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Homotopy Analysis Method to Determine The Concentration Profile of Carbon Dioxide and Two Reactants In Stirred Semi-Batch Tank With a Planar Gas-Liquid

KEYWORDS: absorption, carbon dioxide, homotopy analysis method, mathematical modeling, non-linear boundary value problem

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ABSTRACT *In this work, the mathematical model of the absorption of carbon dioxide into an aqueous solution containing two reactants of 2-amino-2-methyl-1-propanol (AMP) and 1,8-diamino-p-menthane (DAM) in a stirred semi-batch tank with a planar gas-liquid interface has been discussed. This model contains system of non-linear equations. Homotopy analysis method (HAM) is employed to evaluate the concentration of species by solving these non-linear equations. The analytical results are compared with numerical solutions and satisfactory agreement is noted.*

INTRODUCTION

Carbon dioxide (CO_2) is the primary greenhouse gas emitted through human activities. The main human activity that emits CO_2 is the combustion of fossil fuels (coal, natural gas, and oil) for energy and transportation, although certain industrial processes and land-use changes also emit carbon dioxide. Aqueous alkanolamine solutions are frequently used for removal of acidic gases such as carbon dioxide and hydrogen sulfide from gas streams in the natural gas, synthetic, and refinery industries. Industrially important chemical absorbents are alkanolamines [1]. The absorption of CO_2 by solutions of alkanolamines is an operation of such industrial importance that the mechanism and kinetics of the reactions between carbon dioxide, and these alkanolamines are of considerable interest [2]. Utilizing the advantages of each amine, the blended amines have been suggested to be useful in the absorption of acid gases [3]. Hagewiesche et al. [4] investigated the absorption of carbon dioxide into aqueous blends of monoethanolamine and N-methyldiethanolamine.

The reaction kinetics of the absorption of CO_2 into aqueous solutions of piperazine and into mixed aqueous solutions of 2-amino-2-methyl-l-propanol has been investigated by Sun et al. [5]. The absorption of carbon dioxide into piperazine activated aqueous 2-amino-2-methyl-1-propanol solutions has been studied experimentally and theoretically at various temperatures [6]. Puxty et al. [7] measured CO_2 absorption rate into aqueous ammonia as a thin film using a wetted-wall column and compared to monoethanolamine. Kinetics of absorption of carbondioxide into aqueous solution of 2-(1-piperazinyl)-ethylamine has been discussed by Paul et al. [8]. Yu et al. [9] studied the kinetics of the reaction of carbon dioxide in methyldiethanolamine solutions both experimentally and theoretically. Many studies have been done on the mechanisms and kinetics of the reaction of CO_2 with various alkanolamines [10-12].

To the best of our knowledge, no rigorous analytical expression for the absorption of carbon dioxide into an aqueous solution has been reported [13]. In this work, we derive the concentration of species using homotopy analysis method.

MATHEMATICAL FORMULATION OF THE BOUNDARY VALUE PROBLEM

The Zwitterion reaction mechanism in the absorption of CO_2 into aqueous AMP (RNH2) as follows [13]:

$$CO_2+RNH_2=RN^+H_2COO^- \quad \text{(i)}$$

$$RN^+H_2COO^-+H_2O\rightarrow RNH_3^+ +HCO_3^- \quad \text{(ii)}$$

With overall reaction being:

$$CO_2+RNH_2+H_2O\rightarrow RNH_3^+ +HCO_3^- \quad \text{(iii)}$$

And reactions in the absorption of CO_2 into aqueous DAM (H_2NRNH_2) are as follows:

$$CO_2+H_2NRNH_2=H_2NRN^+H_2COO^- \quad \text{(iv)}$$

$$CO_2+H_2NRN^+H_2COO^-=O^-OCH_2N^+RN^+H_2COO^- \quad \text{(v)}$$

$$O^-OCH_2NRN^+H_2COO^-+2H_2O=H_3N^+RN^+H_3+2HCO_3^- \quad \text{(vi)}$$

Overall reaction being:

$$2CO_2+H_2NRNH_2+2H_2O\rightarrow O^-OCHNRNH_2COO^-+H_3N^+RN^+H_3 \quad \text{(vii)}$$

