

APPLICATION OF HOMOTOPY ANALYSIS METHOD AND APPROXIMATE
ANALYTICAL SOLUTION OF NON-LINEAR EQUATION IN CHEMICAL SCIENCE

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ABSTRACT

The analytical solution of the steady state concentrations of carbon dioxide, hydrogen carbonate and carbonate at the gas-liquid phase is discussed. The analytical expression is based on system of reaction diffusion equations containing a non-linear term of the chemical reaction. A simple and closed approximate analytical expression of the steady-state concentrations and effectiveness factor derived for all values of the reaction diffusion parameters. In this paper, Homotopy analysis method is used to solve the system of non-linear differential equations.

Keywords: Absorption, Mass transfer, chemical reactions, interferometry, parametric estimation, Mathematical modelling, Homotopy analysis method.

1. INTRODUCTION

A lot of chemical engineering process is based on chemical reaction between a gas and a component in a liquid phase. It is commonly admitted that the global gas-liquid mass transfer rate is controlled by phenomena occurring in layers close to the gas-liquid interface, especially the coupling between the diffusive transport and the chemical reaction in the liquid phase [1].

Mass transfer is the net movement of mass from one location, usually meaning a stream, phase, fraction or component, to another. Mass transfer occurs in many processes, such as absorption, evaporation, adsorption, drying, precipitation, membrane filtration, and distillation [2-4].

A new experimental tool and an original procedure to study phenomena occurring during the gas-liquid absorption coupled with chemical reactions in the liquid phase. The concentration variation due to the mass absorption and the chemical reaction can modify the refractive index of the liquid. Therefore, digital holographic interferometry can be used to visualize the formation and the development of the diffusion layer during the mass transport in this liquid close to the gas-liquid interface [5]. Overall external mass transfer and pressure drop performance are addressed for a square 2 mm width channel filled with metal foams as catalyst supports for gas-liquid-solid reactions under an applied pulsing regime [6].

Several approaches, such as the two-film theory [6], the penetration theory [7] are presented in the literature to model the global mass transfer rate in a gas-liquid contactor. All these approaches based on mass balance equations in the thin layer of liquid close to the gas-liquid interface. The modelling of the phenomena taking place in the vicinity of the gas-liquid interface when the absorption occurs. As mentioned in Komiya *et al.* [6], one of the key steps in improving the understanding of this phenomenon would be to develop a tool enabling a direct visualization of the absorption at the interface and the reaction diffusion processes in the liquid phase.

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Recently Wylock *et al.* [1] developed a mathematical model for gas-liquid absorption process coupled with chemical reaction in the liquid phase. To the best of our knowledge, till date, no exact analytical solutions of the model have been reported. The purpose of this chapter is to present an analytical expression for the concentrations of carbon dioxide CO_2 , hydrogen carbonate HCO_3^- and carbonate CO_3^{2-} for all possible values of parameters and for short time using Homotopy analysis method.

2. MATHEMATICAL FORMULATION OF THE BOUNDARY VALUE PROBLEM

The reaction scheme for gas-liquid absorption with chemical reactions in the liquid phase can be written as follows:



The diffusion reaction equation in this model can be written in the following form [1]:

$$\frac{\partial[CO_2]}{\partial t} = D_{CO_2} \frac{\partial^2[CO_2]}{\partial x^2} - k_0[CO_2] \frac{[CO_3^{2-}]}{[HCO_3^-]} \tag{2}$$

$$\frac{\partial[HCO_3^-]}{\partial t} = D_{HCO_3^-} \frac{\partial^2[HCO_3^-]}{\partial x^2} + 2k_0[CO_2] \frac{[CO_3^{2-}]}{[HCO_3^-]} \tag{3}$$

$$\frac{\partial[CO_3^{2-}]}{\partial t} = D_{CO_3^{2-}} \frac{\partial^2[CO_3^{2-}]}{\partial x^2} - k_0[CO_2] \frac{[CO_3^{2-}]}{[HCO_3^-]} \tag{4}$$

where CO_2 , HCO_3^- , and CO_3^{2-} are the concentration of carbon dioxide, hydrogen carbonate and carbonate and D_{CO_2} , $D_{HCO_3^-}$ and $D_{CO_3^{2-}}$ are the corresponding diffusion coefficient. k_0 is the kinetic constant. The boundary conditions are,

