International Journal of Mathematical Archive-4(6), 2013, 228-242
Available online through www.ijma.info ISSN 2229 – 5046

ANALYTICAL SOLUTION OF BOUNDARY VALUE PROBLEM IN REACTIVE GAS ABSORPTION

P. Felicia Shirly[1], S. Narmatha[1] and L. Rajendran[2*]

[1]Department of Mathematics, Lady Doak College, Madurai – 625002, Tamil Nadu, India

[2]Department of Mathematics, Madura College, Madurai-625011, Tamil Nadu, India

(Received on: 21-05-13; Revised & Accepted on: 11-06-13)

ABSTRACT

A mathematical model of reactive gas absorption is restudied in this paper. Here He's Homotopy perturbation method is implemented to find the analytical solutions of system of steady-state non-linear reaction diffusion equations containing a non-linear term related to reactive gas absorption. Analytical expressions for concentrations of the gas and liquid reactants have been derived for small values of Hatta number M and all values of parameters rq, a_0, α, β and Ω. Analytical expression of reaction (enhancement) factor for non-volatile and volatile liquid reactant also derived. The Homotopy perturbation method which produces the solutions in terms of convergent series requires no linearization. These analytical results are compared with numerical results and are found to be in good agreement.

Keywords: *Reactive gas absorption, Reaction/diffusion equation, Mathematical modeling, Homotopy perturbation method, Non-linear boundary value problem.*

INTRODUCTION

Absorption of gases in liquid solutions accompanied by chemical reactions is an important industrial operation for the production of basic chemicals. Gas – liquid reactors depend on fundamental understanding of the interactions between transport and chemical reaction phenomena. Mathematical models are developed to describe the effect of chemical reaction on the rate of gas absorption at the microscopic level and are customarily accomplished by invoking inter phase transport models to describe the mechanism of the physical contact between the gas and liquid phases. The most widely used models are film model [1] and surface renewal model [2].

The mathematical formulation of film model gives rise to a boundary value problem which is non linear in most cases of practical importance. Considerable efforts have been directed at the development and application of rigorous and approximate solutions of the local and global boundary value problem models in reactive gas absorption.

Shaikh *et al.* [13] have derived an expression for the reaction factor using a set of algebraic equations. However, to the best of our knowledge, till date there were no analytical results corresponding to the reaction factor for all values of the parameters were reported. The purpose of this communication is to derive an analytical solution for the boundary value problem in reactive gas absorption when the liquid reactant is non volatile and volatile.

MATHEMATICAL FORMULATION OF THE BOUNDARY VALUE PROBLEM FOR NON-VOLATILE LIQUID REACTANT

The mass transfer of a gaseous reactant A through a spherical gas bubble and into a liquid phase which contains a non volatile liquid reactant B is addressed. This reaction scheme is represented in Fig-1. The absorption of A occurs with a non volatile liquid reactant B with an irreversible second order reaction according to the following stoichiometry:

$$A + \nu B \rightarrow \text{products} \qquad (1)$$

A general film model is framed using the relationship between the mass transfer co-efficient and thickness of a boundary layer film. If the size of the gas bubble is independent of reaction, then the film model equations for a gas bubble of radius R, surrounded by a film or boundary layer of thickness δ are given by [13]:

Corresponding author: *L. Rajendran[2*]*
[1]Department of Mathematics, Lady Doak College, Madurai – 625002, Tamil Nadu, India

$$D_A\left[\frac{d^2C_A}{dr'^2}+\frac{2}{r'}\frac{dC_A}{dr'}\right]-kC_AC_B=0 \tag{2}$$

$$D_B\left[\frac{d^2C_B}{dr'^2}+\frac{2}{r'}\frac{dC_B}{dr'}\right]-\nu kC_AC_B=0 \tag{3}$$

with the following boundary conditions

$$C_A=C_{Ai}\ ,\frac{dC_B}{dr'}=0 \text{ when } r'=R \tag{4a}$$

$$-\left[4n\pi(R+\delta)^2\right]D_A\frac{dC_A}{dr'}=kC_AC_B\left\{V_L-\left[\frac{4n\pi}{3}(R+\delta)^3-R^3\right]\right\}+F_L(C_A-C_{A0}),$$

$$C_B=C_{BL} \text{ when } r'=R+\delta \tag{4b}$$

where C_A and C_B are the concentrations of the gas reactant and the liquid reactant , D_A and D_B are the corresponding diffusion coefficients, k is the second order reaction rate constant, ν is the stoichiometric coefficient, r', R, δ are the distance inside the liquid side film, radius of gas bubble and thickness of liquid side film respectively. n, V_L and F_L are the total number of gas bubbles in reactor, volume of liquid phase and volumetric flow rate of phase L respectively.

To cast equations (2) to (4) in dimensionless form, an expression relating the physical mass transfer co-efficient to the thickness of the boundary layer film is needed. Equation (2) can be integrated when the reaction term is dropped to obtain the specific rate of physical absorption. Using the definition of the mass transfer coefficient (rate of gas absorption divided by the driving force) the relationship $k_L{}^0=\frac{D_A}{\delta}\left(1+\frac{1}{\Omega}\right)$ where $\Omega=\frac{r}{\delta}$ is obtained. Introducing the following dimensionless variables,

$$M=\frac{(kD_AC_{BL})^{\frac{1}{2}}}{k_L{}^o},\ a=\frac{C_A}{C_{Ai}},\ b=\frac{C_B}{C_{BL}},\ r=\frac{D_B}{\nu D_A},\ q=\frac{C_{BL}}{C_{Ai}},\ \alpha=\frac{V_Lk_L^o}{a'D_A},\ \beta=\frac{F_L}{a'k_L^o} \tag{5}$$

and utilizing the above relationship, the film model equations (2) and (3)can be normalized as follows:

$$\frac{d^2a}{dx^2}+\frac{2}{x+\Omega}\frac{da}{dx}=\left(1+\frac{1}{\Omega}\right)^2M^2ab \tag{6}$$

$$\frac{d^2b}{dx^2}+\frac{2}{x+\Omega}\frac{db}{dx}=\left(1+\frac{1}{\Omega}\right)^2\frac{M^2}{rq}ab \tag{7}$$