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The irreversible reactions between CO_2 and the reactant (C), as shown in reactions (iii) and (vii) may be formulated as follows:

$A + \nu_1 B_1 + \nu_2 B_2 \rightarrow$ products (viii)

where A, B1 and B2 represents CO_2, AMP, and DAM respectively. v_1 and v_2 are 1 and 0.5 respectively. The mass balance equations are given as follows [13, 14, 15]:

$$D_A \frac{d^2 C_A(z)}{dz^2} = k_1 C_A(z) C_{B1}(z) + k_2 C_A(z) C_{B2}(z) \quad (1)$$

$$D_{B1} \frac{d^2 C_{B1}(z)}{dz^2} = \nu_1 k_1 C_A(z) C_{B1}(z) \quad (2)$$

$$D_{B2} \frac{d^2 C_{B2}(z)}{dz^2} = \nu_2 k_2 C_A(z) C_{B2}(z) \quad (3)$$

where C_A, C_{B1}, and C_{B2} are the concentration of carbon dioxide, 2-amino-2-methyl-1-propanol and 1, 8-diamino-p-menthane respectively. D_A, D_{B1} and D_{B2} are the diffusivity of carbon dioxide, APM and DAM respectively. k_j is the reaction rate constant of species, j and ν_j is the stoichiometric coefficients of species, j. The boundary conditions are

$$z = 0;\ C_A = C_{Ai};\ C_{B1} = C_{B1i};\ C_{B2} = C_{B2i} \quad (4)$$

$$z = \delta;\ C_A = 0;\ C_{B1} = C_{B10};\ C_{B2} = C_{B20} \quad (5)$$

where C_{Ai}, C_{B1i} and C_{B2i} are the solubility of carbon dioxide, APM and DAM respectively. z is the diffusion coordinate of gas and δ is the thickness of diffusion film. The molar flux of A is defined as given below:

$$N_A = -D_A \left.\frac{dC_A}{dz}\right|_{z=0} \quad (6)$$

where N_A is the molar flux of carbon dioxide. By introducing the following dimensionless parameters

$$X = \frac{z}{\delta};\ U = \frac{C_A}{C_{Ai}};\ V = \frac{C_{B1}}{C_{B1i}};\ W = \frac{C_{B2}}{C_{B2i}} \quad (7)$$

$$\alpha = \frac{\delta^2 k_1 C_{B1i}}{D_A};\ \beta = \frac{\delta^2 k_2 C_{B2i}}{D_A};\ \gamma = \frac{\delta^2 k_1 C_{Ai}}{D_{B1}};\ \mu = \frac{\delta^2 k_2 C_{Ai}}{D_{B2}} \quad (8)$$

the differential equations (Eqs.(1)-(3)) with the boundary conditions in the dimensionless form is given below:

$$\frac{d^2 U(X)}{dX^2} = \alpha\, U(X)\, V(X) + \beta\, U(X)\, W(X) \quad (9)$$

$$\frac{d^2 V(X)}{dX^2} = \nu_1 \gamma\, U(X)\, V(X) \quad (10)$$

$$\frac{d^2 W(X)}{dX^2} = \nu_2\, \mu\, U(X)\, W(X) \quad (11)$$

$$X = 0:\ U = 1;\ \ V = 1;\ \ W = 1 \quad (12)$$

$$X = 1:\ U = 0;\ V = \frac{C_{B10}}{C_{B1i}} = k;\ W = \frac{C_{B20}}{C_{B2i}} = c \quad (13)$$

The dimensionless flux is

$$\psi = -\frac{D_A C_{Ai}}{\delta} \left.\frac{dU}{dX}\right|_{X=0} \quad (14)$$

APPROXIMATION OF ANALYTICAL EXPRESSION

HOMOTOPY ANALYSIS METHOD (HAM):

The HAM was devised by Shijun Liao [16-21] which is a powerful analytical method for solving nonlinear problems. The greater generality of this method often allows for strong convergence of the solution over larger spacial and parameter domains. This method provides an analytical solution in terms of an infinite power series.