$$t = 0, [CO_2] = [CO_2]_0, [HCO_3^-] = [HCO_3^-]_0, [CO_3^{2-}] = [CO_3^{2-}]_0 \tag{5}$$

$$x = 0, [CO_2] = n \frac{p_{CO_2}}{RT}, \frac{\partial[HCO_3^-]}{\partial x} = 0, \frac{\partial[CO_3^{2-}]}{\partial x} = 0 \tag{6}$$

$$x \rightarrow \infty, \frac{\partial[CO_2]}{\partial x} = 0, \frac{\partial[HCO_3^-]}{\partial x} = 0, \frac{\partial[CO_3^{2-}]}{\partial x} = 0 \tag{7}$$

where $[CO_2]_0$, $[HCO_3^-]_0$ and $[CO_3^{2-}]_0$ be the initial concentrations, n is the CO_2 solubility, p_{CO_2} is the CO_2 partial pressure in the gaseous phase, R is the perfect gas constant and T is the absolute temperature. Now, using the following dimensionless parameters

$$a = \frac{[CO_2]}{[CO_2]_0}, \quad b = \frac{[HCO_3^-]}{[HCO_3^-]_0}, \quad c = \frac{[CO_3^{2-}]}{[CO_3^{2-}]_0}, \quad X = x \sqrt{\frac{\alpha}{D}}, \tag{8}$$

$$T = \alpha t, \quad \alpha = \frac{1}{s} [CO_2][CO_3^{2-}], \quad k_1 = \frac{k_0[HCO_3^-]}{\alpha[CO_3^{2-}]}$$

We get the dimensionless non-linear reaction diffusion equations for the concentration as follows:

$$\frac{\partial a}{\partial T} = \frac{\partial^2 a}{\partial X^2} - k_1 \frac{ac}{b} \tag{9}$$

$$\frac{\partial b}{\partial T} = \frac{\partial^2 b}{\partial X^2} + 2k_1 \frac{ac}{b} \tag{10}$$

$$\frac{\partial c}{\partial T} = \frac{\partial^2 c}{\partial X^2} - k_1 \frac{ac}{b} \tag{11}$$

where, a , b and c are the dimensionless concentration of carbon dioxide CO_2 , hydrogen carbonate HCO_3^- and carbonate CO_3^{2-} , k_1 is the dimensionless rate constant. The initial and boundary conditions are represented as follows:

$$T = 0, a = 1, b = 1, c = 1 \tag{12}$$

$$X = 0, \quad a = l, \quad \frac{\partial b}{\partial X} = 0, \quad \frac{\partial c}{\partial X} = 0 \tag{13}$$

$$X \rightarrow \infty, \quad \frac{\partial a}{\partial X} = 0, \quad \frac{\partial b}{\partial X} = 0, \quad \frac{\partial c}{\partial X} = 0 \tag{14}$$

3. ANALYTICAL SOLUTIONS OF THE PROBLEM USING HOMOTOPY ANALYSIS METHOD

Liao [9-11] proposed a powerful analytical method for solving the nonlinear problems, namely the Homotopy analysis method. Different from all perturbation and non-perturbation techniques, the Homotopy analysis method [12-14] itself provides us with a convenient way to control and adjust the convergence region and rate of approximation series, when necessary. Briefly speaking, the Homotopy analysis method has the following advantages: It is valid even if a given nonlinear problem does not contain any small/large parameters at all; it can be employed to efficiently approximate a nonlinear problem by choosing different sets of base functions.

Now, more and more researchers have been successfully applying this method to various nonlinear problems in science and engineering. In this paper we apply HAM to solve the nonlinear differential equations (Eqns. (9) - (11)). The basic concept of Homotopy analysis method is given in Appendix A. By solving the equations (9) - (11), using Homotopy analysis method (see Appendix B) we can obtain the following new approximate expression for the concentrations as follows:

$$a(X, s) = 1 + (l-1)erfc\left(\frac{X}{2\sqrt{t}}\right) - hk_1 \left[\left(\frac{x^2}{2} + t\right)erfc\left(\frac{X}{2\sqrt{t}}\right) - X\sqrt{\frac{t}{\pi}}e^{-X^2/4t} \right] + hk_1 t + \frac{hk_1(l_1-1)}{2} \left[2\sqrt{\frac{t}{\pi}}e^{-\frac{X^2}{4t}} - Xerfc\left(\frac{X}{2\sqrt{t}}\right) \right] X \tag{15}$$

