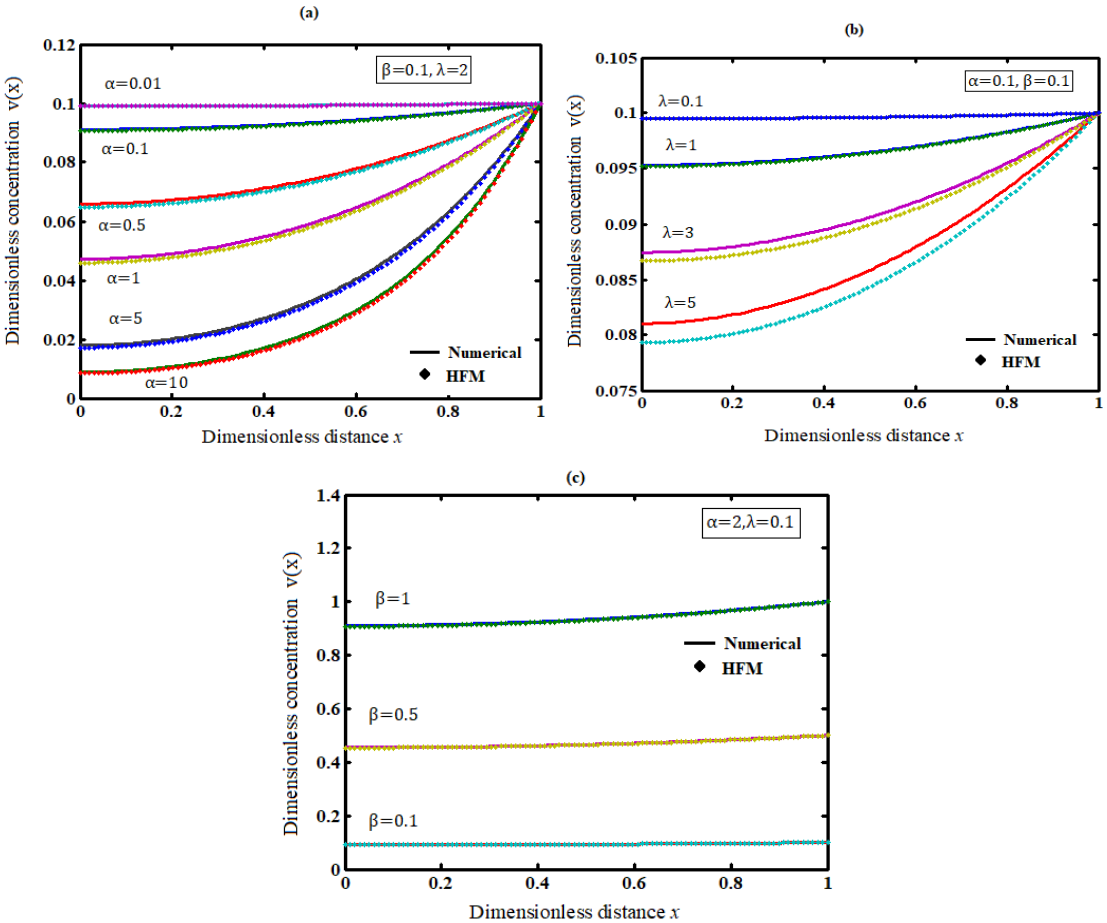


Fig. 2. Comparison of analytical expression (Eq. (10)) of concentration of species $v(x)$ with simulation result for all value of parameters α, λ and β.