The homotopy analysis method [22] is a good technique comparing to another perturbation method. The HAM gives excellent flexibility in the expression of the solution and how the solution is explicitly obtained. Different from all reported perturbation and

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non perturbative techniques, the homotopy analysis method 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 parameter at all; it can be employed to efficiently approximate a nonlinear problem by choosing different sets of base functions. In this paper we employ HAM (see Appendix A) to solve the nonlinear equations (9)-(11).

ANALYTICAL EXPRESSION FOR THE CONCENTRATIONS OF CARBON DIOXIDE, 2-AMINO-2-METHYL-1-PROPANOL AND 1, 8-DIAMINO-P-MENTHANE:

Using HAM, we can obtain the dimensionless concentration of species (see Appendix B) as follows:

$$U(X) = 1 - \left[1 - \frac{h}{12}\left(\alpha(k+3) + \beta(c+3)\right)\right]X - h\left[\frac{(\alpha+\beta)}{2}X^2 + \frac{\left(\alpha(k-2)+\beta(c-2)\right)}{6}X^3 - \frac{\left(\alpha(k-1)+\beta(c-1)\right)}{12}X^4\right] \quad (15)$$

$$V(X) = 1 - \left(1 - k - \frac{hv_1\gamma(k+3)}{12}\right)X - hv_1\gamma\left[\frac{X^2}{2} + \frac{(k-2)}{6}X^3 - \frac{(k-1)}{12}X^4\right] \quad (16)$$

$$W(X) = 1 - \left(1 - c - \frac{hv_2\mu(c+3)}{12}\right)X - hv_2\mu\left[\frac{X^2}{2} + \frac{(c-2)}{6}X^3 - \frac{(c-1)}{12}X^4\right] \quad (17)$$

DETERMINATION OF MOLAR FLUX:

The dimensionless molar flux is

$$\psi = \frac{D_A C_{Ai}}{\delta}\left[1 - \frac{h}{12}\left(\alpha(k+3) + \beta(c+3)\right)\right] \quad (18)$$

NUMERICAL SIMULATION

The diffusion equations (Eqs.(9)-(11)) for the boundary conditions (Eqs. (12) and (13)) are solved by numerical methods. The function pdex4 in Mat lab software, which is a function of solving boundary value problems for partial differential equations, is used to solve these non-linear equations. Numerical solution obtained from this function is compared with the analytical results which are depicted in Figs.1-3. Satisfactory agreement is noted. The corresponding Mat lab program is made available in Appendix D

DISCUSSION

Eqs. (15) - (17) represent the approximate analytical expression of steady state concentration of carbon dioxide, 2-amino-2-methyl-1-propanol and 1, 8-diamino-p-menthane. The molar flux of carbon dioxide is calculated using the gradient concentration of carbon dioxide as shown in Eq. (23). Figs. 1-4 represent the comparison between our analytical results (Eqs. (15) - (17)) and the numerical results.

Fig.1(a) shows the plot of dimensionless concentration of carbon dioxide U versus dimensionless diffusion coordinate of gas X using Eq. (15). From this figure, it is evident that when the dimensionless parameter $\alpha \geq 0.5$ (i.e. the reaction rate constant of CO_2 increases) and small value of $\beta \leq 0.01$, the concentration U depends on the dimensionless diffusion coordinate of gas X. In Fig.1(b), plot of dimensionless concentration of 2-amino-2-methyl-1-propanol V versus dimensionless diffusion coordinate of gas X using Eq. (16). For small value of stoichiometric coefficients $v_1 = 0.01$, it is clear that the concentration decreases when γ increases. Fig.1(c) represents the plot of dimensionless concentration of 1, 8-diamino-p-menthane W versus dimensionless diffusion coordinate of gas X using Eq. (17). For small value