with boundary conditions

$$\text{At } x=0,\quad a=1,\quad \frac{db}{dx}=0 \tag{8a}$$

$$\text{At } x=1,\quad -\frac{da}{dx}=M^2\left[\left(\frac{\Omega}{1+\Omega}\right)\alpha-\left(1+\frac{1}{\Omega}+\frac{1}{3\Omega^2}\right)\right]a-\left(\frac{\Omega}{1+\Omega}\right)\beta(a-u_0),\quad b=1 \tag{8b}$$

where a and b are dimensionless concentrations of the gas and liquid reactants respectively and x is the dimensionless distance inside the liquid film. The other dimensionless parameters are the Hatta number M, the concentration ratio rq and u_0, α, β, Ω. The equations (6) and (7) are the system of non linear differential equations. This non linear boundary value problem does not have a general analytic solution. Shaikh and coworkers [13] have solved these equations using Van Krevelen- Hoftijzer approach [14] which is given in the next section.

PREVIOUS WORK

As per Van Krevelen- Hoftijzer approach, the concentration of the liquid reactant within the film is equal to its concentration at the interface (i.e.) $b(x) = b_1$ for $x \in (0,1)$. This uncouples equation (6) from (7) and using the boundary

condition equation (8) can be solved to obtain *a(x)*. This function can be used to obtain an expression for the reaction factor which is defined as the ratio of the actual rate of absorption to the maximum possible rate of physical absorption given by

$$E_A^* = \frac{\left[-D_A\, dC_A/dr'\right]_{r'=R}}{k_L{}^0 C_{Ai}} = -\frac{\Omega}{1+\Omega}\left[\frac{da}{dx}\right]_{x=0} \tag{9}$$

Shaikh *et al* [13] obtained the expression for E_A^* using the following set of simultaneous algebraic equations.

$$E_A^* = M\sqrt{b_i}\left\{\frac{\Omega\left[M_1(1+\Omega)-1\right]+(1+\Omega)^2 M\sqrt{b_i}\tanh\left[\left(1+\frac{1}{\Omega}\right)M\sqrt{b_i}\right]}{\Omega\left[M_1(1+\Omega)-1\right]\tanh\left[\left(1+\frac{1}{\Omega}\right)M\sqrt{b_i}\right]+(1+\Omega)^2 M\sqrt{b_i}}\right\}+\frac{1}{1+\Omega}$$
$$-\frac{\Omega(1+\Omega)\beta a_0}{\Omega\left[M_1(1+\Omega)-1\right]\sinh\left[\left(1+\frac{1}{\Omega}\right)M\sqrt{b_i}\right]+(1+\Omega)^2 M\sqrt{b_i}\cosh\left[\left(1+\frac{1}{\Omega}\right)M\sqrt{b_i}\right]} \tag{10}$$

$$b_i = \frac{(1+rq)-E_A^*-a_L}{rq} \tag{11}$$

$$a_L = \frac{\Omega(1+\Omega)M\sqrt{b_i}+\Omega^2\beta u_0\sinh\left[\left(1+\frac{1}{\Omega}\right)M\sqrt{b_i}\right]}{\Omega\left[M_1(1+\Omega)-1\right]\sinh\left[\left(1+\frac{1}{\Omega}\right)M\sqrt{b_i}\right]+(1+\Omega)^2 M\sqrt{b_i}\cosh\left[\left(1+\frac{1}{\Omega}\right)M\sqrt{b_i}\right]} \tag{12}$$

$$M_1 = M^2\left\{\left[\frac{\Omega}{1+\Omega}\right]\alpha-\left[1+\frac{1}{\Omega}+\frac{1}{3\Omega^2}\right]\right\}+\left[\frac{\Omega}{1+\Omega}\right]\beta = M^2 l + n\beta \tag{13}$$

where

$$l = \frac{\alpha\,\Omega}{1+\Omega}-\left(1+\frac{1}{\Omega}+\frac{1}{3\Omega^2}\right)\quad,\quad n=\frac{\Omega}{1+\Omega} \tag{14}$$

ADVANTAGES OF HOMOTOPY PERTURBATION METHOD

Recently, many authors have applied the HPM to various problems and demonstrated the efficiency of the HPM for handling non-linear structures and solving various physics and engineering problems [3-6]. Homotopy perturbation method is a series expansion method used in the solution of non linear partial differential equations. This method employs a homotopy transform to generate a convergent series solution of differential equations. This method has been used by many authors to obtain solutions of a large class of linear and non- linear equations. The HPM was introduced by Ji-Huan He. The basic concept of HPM [7-10] is given in Appendix-A. In this paper HPM [11-12] is employed to solve the system of non-linear differential equations (6) and (7).

ANALYTICAL EXPRESSIONS OF THE CONCENTRATIONS OF GAS AND LIQUID REACTANTS FOR NON-VOLATILE LIQUID REACTANT USING HOMOTOPY PERTURBATION METHOD

The dimensionless concentration of gas and liquid reactants can be obtained by solving the non – linear equation (6) and (7) using HPM (see Appendix B)

$$a(x) = \left[\frac{\left(\left(\Omega(1-M_1(1+\Omega))+n\beta u_0(1+\Omega)^2\right)x\right)+\Omega(\Omega+M_1(1+\Omega))}{(x+\Omega)(\Omega+M_1(1+\Omega))}\right]$$
$$+\frac{1}{x+\Omega}\left[\frac{M^2(\Omega(1-M_1(1+\Omega))+n\beta u_O(1+\Omega)^2)\,x^3}{6n^2(\Omega+M_1(1+\Omega))}+\frac{M^2\Omega x^2}{2n^2}\right]$$

$$-\frac{x}{x+\Omega}\left[\frac{M^2}{6n^2(\Omega+M_1(1+\Omega))^2}\left[\begin{array}{l}2\Omega+n\beta(1+\Omega)\Big((1+\Omega)\Big[(M_1(1+\Omega)+3\Omega+2)u_0+2\Omega\Big(M_1+M^2l\Big)\Big]+2\Omega(3\Omega+1)\Big)\\+(1+\Omega)((2M^4l^2\Omega(1+\Omega)+6\Omega^2+2M^2l\ \ \Omega(3\Omega+1))\end{array}\right]\right] \quad (15)$$