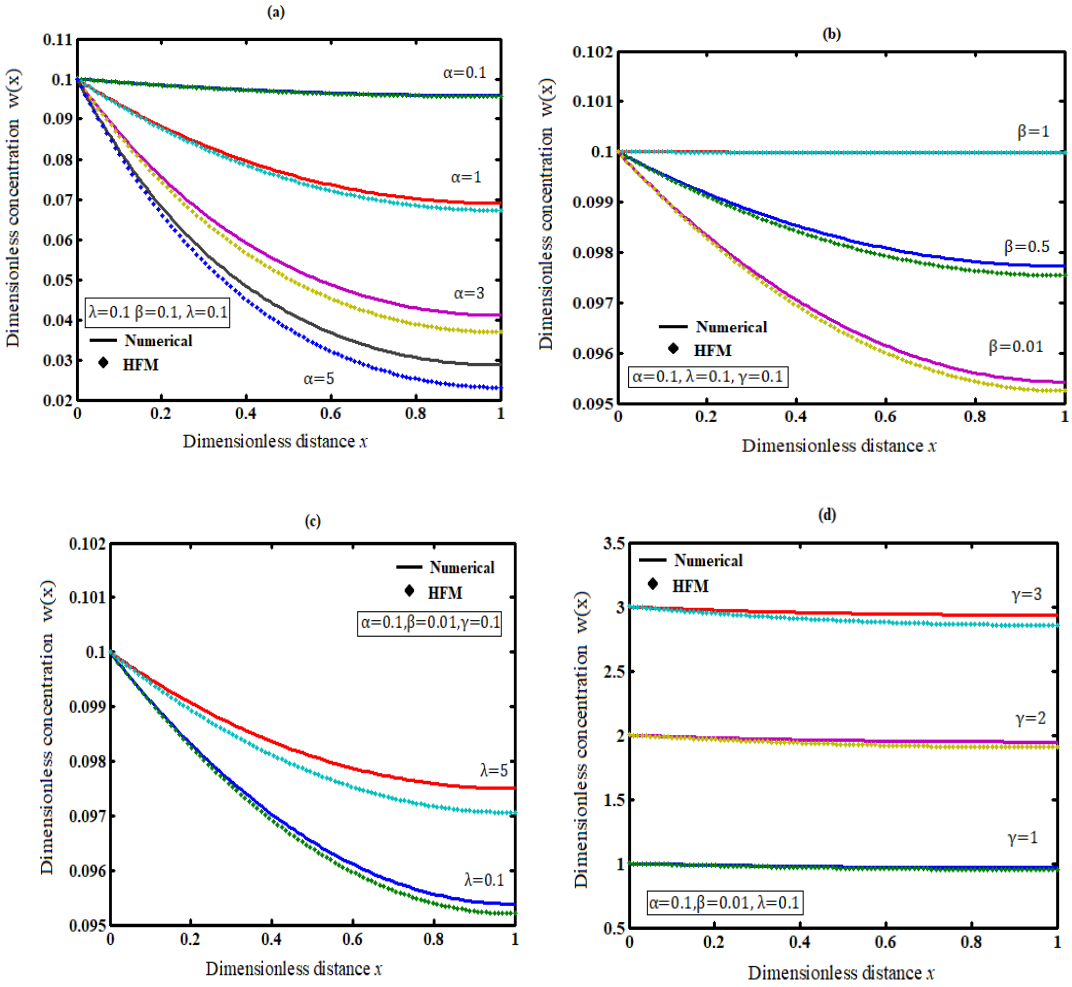


Fig. 3. Comparison of analytical expression (Eq. (11)) of concentration of species $w(x)$ with simulation result for all value of parameters α, β, γ and λ.