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of reaction rate constant $v_2 \le 0.01$, it is clear that the concentration is uniform. Fig.2(a) shows the plot of dimensionless concentration of carbon dioxide U versus dimensionless diffusion coordinate of gas X using Eq. (15). From this figure, it is evident that for the increasing values of thickness of diffusion film (or) the reaction rate constant of CO_2 and large value of reaction rate constant $\beta \ge 5$, the concentration U remains the same. In Fig.2(b), plot of dimensionless concentration of 2-amino-2-methyl-1-propanol V versus dimensionless diffusion coordinate of gas X using Eq. (16). For large value of stoichiometric coefficients ($v_1 \ge 5$), it is clear that the concentration decreases when γ increases. Fig.2(c) represents the plot of dimensionless concentration of 1, 8-diamino-p-menthane W versus dimensionless diffusion coordinate of gas X using Eq. (17). For large value of reaction rate constant $\mu \ge 5$, it is clear that the concentration decreases when v_2 increases.

Fig.3(a) shows the plot of dimensionless concentration of carbon dioxide U versus dimensionless diffusion coordinate of gas X using Eq. (15). From this figure, it is evident that for the increasing values of thickness of diffusion film α (or) the reaction rate constant of CO_2 and large value of reaction rate constant $\beta \ge 10$, the concentration U deviates from the linear form. In Fig.3(b), plot of dimensionless concentration of 2-amino-2-methyl-1-propanol V versus dimensionless diffusion coordinate of gas X using Eq. (16). For small value of stoichiometric coefficients $v_1 \le 10$, it is clear that the concentration decreases when γ increases. In Fig.3(c) represents the plot of dimensionless concentration of 1, 8-diamino-p-menthane W versus dimensionless diffusion coordinate of gas X using Eq. (17). For small value of reaction rate constant $\mu \ge 10$, it is clear that the concentration decreases when v_2 increases. Fig.4(a)-(b) illustrates the dimensionless parameter α versus dimensionless molar flux ψ using Eq. (18). From these figures, the flux increases for increasing reaction rate constant α. Fig.4(c)-(d) represents the dimensionless parameter β versus dimensionless molar flux ψ using Eq. (18). From these figures, the flux increases for increasing thickness of diffusion film or decreasing diffusion D_A.

CONCLUSION

The absorption of carbon dioxide into an aqueous solution containing two reactants of 2-amino-2-methyl-1-propanol (AMP) and 1,8- diamino-p-menthane (DAM) was studied theoretically. The approximate analytical expression for the concentration of carbon dioxide, 2-amino-2-methyl-1-propanol and 1, 8-diamino-p-menthane was obtained using homotopy analysis method. A satisfactory agreement with the numerical result is noted. Furthermore, we have also presented a closed form expression for the molar flux.

Appendix A

Basic idea of Liao's [15] Homotopy analysis method

Consider the following differential equation [23]:

$$N[u(t)] = 0 \qquad \text{(A1)}$$

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:

$$(1-p)\,L[\varphi(t;p) - u_0(t)] = p\,h\,H(t)\,N[\varphi(t;p)] \qquad \text{(A2)}$$

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where $p \in [0,1]$ is the embedding parameter, $h \neq 0$ is a nonzero auxiliary parameter, $H(t) \neq 0$ is an auxiliary function, L is an auxiliary linear operator, $u_0(t)$ is an initial guess of $u(t)$ and $\varphi(t:p)$ 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:

$$\varphi(t;0) = u_0(t) \text{ and } \varphi(t;1) = u(t) \quad \text{(A3)}$$

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

$$\varphi(t;p) = u_0(t) + \sum_{m=1}^{+\infty} u_m(t) p^m \quad \text{(A4)}$$

where

$$u_m(t) = \frac{1}{m!} \frac{\partial^m \varphi(t;p)}{\partial p^m} |_{p=0} \quad \text{(A5)}$$