$$b(x)=1-\frac{M^2}{6(x+\Omega)n^2rq(\Omega+M_1(1+\Omega))(1+\Omega)}\left[\begin{array}{l}\Big((1+\Omega)\Big[-n\beta u_o(1+\Omega)^2+\Omega(1+\Omega)M_1-\Omega\Big]\Big)x^3+\\(-3\Omega(1+\Omega)(M_1(1+\Omega)+\Omega))x^2+\\\Big((1+\Omega)[n\beta u_o(1+\Omega)+2\Omega M_1]+\Omega\ \ (3\Omega+1)\Big)x+\\\Big((1+\Omega)\Big[n\beta u_o\Omega(1+\Omega)+2\Omega^2M_1\Big]+\Omega^2(3\Omega+1)\Big)\end{array}\right] \quad (16)$$

From equation (15) the reaction factor can be obtained as follows:

$$E_A^{\ *}=-\frac{\Omega}{(1+\Omega)}\left[\frac{da}{dx}\right]_{x=0}$$

$$=-\frac{\Omega}{(1+\Omega)}\left[\begin{array}{l}\frac{\Omega(1-M_1(1+\Omega))+n\beta u_0(1+\Omega)^2}{\Omega(\Omega+M_1(1+\Omega))}-\frac{1}{\Omega}\\-\frac{M^2}{6\Big(\Omega n^2(\Omega+M_1(1+\Omega))^2\Big)}\left(\begin{array}{l}2\Omega+n\beta(1+\Omega)\Big((1+\Omega)\Big((M_1(1+\Omega)+3\Omega+2)u_0+2\Omega\Big(M_1+M^2l\Big)\Big)+2\Omega(3\Omega+1)\Big)\\+(1+\Omega)\Big(2M^4l^2\Omega(1+\Omega)+6\Omega^2+2M^2l\Omega(3\Omega+1)\Big)\end{array}\right)\end{array}\right] \quad (17)$$

DISCUSSION

Equations (15) and (16) represent the new analytical expressions of concentration of gas reactant and liquid reactant for small values of parameters. Equation (17) represents the new simple closed form of an analytical expression of reaction factor. Tables 1-4 show the comparison between analytical and numerical values of reaction factor in non volatile liquid reactant model for small values of Hatta number *M*. From the tables it is evident that as the value of Hatta number increases, the value of reaction factor also increases. Further, when the value ofΩ increases the value of reaction factor decreases.

MATHEMATICAL FORMULATION OF THE BOUNDARY VALUE PROBLEM FOR VOLATILE LIQUID REACTANT

The absorption of gaseous species A accompanied by simultaneous reaction with volatile liquid species B according to irreversible second-order kinetics is described. A linear approximation for the concentration profile of species B is applied in a film model to obtain an analytical expression for the reaction factor which can be applied to all reaction regimes. On the basis of the film model and a plane interface, the absorption of species A accompanied by irreversible second order reaction with volatile species B is mathematically described as follows [9]:

$$D_A\frac{d^2C_A}{dz^2}-kC_AC_B=0 \quad (18)$$

$$D_B\frac{d^2C_B}{dz^2}-\nu kC_AC_B=0 \quad (19)$$

The boundary conditions are

$$C_A=C_{Ai} \quad \text{at} \quad z=0 \quad (20a)$$

$$D_B\frac{dC_B}{dz}=k_{GB}^0K_B(C_B-C_{BG}) \quad \text{at} \quad z=0 \quad (20b)$$

$$-a'D_A\frac{dC_a}{dz}=kC_AC_B(V_L-a'z)+F_L(C_A-C_{A0}) \text{ at } z=z_L \quad (21a)$$

$$C_B=C_{BL} \text{ at } z=z_L \quad (21b)$$

To cast equations (18) to (21) in dimensionless form, an expression relating the physical mass transfer co-efficient to the thickness of the boundary layer film is used. Using the definition of the mass transfer coefficient the relationship $k_L{}^0 = D_A/z_L$ is obtained. Introducing the following dimensionless variables,

$$M = \frac{(kD_A C_{BL})^{\frac{1}{2}}}{k_L{}^o},\ a = \frac{C_A}{C_{Ai}},\ b = \frac{C_B}{C_{BL}},\ r = \frac{D_B}{\nu D_A},\ q = \frac{C_{BL}}{C_{Ai}},\ \alpha = \frac{V_L k_L^o}{a' D_A},\ \beta = \frac{F_L}{a' k_L^o} \tag{22}$$

and utilizing the above relationship, the film model equations can be normalized as follows:

$$\frac{d^2 a}{dx^2} = M^2 ab \tag{23}$$

$$\frac{d^2 b}{dx^2} = \frac{M^2}{rq} ab \tag{24}$$

with boundary conditions

$$\text{At } x = 0,\quad a = 1,\quad \frac{db}{dx} = \gamma(1 - b_G)b \tag{25}$$

$$\text{At } x = 1,\quad -\frac{da}{dx} = M^2(\alpha - 1)a - \beta(a - u_0),\quad b = 1 \tag{26}$$

where γ is the volatility of the liquid reactant and b_G is the dimensionless concentration. The equations (23) and (24) are the system of non linear differential equations. This non linear boundary value problem does not have a general analytic solution. While no general method of solving these non-linear problems has been proposed, homotopy perturbation method has been applied here to solve these non linear differential equations.

ANALYTICAL EXPRESSIONS OF THE CONCENTRATIONS OF GAS AND LIQUID REACTANTS FOR VOLATILE LIQUID REACTANT USING HOMOTOPY PERTURBATION METHOD

Using HPM (see Appendix C), the analytical expression of concentrations of gas and liquid reactants are obtained as follows:

$$a(x) = c_1 rq \cosh\left(\frac{Mx}{\sqrt{rq}}\right) + c_2 rq \sinh\left(\frac{Mx}{\sqrt{rq}}\right) + c_3 x + c_4 \tag{27}$$

$$b(x) = c_1 \cosh\left(\frac{Mx}{\sqrt{rq}}\right) + c_2 \sinh\left(\frac{Mx}{\sqrt{rq}}\right) \tag{28}$$

where the constants c_1 to c_4 and M_1 are defined in the equations (C6), (C7), (C10) and (C11).