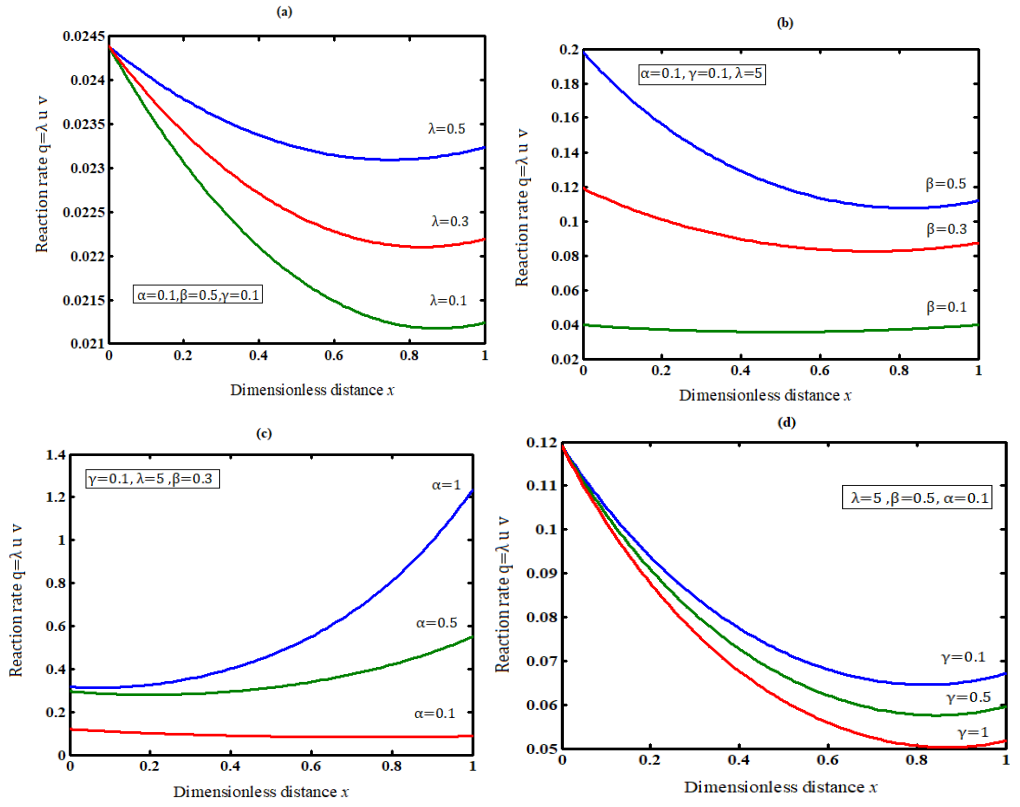


Fig. 4. Reaction rate versus dimensionless distance for all value of parameters α, β, γ and λ using Eq. (14).

## V. CONCLUSION

The steady-state nonlinear differential equations have been solved analytically. Approximate analytical expressions about the concentrations of species for all the values of parameters are obtained using the hyperbolic function method. The numerical simulation compares and validates the obtained species concentrations for all parameter values. These results were in agreement, therefore providing a good understanding of the system and optimising the parameters in the chemical reaction model.

## APPENDIX

**Nomenclature**

| Symbols | Description | Units |
|---|---|---|
| $u(x)$ | Dimensionless concentration of chemical species A | None |
| $v(x)$ | Dimensionless concentration of chemical species B | None |
| $w(x)$ | Dimensionless concentration of chemical species C | None |
| $x$ | Dimensionless distance | None |
| α | Fixed concentration of chemical species A | None |
| β | Fixed concentration of chemical species B | None |
| γ | Fixed concentration of chemical species C | None |
| λ | Dimensionless parameter | None |
| $q$ | Dimensionless reaction rate | None |

### *A. Appendix A: Analytical Solution of Nonlinear Equations (3)- (5) Using HFM*

Assume that the solution to Eqs. (3-5) is of the following hyperbolic function form:

$$u(x) = A_0 \cosh(m\,x) + B_0 \sinh(m\,x) \quad \text{(A1)}$$
$$v(x) = A_1 \cosh(n\,x) + B_1 \sinh(n\,x) \quad \text{(A2)}$$
$$w(x) = A_2 \cosh(p\,x) + B_2 \sinh(p\,x) \quad \text{(A3)}$$

where $A_0, A_1, A_2, B_0, B_1, B_2, m, n$ and $p$ are constant. The values of $A_0, A_1, A_2, B_0, B_1, B_2$ are found easily from boundary conditions (6) and (7), that is

$$A_0 = \alpha\,, B_0 = \frac{-\alpha \sinh(m)}{\cosh(m)}, A_1 = \frac{\beta}{\cosh(n)}\,, B_1 = 0, A_2 = \gamma\,,\ and\ B_2 = \frac{-\gamma \sinh(p)}{\cosh(p)} \quad \text{(A4)}$$