If the auxiliary linear operator, the initial guess, the auxiliary parameter h, and the auxiliary function are so properly chosen, the series Eq. (A4) converges at p =1 then we have:

$$u(t) = u_0(t) + \sum_{m=1}^{+\infty} u_m(t). \quad \text{(A6)}$$

Define the vector

$$\vec{u}_n = \{u_0, u_1, ..., u_n\} \quad \text{(A7)}$$

Differentiating Eq. (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 m^{th}-order deformation equation as:

$$L[u_m - \chi_m u_{m-1}] = h H(t) \Re_m(\vec{u}_{m-1}) \quad \text{(A8)}$$

where

$$\Re_m(\vec{u}_{m-1}) = \frac{1}{(m-1)!} \frac{\partial^{m-1} N[\varphi(t;p)]}{\partial p^{m-1}} |_{p=0} \quad \text{(A9)}$$

and

$$\chi_m = \begin{cases} 0, & m \leq 1, \\ 1, & m > 1. \end{cases} \quad \text{(A10)}$$

Applying L^{-1} on both side of equation (A8), we get

$$u_m(t) = \chi_m u_{m-1}(t) + hL^{-1}[H(t)\Re_m(\vec{u}_{m-1})] \quad \text{(A11)}$$

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

$$u(t) = \sum_{m=0}^{M} u_m(t)$$

When $M \to +\infty$, we get an accurate approximation of the original equation (A1). For the convergence of the above method we refer the reader to Liao [23]. If equation (A1) admits unique solution, then this method will produce the unique solution. If equation (A1) does not possess unique solution, the HAM will give a solution among many other (possible) solutions.

Appendix B

Solution of Eq. (9) using Homotopy analysis method

In this appendix, we indicate how the solution of Eq. (9) in this paper is derived. The Homotopy analysis method was constructed to determine the solution of Eqs. (9) as follows:

$$\frac{d^2U}{dX^2} = \alpha UV + \beta UW \quad \text{(B1)}$$

In order to solve Eq. (B1) by means of the HAM, we first construct the zeroth-order deformation equation by taking H(t) = 1.

$$(1-p)\left[\frac{d^2U}{dX^2}\right] = ph\left[\frac{d^2U}{dX^2} - \alpha UV - \beta UW\right] \quad \text{(B2)}$$

The approximate solutions of Eq. (B2) is as follows

$$U = U_0 + pU_1 + pU_2 + ... \quad \text{(B3)}$$

Substituting Eq. (B3) into Eq. (B1) and comparing the coefficients of like powers of p, we get

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$$p^0 : \frac{d^2U_0}{dX^2} = 0 \qquad \text{(B4)}$$

$$p^1 : \frac{d^2U_1}{dX^2} - \frac{d^2U_0}{dX^2} = h\left[\frac{d^2U_0}{dX^2} - \alpha U_0 V_0 - \beta U_0 W_0\right] \qquad \text{(B5)}$$

$$p^2 : \frac{d^2U_2}{dX^2} - \frac{d^2U_1}{dX^2} = h\left[\frac{d^2U_1}{dX^2} - \alpha U_0 V_1 - \alpha U_1 V_0 - \beta U_0 W_1 - \beta U_1 W_0\right] \qquad \text{(B6)}$$

The boundary conditions are

$U_0 = 1$ when $X = 0$ and $U_0 = 0$ when $X = 1$ (B7)

$U_i = 0$ when $X = 0$ and $U_i = 0$ when $X = 1$ for all $i = 1,2,3,\ldots$ (B8)

Now applying the boundary conditions (B7) in (B4) we get

$$U_0(X) = 1 - X \qquad \text{(B9)}$$

Substituting the value of U_0 in Eq. (B5) and solving the equation using the boundary conditions (B8) we obtain the following results:

$$U_1(X) = -h\left[\frac{(\alpha(k+3)+\beta(c+3))}{12}X + \frac{(\alpha+\beta)}{2}X^2 + \frac{(\alpha(k-2)+\beta(c-2))}{6}X^3 - \frac{(\alpha(k-1)+\beta(c-1))}{12}X^4\right] \qquad \text{(B10)}$$

Upon solving the Eq. (B6) by substituting the values of $U_0(X)$ and $U_1(X)$, and using the boundary conditions Eq. (B8), we can find the results for $U_2(X)$.

After three successive iterations the solutions of $U(X)$ reach the better approximation. By adding, we get Eq. (9) in the text. Similarly we can solve Eq. (10) and Eq. (11) by using homotopy analysis method.