NUMERICAL SIMULATION

To show the efficiency of the present method , the analytical solutions (27) and (28) is compared with numerical solution. The SCILAB/MATLAB program is also given in Appendix D. The dimensionless concentrations of gas and liquid reactants which are derived from HPM are compared with simulation results in Figs 2 and 3.

Limiting case

When $b_G = 1, \alpha = 1,\ a = u_0$, the boundary conditions (25) and (26) become as follows:

$$\text{At } x = 0,\quad a = 1,\quad \frac{db}{dx} = 0 \tag{29}$$

$$\text{At } x = 1,\quad \frac{da}{dx} = 0,\quad b = 1 \tag{30}$$

In this case, the dimensionless concentrations of the gas and liquid reactants can be obtained using Homotopy perturbation method as follows:

$$a(x) = 1 + \frac{M^2 x^2}{2} - M^2 x + \frac{M^4}{2rq}\left(\frac{x^4(1+rq)}{12} - \frac{x^2}{2} - \frac{rqx^3}{3}\right) + \frac{M^4(1+rq)x}{3rq} \tag{31}$$

$$b(x) = 1 + \frac{M^2 x^2}{2rq} - \frac{M^2}{2rq} + \frac{M^4}{2r^2q^2}\left(\frac{x^4(1+rq)}{12} - \frac{x^2}{2} - \frac{rqx^3}{3}\right) + \frac{M^4(5+3rq)}{24r^2q^2} \tag{32}$$

The dimensionless concentrations of gas and liquid reactants (eqns 31 and 32) which are derived from HPM are compared with simulation results in Figs 4 and 5. The SCILAB/MATLAB program is also given in appendix E.

CONCLUSION

Approximate solution of two non linear boundary value problems in reactive gas absorption are obtained using Homotopy perturbation method. Simple and closed form of an analytical expression of the enhancement factor is reported for both volatile and non volatile reactants. This theoretical result is very much useful to analyze the spherical-effect of gas – liquid reactions.

APPENDIX A: Basic concepts of the Homotopy perturbation method

Homotopy perturbation method has overcome the limitations of traditional perturbation methods. It can take full advantage of the traditional perturbation techniques, so a considerable deal of research has been conducted to apply the homotopy technique to solve various strong non-linear equations. To explain this method, let us consider the following function:

$$D_O(u) - f(r) = 0, \quad r \in \Omega \tag{A1}$$

with the boundary conditions of

$$B_O(u, \frac{\partial u}{\partial n}) = 0, \qquad r \in \Gamma \tag{A2}$$

where D_O is a general differential operator, B_O is a boundary operator, $f(r)$ is a known analytical function and Γ is the boundary of the domain Ω. In general, the operator D_O can be divided into a linear part L and a non-linear part N. Eq. (A1) can therefore be written as

$$L(u) + N(u) - f(r) = 0 \tag{A3}$$

By the homotopy technique, we construct a homotopy $v(r, p) : \Omega \times [0,1] \to \Re$ that satisfies

$$H(v, p) = (1-p)[L(v) - L(u_0)] + p[D_O(v) - f(r)] = 0. \tag{A4}$$

$$H(v, p) = L(v) - L(u_0) + pL(u_0) + p[N(v) - f(r)] = 0. \tag{A5}$$

where $p \in [0, 1]$ is an embedding parameter, and u_0 is an initial approximation of Eq. (A1) that satisfies the boundary conditions. From Eq. (A4) and Eq. (A5), we have

$$H(v,0) = L(v) - L(u_0) = 0 \tag{A6}$$

$$H(v,1) = D_O(v) - f(r) = 0 \tag{A7}$$

When p=0, Eq. (A4) and Eq. (A5) become linear equations. When p =1, they become non-linear equations. The process of changing p from zero to unity is that of $L(v) - L(u_0) = 0$ to $D_O(v) - f(r) = 0$. We first use the embedding parameter p as a "small parameter" and assume that the solutions of Eq. (A4) and Eq. (A5) can be written as a power series in p :

$$v = v_0 + pv_1 + p^2 v_2 + \ldots \tag{A8}$$

Setting $p = 1$ results in the approximate solution of Eq. (A1):

$$u = \lim_{p \to 1} v = v_0 + v_1 + v_2 + \ldots \tag{A9}$$

This is the basic idea of the HPM.

APPENDIX B

Solution of equations (6) and (7) using Homotopy perturbation method

The Homotopy for the equations (6) and (7) can be constructed as follows:

$$(1-p)\left(\frac{d^2a}{dx^2} + \frac{2}{x+\Omega}\frac{da}{dx}\right) + p\left(\frac{d^2a}{dx^2} + \frac{2}{x+\Omega}\frac{da}{dx} - \frac{M^2ab}{n^2}\right) = 0 \tag{B1}$$

$$(1-p)\left(\frac{d^2b}{dx^2} + \frac{2}{x+\Omega}\frac{db}{dx}\right) + p\left(\frac{d^2b}{dx^2} + \frac{2}{x+\Omega}\frac{db}{dx} - \frac{M^2ab}{n^2rq}\right) = 0 \tag{B2}$$

The boundary conditions (8a) and (8b) can be written as follows:

$$At \quad x = 0, \quad a = 1, \qquad \frac{db}{dx} = 0 \tag{B3a}$$

$$At \quad x = 1, \quad -\frac{da}{dx} = \left(M^2 l + n\beta\right)a - n\beta u_0 == M_1 a - n\beta u_0, \quad b = 1 \tag{B3b}$$

where *l* and *n* are given by (14). The approximate solutions of (B1) and (B2) are

$$a(x) = a_0 + a_1 p + a_2 p^2 + \ldots \tag{B4}$$

$$b(x) = b_0 + b_1 p + b_2 p^2 + \ldots \tag{B5}$$

Substituting equations (B4),(B5) in equations (B1),(B2) and comparing the coefficients of like powers of p, the following equations are obtained.