$$b(X, s) = 1 - 2hk_1 t - hk_1(l-1) \left[\left(t + \frac{X^2}{2}\right)erfc\left(\frac{X}{2\sqrt{t}}\right) - X\sqrt{\frac{t}{\pi}}e^{-X^2/4t} \right] - hk_1(l-1)X \left[2\sqrt{\frac{t}{\pi}}e^{-X^2/4t} - Xerfc\left(\frac{X}{2\sqrt{t}}\right) \right] \tag{16}$$

$$c(X, s) = l \left[2\sqrt{\frac{T}{\pi}}e^{-X^2/4T} - Xerfc\left(\frac{X}{2\sqrt{T}}\right) \right] - \frac{hk_1 l}{2} \left[\frac{1}{3}\sqrt{\frac{T}{\pi}}e^{-X^2/4T} (4T + X^2) - \frac{1}{6}(6TX + X^3)erfc\left(\frac{X}{2\sqrt{T}}\right) \right] + hk_1 T - \frac{hk_1 l X}{2} \left[\left(\frac{X^2}{2} + T\right)erfc\left(\frac{X}{2\sqrt{T}}\right) - X\sqrt{\frac{T}{\pi}}e^{-X^2/4T} \right] \tag{17}$$

The analytical expression represented by Eqns. (9) - (11) contains the auxiliary parameters *h*, which gives the convergence region and the rate of approximation for HAM. The auxiliary parameter *h* controls the convergence and accuracy of the solution series [15]. The parameter *h* ∈ [-1, 1], throughout this chapter we choose *h* = -1, to show the accuracy of solution and it gives better results.

4. RESULTS AND DISCUSSION

Equations (9)-(11) are the new approximate analytical expression of dimensionless concentration of carbon dioxide CO₂, hydrogen carbonate HCO₃⁻ and carbonate CO₃²⁻ for all values of the dimensionless parameters *k*₁, *l* and *π*. It satisfies the initial condition Eqn. (12) - (14).

Fig. (1-2) represents the dimensionless concentration of CO_2 versus depth in the liquid from the interface X for all values of dimensionless rate constants k_1, l and π . From Fig. 1, it is inferred that the concentration of CO_2 decreases when k_1 increases. Fig. 2 shows that concentration of CO_2 increases when interfacial concentration of carbon dioxide in the liquid face l is increases.

Fig. (3-4) shows that the dimensionless concentration of HCO_3^- versus depth in the liquid from the interface X for various values of parameters. From this figures we can see that the concentration of HCO_3^- gradually increases when interfacial concentration of carbon dioxide l and k_1 increases.

Fig. (5-6) shows that the dimensionless concentration of CO_3^{2-} versus depth in the liquid from the interface X for various values of parameters. From this figures we can see that the concentration of CO_3^{2-} gradually decreases when l and k_1 increases.

5. CONCLUSIONS

In this chapter, the system of time dependent non-linear differential equations in gas-liquid absorption process has been solved analytically using homotopy analysis method. We have presented an approximate analytical expression of the concentrations for various values of the dimensionless parameters k_1, π and l for steady state conditions. This analytical result presented in this chapter is useful for the optimization of parameters and validation of the experimental result. This work can be easily extended to find the solution for other non-linear systems in gas-liquid absorption process for various complex boundary conditions.

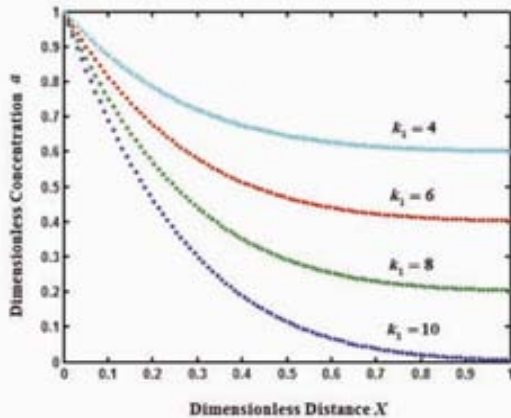


Fig. 1 Plot of the dimensionless concentration of carbon dioxide CO_2 (a) versus the depth in the liquid from the interface X . The concentrations were computed using Eq. (14) for various values of k_1 and the parameter $l = 1$.