Appendix C

Determining the region of *h* for validity

The analytical solution should converge. It should be noted that the auxiliary parameter h controls the convergence and accuracy of the solution series. The analytical solution represented by Eqs. (15) - (17) contains the auxiliary parameter h, which gives the convergence region and rate of approximation for the Homotopy analysis method. In order to define region such that the solution series is independent of h, a multiple of h curves are plotted. The region where the dimensionless concentration of species j ($j = U(X), V(X)$ and $W(X)$) and gradient ($U'(X), V'(X)$ and $W'(X)$) versus h is a horizontal line known as the convergence region for the corresponding function. The common region among concentration of species j and its derivatives are known as the overall convergence region. To study the influence of h on the convergence of solution, h- curves of concentration of species j and gradient of species j are plotted in Fig. (5) respectively. These figures clearly indicate that the valid region of h is about (-0.6 to -0.5). Similarly we can find the value of the convergence control parameter h for different values of the constant parameters.

Appendix D

The Matlab code to find the numerical simulation of Eqs. (9)-(11) is as follows:

```
function pdex4
m = 0;
x = linspace(0,1);
t=linspace(0,100000);
```

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```
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('u3(x,t)')
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;
 alpha=0.01 ; beta=10 ; v1=10; v2=0.01 ;
gamma=0.01 ; mu=10 ;
 F1 = -alpha*u(1)*u(2)-beta*u(1)*u(3);
 F2 = -v1*gamma*u(1)*u(2);
 F3= -v2*mu*u(1)*u(3);
 s=[F1; F2; F3];
% ----------------------------------------------------------------
function u0 = pdex4ic(x) %create a initial conditions
u0 = [0; 0; 0];
% ----------------------------------------------------------------
function [pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t) %create a
boundary conditions
k=1 ; c=1;
pl = [ul(1)-1; ul(2)-1; ul(3)-1];
ql = [0; 0; 0];
pr = [ur(1)-0; ur(2)-k; ur(3)-c];
qr = [0; 0; 0];
```

Nomenclature

C_A	Concentration of carbon dioxide (kmol/m^3)
C_{B1}	Concentration of 2-amino-2-methyl-1-propanol (kmol/m^3)
C_{B2}	Concentration of 1, 8-diamino-p-menthane (kmol/m^3)
C_{B1i}	Solubility of 2-amino-2-methyl-1-propanol (kmol/m^3)
C_{B2i}	Solubility of 1, 8-diamino-p-menthane (kmol/m^3)