$$p^0: \quad \frac{d^2a_0}{dx^2} + \frac{2}{x+\Omega}\frac{da_0}{dx} = 0 \tag{B6}$$

$$p^1: \quad \frac{d^2a_1}{dx^2} + \frac{2}{x+\Omega}\frac{da_1}{dx} - \frac{M^2a_o b_o}{n^2} = 0 \tag{B7}$$

$$p^0: \quad \frac{d^2b_0}{dx^2} + \frac{2}{x+\Omega}\frac{db_0}{dx} = 0 \tag{B8}$$

$$p^1: \quad \frac{d^2b_1}{dx^2} + \frac{2}{x+\Omega}\frac{db_1}{dx} - \frac{M^2a_o b_o}{n^2rq} = 0 \tag{B9}$$

The boundary conditions become

$$At \ x = 0, \quad a_0 = 1, \ \frac{db_0}{dx} = 0 \tag{B10}$$

$$a_1 = 0,\ \frac{db_1}{dx} = 0 \tag{B11}$$

$$At\ x = 1, \quad -\frac{da_0}{dx} = M_1 a_0 - n\beta u_0\,,\ b_0 = 1 \tag{B12}$$

$$-\frac{da_1}{dx} = M_1 a_1,\ \ b_1 = 0 \tag{B13}$$

Solving equations (B6) to (B9) using the boundary conditions (B10) to (B13), we obtain the following results:

$$a_o(x) = \frac{\left((\Omega(1-M_1(1+\Omega)) + n\beta u_o(1+\Omega)^2)x + \Omega(\Omega + M_1(1+\Omega)\right)}{(x+\Omega)(\Omega + M_1(1+\Omega))} \tag{B14}$$

$$a_1(x) = \frac{1}{x+\Omega}\left(\frac{M^2(\Omega(1-M_1(1+\Omega)) + n\beta u_o(1+\Omega)^2)\,x^3}{6n^2(\Omega + M_1(1+\Omega))} + \frac{M^2\Omega x^2}{2n^2}\right)$$
$$-\frac{x}{x+\Omega}\left[\frac{M^2}{6\left(n^2(\Omega + M_1(1+\Omega))^2\right)}\left[\begin{array}{l} 2\Omega + n\beta(1+\Omega)\left((1+\Omega)\left[(M_1(1+\Omega) + 3\Omega + 2)u_0 + 2\Omega\left(M_1 + M^2 l\right)\right] + 2\Omega(3\Omega+1)\right)\right] \\ +(1+\Omega)((2M^4 l^2\Omega(1+\Omega) + 6\Omega^2 + 2M^2 l\ \ \Omega(3\Omega+1)) \end{array}\right]\right] \tag{B15}$$

$$b_0(x) = 1 \tag{B16}$$

$$b_1(x) = -\frac{M^2}{6(x+\Omega)n^2 rq\left(\Omega + M_1(1+\Omega)\right)(1+\Omega)}\left[\begin{array}{l} \left((1+\Omega)\left[-n\beta u_o(1+\Omega)^2 + \Omega(1+\Omega)M_1 - \Omega\right]\right)x^3 \\ +\left(-3\Omega(1+\Omega)\left(M_1(1+\Omega) + \Omega\right)\right)x^2 \\ +\left((1+\Omega)\left[n\beta u_o(1+\Omega) + 2\Omega M_1\right] + \Omega\ \ (3\Omega+1)\right)x \\ +\left((1+\Omega)\left[n\beta u_o\Omega(1+\Omega) + 2\Omega^2 M_1\right] + \Omega^2(3\Omega+1)\right) \end{array}\right] \tag{B17}$$

According to HPM, we conclude that

$$a\ (x) = \lim_{p\to 1}\left(a_0 + a_1 p + a_2 p^2 + \ldots\right) \cong a_0 + a_1 \tag{B18}$$

$$b\ (x) = \lim_{p\to 1}\left(b_0 + b_1 p + b_2 p^2 + \ldots\right) \cong b_0 + b_1 \tag{B19}$$

From the above equations we can obtain the equations (15) and (16) in the text.

APPENDIX C

Solution of equations (23) and (24) using Homotopy perturbation method

Consider the equations

$$\frac{d^2 a}{dx^2} = M^2 ab \tag{C1}$$

$$\frac{d^2 b}{dx^2} = \frac{M^2 ab}{rq} \tag{C2}$$

with the following boundary conditions,

$$At \quad x=0, \quad a=1, \qquad \frac{db}{dx}=\gamma(1-b_G)b \tag{C3a}$$

$$At \quad x=1, \quad -\frac{da}{dx}=M^2(\alpha-1)a+\beta(a-u_0)=M_1a-\beta u_0 \ , \ b=1 \tag{C3b}$$

where $M_1=M^2(\alpha-1)+\beta$. Substituting the boundary condition $a=1$ when $x=0$ in (C2), we get,

$$\frac{d^2b}{dx^2}=\frac{M^2b}{rq} \tag{C4}$$

The complementary function for the above equation is

$$b=c_1\cosh\left(\frac{M}{\sqrt{rq}}x\right)+c_2\sinh\left(\frac{M}{\sqrt{rq}}x\right) \tag{C5}$$

Using the boundary condition at x=0, $\frac{db}{dx}=\gamma(1-b_G)b$ and at x=1, b=1, the following constants are obtained.

$$c_1=\frac{1}{\cosh\left(\frac{M}{\sqrt{rq}}\right)+\frac{\gamma(1-b_G)\sqrt{rq}}{M}\sinh\left(\frac{M}{\sqrt{rq}}\right)} \tag{C6}$$

$$c_2=\frac{1}{\frac{M}{\gamma(1-b_G)\sqrt{rq}}\cosh\left(\frac{M}{\sqrt{rq}}\right)+\sinh\left(\frac{M}{\sqrt{rq}}\right)} \tag{C7}$$

Substituting this value of b and a=1 in (C1), we get

$$\frac{d^2a}{dx^2}=M^2\left[c_1\cosh\left(\frac{M}{\sqrt{rq}}x\right)+c_2\sinh\left(\frac{M}{\sqrt{rq}}x\right)\right] \tag{C8}$$