As a result, Eqs. (A1-A3) becomes

$$u(x) = \frac{\alpha \cosh m\,(1-x)}{\cosh m}\,,\ v(x) = \frac{\beta \cosh(nx)}{\cosh(n)} \text{ and } w(x) = \frac{\gamma \cosh p\,(1-x)}{\cosh p} \quad \text{(A5)}$$

We use the general form of Eqs. (3)-(5) to find the constant $m, n\ and\ p$ in Eq. (A5).

$$F(x) = \frac{d^2u(x)}{d\,x^2} - \lambda\,u(x)v(x) - u(x)w(x) = 0 \quad \text{(A6)}$$
$$G(x) = \frac{d^2v(x)}{d\,x^2} - \lambda\,u(x)v(x) = 0 \quad \text{(A7)}$$
$$H(x) = \frac{d^2w(x)}{d\,x^2} + \lambda\,u(x)v(x) - u(x)w(x) = 0 \quad \text{(A8)}$$

We obtain Eqs. (A6)-(A8) by substituting it for Eqs. (A5)

$$F(x)|_{x=0} = m^2 - \lambda\beta \operatorname{sech}\sqrt{\lambda\,\alpha)} - \gamma = 0 \quad \text{(A9)}$$
$$G(x)|_{x=0} = n^2 - \lambda\,\alpha = 0 \quad \text{(A10)}$$
$$H(x)|_{x=0} = p^2\gamma + \alpha\beta\lambda \operatorname{sech}\sqrt{\lambda\,\alpha)} - \alpha\gamma = 0 \quad \text{(A11)}$$

it shows that

$$m^2 - \lambda\beta \operatorname{sech}\sqrt{\lambda\,\alpha)} - \gamma = 0 \quad \text{(A12)}$$
$$n = \sqrt{\lambda\,\alpha)} \quad \text{(A13)}$$
$$p^2\gamma + \alpha\beta\lambda \operatorname{sech}\sqrt{\lambda\,\alpha)} - \alpha\gamma = 0 \quad \text{(A14)}$$

*B. Appendix B: MATLAB Code for Numerical Solutions of the Nonlinear Reaction -Diffusion Equations (3)-(5).*

```
function pdex2

    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,1)')
    %-------------------------------------------------------------------
    figure
    plot(x,u2(end,:))
    title('u2(x,t)')
    xlabel('Distance x')
    ylabel('u2(x,2)')
    % -------------------------------------------------------------------
    figure
    plot(x,u3(end,:))
    title('u3(x,t)')
    xlabel('Distance x')
    ylabel('u3(x,3)')
    %-------------------------------------------------------------------
    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);
    h=0.1;
    F=-h*y-y1;
    F1=-h*y;
    F2=h*y-y1;
    s=[F;F1;F2];
    function u0 = pdex4ic(x);
    %create a initial conditions
    u0 = [0; 1; 0];
    function [pl, ql, pr, qr] =pdex4bc(xl, u1, xr, ur, t)
    %create a boundary condition
    pl = [u1(1)-2; 0; u1(3)-0.001];
    ql =[0; 1; 0];
    pr = [0; ur(2)-0.5; 0];
    qr = [1; 0; 1];
```

## ACKNOWLEDGMENT

The authors are thankful to the reviewers for their valuable comments. They express their gratitude to Shri J. Ramachandran, Chancellor,Col. Dr. G. Thiruvasagam, Vice-Chancellor and Dr. M.Jayaprakashvel, Registrar, Academy of Maritime Education and Training (AMET), Chennai, Tamil Nadu for their continuous encouragement.

## CONFLICT OF INTEREST

Authors declare that they do not have any conflict of interest

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