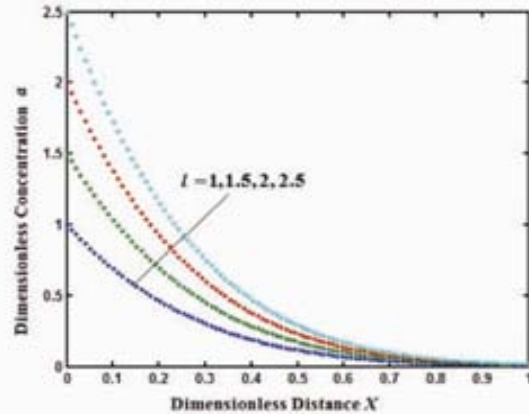


Fig. 2 Plot of the dimensionless concentration of carbon dioxide CO_2 (a) versus the depth in the liquid from the interface X . The concentrations were computed using Eq. (14) for various values of l and the parameters $k_1 = 10$.

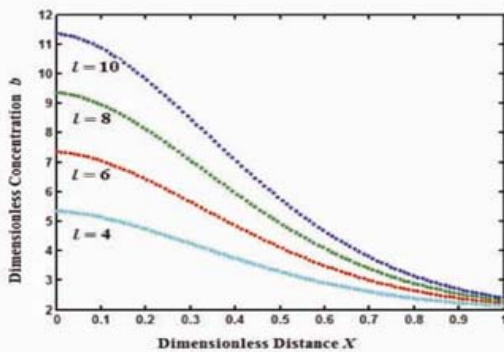


Fig. 3 Plot of the dimensionless concentration of hydrogen carbonate HCO_3^- (b) versus the depth in the liquid from the interface X . The concentrations were computed using Eq.(15) for various values of l and the parameters $k_1 = 10$.

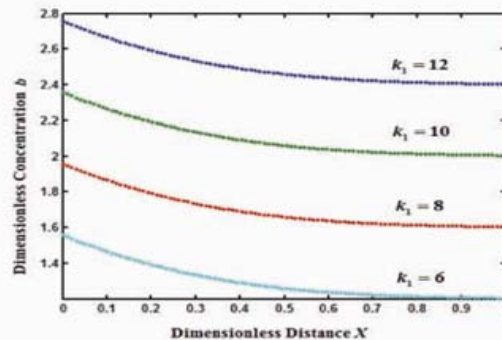


Fig. 4 Plot of the dimensionless concentration of hydrogen carbonate HCO_3^- (b) versus the depth in the liquid from the interface X . The concentrations were computed using Eq. (15) for various values of l and the parameters $k_1 = 10$.

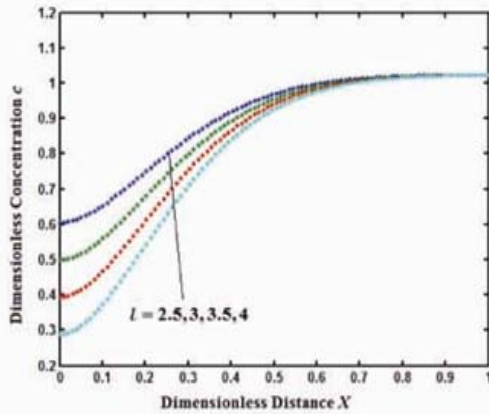


Fig. 5 Plot of the dimensionless concentration of carbonate CO_3^{2-} (c) versus the depth in the liquid from the interface X. The concentrations were computed using Eq. (16) for various values of l and the parameters $k_l=10$

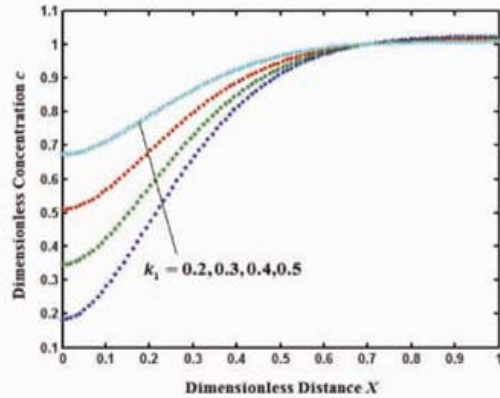


Fig. 6 Plot of the dimensionless concentration of carbonate CO_3^{2-} (c) versus the depth in the liquid from the interface X. The concentrations were computed using Eq. (16) for various values of k_l and the parameters $l=1$.

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