Using the boundary condition that *at* x=0, a=1 and at x=1, $-\frac{da}{dx}=M_1a-\beta u_0$, we get

$$a(x)=c_1rq\cosh\left(\frac{Mx}{\sqrt{rq}}\right)+c_2rq\sinh\left(\frac{Mx}{\sqrt{rq}}\right)+c_3x+c_4 \tag{C9}$$

where

$$c_3=-\frac{1}{M_1+1}\left[rq\cosh\left(\frac{M}{\sqrt{rq}}\right)\left(c_2\frac{M}{\sqrt{rq}}+M_1c_1\right)+rq\sinh\left(\frac{M}{\sqrt{rq}}\right)\left(\frac{c_1M}{\sqrt{rq}}+M_1c_2\right)+M_1c_4-\beta u_0\right] \tag{C10}$$

$$c_4=1-c_1rq \tag{C11}$$

and the constants c_1 and c_2 are given in the equation (C6) and (C7).

APPENDIX D

Scilab/matlab program to find the numerical solution of Eqns.23 and 24.

```
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);
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)')
% ————————————————————————————
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1];
f = [1; 1] .* DuDx;
M = 0.5;
r = 75;
q = 1;
F = -M^2*u(1)*u(2);
F1 = -(M^2)*u(1)*u(2)/(r*q);
s=[F; F1];
% ————————————————————————————
function u0 = pdex4ic(x);
u0 = [1; 1];
% ————————————————————————————
function [pl, ql, pr, qr] = pdex4bc(xl, ul, xr, ur, t)
M = 0.5;
r = 75;
q = 1;
g = 0.2;
h = 0.1;
j = 50;
k = 0.01;
u0 = 0;
pl = [ul(1)-1; -g*(1-h)*ul(2)];
ql = [0; 1];
pr = [M^2*(j-1)*ur(1)+k*(ur(1)-u0); ur(2)-1];
qr = [1; 0];
```

APPENDIX E

Scilab/matlab program to find the numerical solution of Eqns.in the limiting case.

```
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);
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)')
% ————————————————————————————
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = [1; 1];
f = [1; 1] .* DuDx;
M = 0.5;
r = 100;
```



```
q = 1;
F = -M^2*u(1)*u(2);
F1 = -(M^2)*u(1)*u(2)/(r*q);
s=[F; F1];
% ————————————————————————————
function u0 = pdex4ic(x);
u0 = [1; 1];
% ————————————————————————————
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
M = 0.5;
r = 100;
q = 1;
pl = [ul(1)-1; 0];
ql = [0; 1];
pr = [0; ur(2)-1];
qr = [1; 0];
```

NOMENCLATURE

a	dimensionless concentration of gas reactant, C_A/C_{Ai}
a'	interfacial area
b	dimensionless concentration of liquid reactant, C_B/C_{BL}
b_G	dimensionless concentration, defined as C_{GB}/C_{BL}
D_j	diffusion coefficient of species j,j=A,B
E_A^*	reaction factor
F_p	volumetric flow rate of phase p, p=L,G
k	second order reaction rate constant
k_{GB}^0	gas – side mass transfer coefficient for species B
k_L^0	liquid – side mass transfer coefficient
k_B	equilibrium constant for species B
M	Hatta number, defined as $(kD_AC_{BL})^{\frac{1}{2}}/k_L^0$
M_1	dimensionless parameter
n	total number of gas bubbles in reactor
q	dimensionless ratio of concentrations, C_{BL}/C_{AI}
r	dimensionless ratio of diffusion coefficients $D_B/\nu D_A$
r'	distance inside liquid - side film
R	radius of gas bubble
V_L	volume of liquid phase
x	dimensionless distance inside liquid side film
z	distance inside liquid side film
z_L	thickness of liquid side film

Greek letters

α	ratio of total liquid volume to film volume, $V_L k_L^0/a' D_A$
β	dimensionless parameter, $F_L/a'\ k_L^0$
δ	thickness of liquid side film
γ	dimensionless voltality parameter $D_AK_B - k_{GB}^0/D_B k_L^0$
γ'	dimensionless parameter, $(1-b_G)\ \gamma$
ν	stoichiometric coefficient
Ω	dimensionless ration of bubble radius to film thickness

Subscripts

G	bulk gas phase
I	gas – liquid interphase
L	bulk liquid phase
0	liquid food

ACKNOWLEDGEMENTS

This work was supported by the University Grants Commission (F. no. 39-58/2010 (SR)), New Delhi, India. The authors are thankful to Dr. R. Murali, The Principal, The Madura College, Madurai, and Mr. S. Natanagopal, The Secretary, Madura College Board, Madurai, for their encouragement. They also thank the reviewers for their valuable comments to improve the quality of the paper.

REFERENCES

[1] Astarita G., Mass Transfer with Chemical Reaction, Elsevier, Amsterdam, 1967

[2] Danckwerts P.V., Gas-liquid Reactions, McGraw-Hill, New York, 1970.

[3] Eswari. A,Rajendran. L,Analytical solution of steady state current at a microdisk biosensor, Journal of Electroanalytical Chemistry, 641 (2010) 35–44.

[4] Ghori Q.K., Ahmed M. and Siddiqui A.M., "Application of Homotopy Perturbation Method to Squeezing Flow of a Newtonian Fluid," International Journal of Nonlinear Science and Numerical Simulation, Vol. 8, No. 2, 2007, pp. 179-184.

[5] He J.H., "Homotopy Perturbation Technique," Computer Methods in Applied Mechanics and Engineering, Vol. 178, No. 3-4, 1999, pp. 257-262.

[6] He J.H., "Homotopy Perturbation Method: A New Nonlinear Analytical Technique," Applied Mathematics and Computation, Vol. 135, No. 1, 2003, pp. 73-79.

[7] Li S.J. and Liu Y.X., "An Improved Approach to Nonlinear Dynamical System Identification Using PID Neural Networks," International Journal of Nonlinear Science and Numerical Simulation, Vol. 7, No. 2, 2006, pp. 177-182.

[8] Loghambal. S, Rajendran. L, Mathematical modeling of diffusion and kinetics of amperometric Immobilized enzyme electrodes, Electrochimica Acta, Vol. 55, No. 18, 2010, pp. 5230-5238.

[9] Margret. V, Rajendran. L, Analytical expression of non steady-state concentration profiles at planar electrode for the CE mechanism, Natural Science, 2(11) (2010) 1318-1325.

[10] Meena. A, Rajendran. L, Mathematical modeling of amperometric and potentiometric biosensors and system of non-linear equations-Homotopy perturbation approach, Journal of Electroanalytical Chemistry 644 (2010) 50-59.

[11] Mousa M.M. and Ragab S.F., "Application of the Homotopy Perturbation Method to Linear and Nonlinear Schrödinger Equations," Zeitschrift fur Naturforschung, Vol. 63, 2008, pp. 140-144.

[12] Ozis T. and Yildirim A., "A comparative Study of He's Homotopy Perturbation Method for Determining Frequency-Amplitude Relation of a Nonlinear Oscillater with Discontinuities," International Journal of Nonlinear Science and Numerical Simulation, Vol. 8, No. 2, 2007, pp. 243-248.

[13] Shaikh A.A., Jamal A., Zarook S.M., The Chemical Engineering Journal, 57(1995)27-38

[14] Van Krevelen D.W., Hoftijzer P.J., Rec. Trav. Chem. Pays-Bas, 67(1948)563

Table 1: Comparison between analytical (Eq. (17)) and numerical values of reaction factor when $u_0 = 0$, rq=5, α=200, β=5

Ω	M	Numerical value of E_A^* [13]	Analytical value of E_A^* (Eqn.(17)	% deviation
50	0.01	0.834	0.834	0
	0.05	0.847	0.847	0
	0.08	0.865	0.865	0
	0.1	0.879	0.879	0
	0.2	0.943	0.943	0
	0.3	0.990	0.990	0
	0.4	1.029	1.029	0
	0.5	1.066	1.068	0.18

Table 2: Comparison between analytical (Eq. (17)) and numerical values of reaction factor when $u_0 = 0$, rq=5, α=200 and β=5

Ω	M	Numerical value of E_A^* [13]	Analytical value of E_A^* Eqn.(17)	% deviation
0.5	0.01	0.834	0.834	0
	0.05	0.849	0.849	0
	0.08	0.871	0.871	0
	0.1	0.888	0.888	0
	0.2	0.977	0.977	0
	0.3	1.060	1.060	0
	0.4	1.135	1.147	1.05
	0.5	1.203	1.246	3.57

Table 3: Comparison between analytical (Eq. (17)) and numerical values of reaction factor when $u_0 = 0$, rq=50, α=200, β=5

Ω	M	Numerical value of E_A^* [13]	Analytical value of E_A^* Eqn.(17)	% deviation
50	0.01	0.834	0.834	0
	0.05	0.847	0.847	0
	0.08	0.865	0.865	0
	0.1	0.879	0.879	0
	0.2	0.943	0.943	0
	0.3	0.990	0.990	0
	0.4	1.029	1.029	0

Table 4: Comparison between analytical (Eq. (17)) and numerical values of reaction factor when $u_0 = 0$, rq=50, α=200, β=5

Ω	M	Numerical value of E_A^* [13]	Analytical value of E_A^* Eqn.(17)	% deviation
0.5	0.01	0.834	0.834	0
	0.05	0.849	0.849	0
	0.08	0.871	0.871	0
	0.1	0.888	0.888	0
	0.2	0.977	0.977	0
	0.3	1.060	1.060	0
	0.4	1.135	1.147	1.05
	0.5	1.209	1.246	3.06

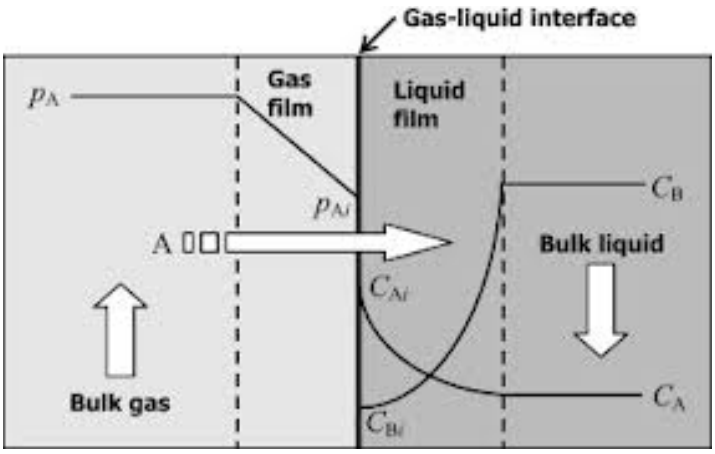

Fig. 1: General reaction scheme

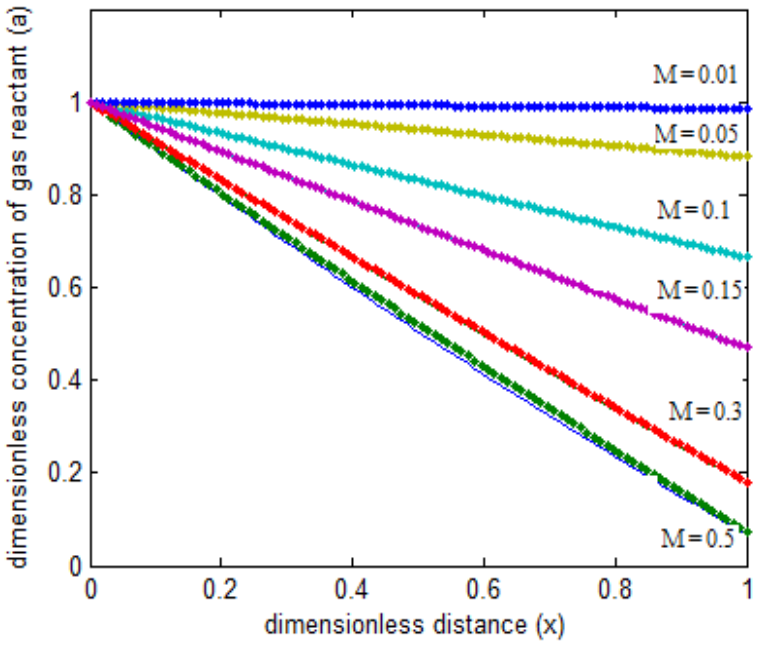

Fig. 2: Dimensionless concentration of gas reactant $a(x)$ versus dimensional distance x for various values of M and some fixed values of other parameters (a_0=0, rq=100, $\alpha = 50, \beta = 0.01$). Solid lines represent analytical result (eqn (27)) and dotted lines represent numerical results.

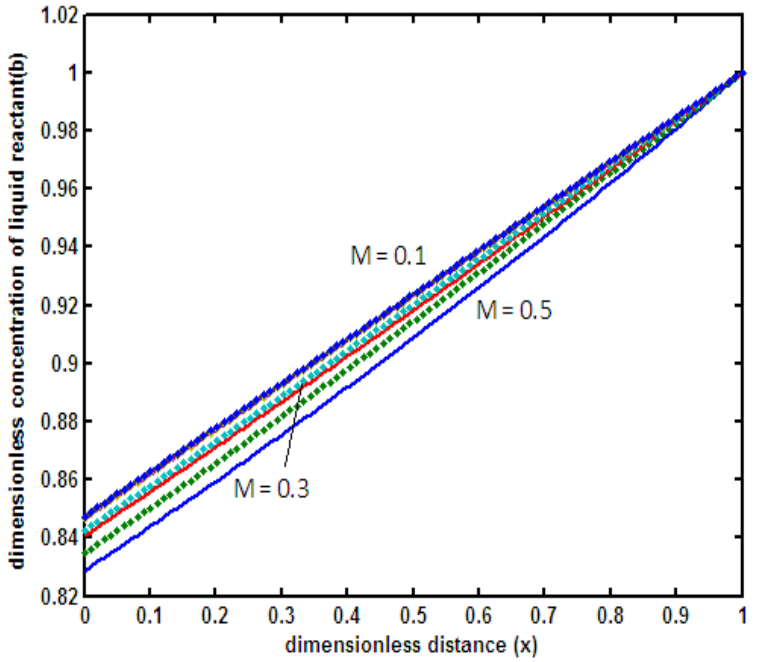

Fig. 3: Dimensionless concentration of liquid reactant $b(x)$ versus dimensional distance x for various values of M and some fixed values of other parameters (a_0=0, rq=100, $\alpha = 50, \beta = 0.01$). Solid lines represent analytical result (eqn (28)) and dotted lines represent numerical results.

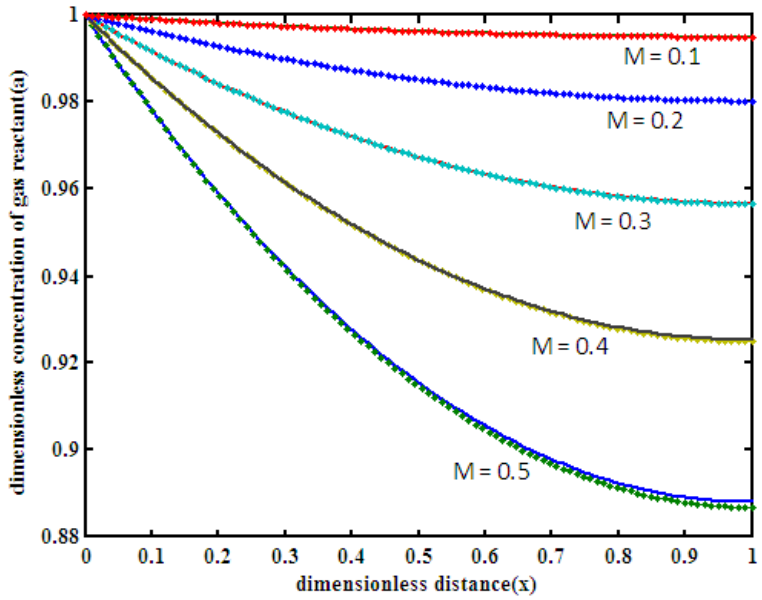

Fig. 4: Dimensionless concentration of gas reactant *a(x)* vesus dimensional distance *x* for various values of M and for fixed value of *rq*=100. Solid lines represent analytical result (eqn (31)) and dotted lines represent numerical results.

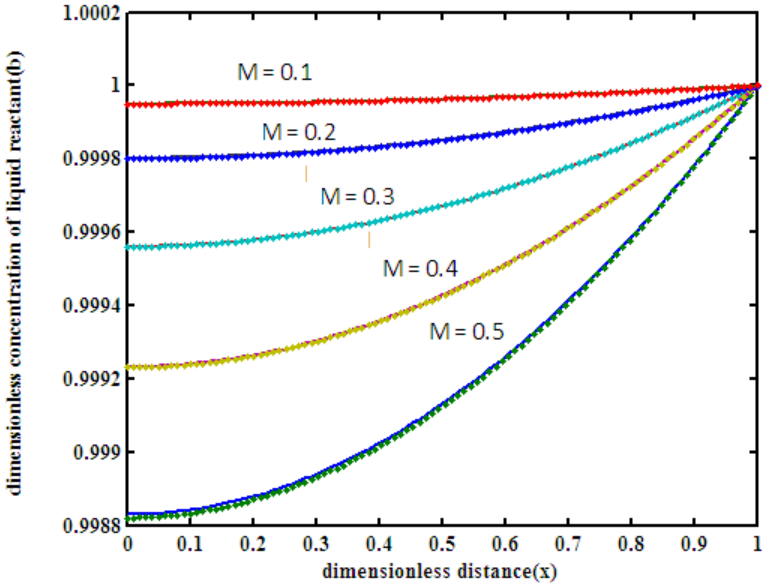

Fig. 5: Dimensionless concentration of liquid reactant *b*(*x*) versus dimensional distance *x* for various values of M and for fixed value of *rq*=100. Solid lines represent analytical result (eqn. (32)) and dotted lines represent numerical results.

Source of support: University Grants Commission (F. no. 39-58/2010 (SR)), New Delhi, India,
Conflict of interest: None Declared