D_A	Diffusivity of carbon dioxide (m^2/s)
D_{B1}	Diffusivity of 2-amino-2-methyl-1-propanol (m^2/s)
D_{B2}	Diffusivity of 1, 8-diamino-p-menthane (m^2/s)
k_j	Reaction rate constant of species, j (m^3/kmol·s)
v_j	Stoichiometric coefficients of species, j (none)
N_A	Molar flux of carbon dioxide (kg mol/m^2.s)
z	Diffusion coordinate of gas (m)
δ	Thickness of diffusion film (m)
U	Dimensionless concentration of carbon dioxide (none)
V	Dimensionless concentration of 2-amino-2-methyl-1-propanol (none)
W	Dimensionless concentration of 1, 8-diamino-p-menthane (none)
ψ	Dimensionless molar flux of carbon dioxide (none)
X	Dimensionless diffusion coordinate of gas (none)
$\alpha = \frac{\delta^2 k_1 C_{B1i}}{D_A}$	Dimensionless parameter (none)
$\beta = \frac{\delta^2 k_2 C_{B2i}}{D_A}$	Dimensionless parameter (none)
$\gamma = \frac{\delta^2 k_1 C_{Ai}}{D_{B1}}$	Dimensionless parameter (none)

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Subscripts

A: CO_2

B1: AMP

B2: DAM

j: species

Figures

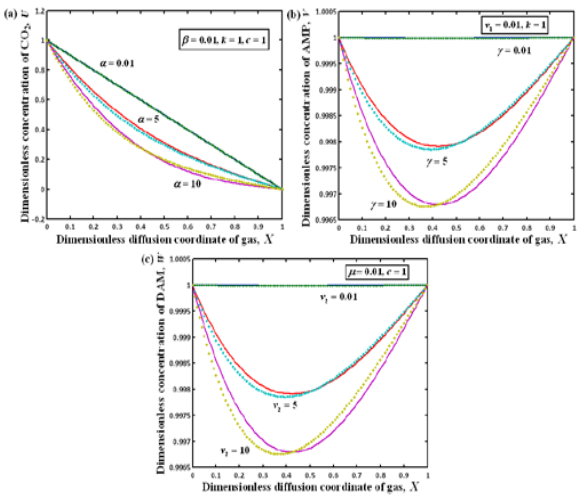

Fig. 1. Plot of dimensionless concentration of species j ($j = U, V$ and W) versus dimensionless distance X. The concentrations were computed for various values of the dimensionless parameters α, γ and v_2 when (a) $\beta = 0.01$, $k = 1$, $c = 1$ (b) $v_1 = 0.01$, $k = 1$ and (c) $\mu = 0.01$, $c = 1$ respectively. The curves are plotted using Eq. (15). (—) denotes the analytical results and (• • •) denotes the numerical simulations.

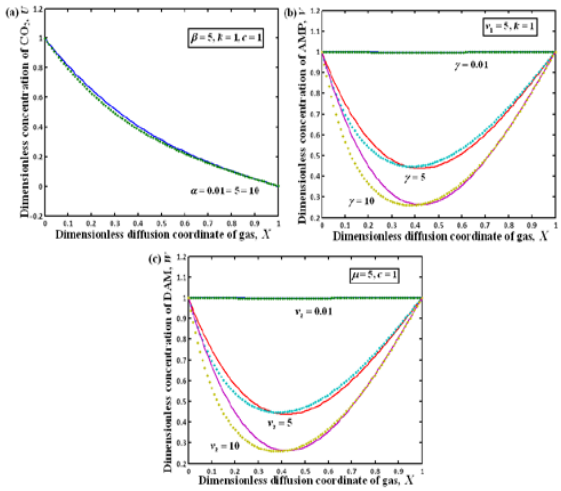

Fig. 2. Plot of dimensionless concentration of species j ($j = U, V$ and W) versus dimensionless distance X. The concentrations were computed for various values of the dimensionless parameters α, γ and v_2 when (a) $\beta = 5$, $k = 1$, $c = 1$ (b) $v_1 = 5$, $k = 1$ and (c) $\mu = 5$, $c = 1$ respectively. The curves are plotted using Eq. (16). (—) denotes the analytical results and (• • •) denotes the numerical simulations.

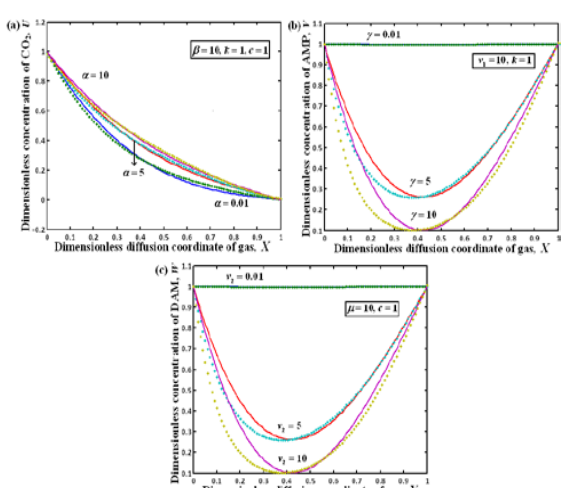

Fig. 3. Plot of dimensionless concentration of species j ($j = U, V$ and W) versus dimensionless distance X. The concentrations were computed for various values of the dimensionless parameters α, γ and v_2

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when (a) $\beta = 10,\ k = 1,\ c = 1$ (b) $v_1 = 10,\ k = 1$ and (c) $\mu = 10,\ c = 1$ respectively. The curves are plotted using Eq. (17). (—) denotes the analytical results and (• • •) denotes the numerical simulations.

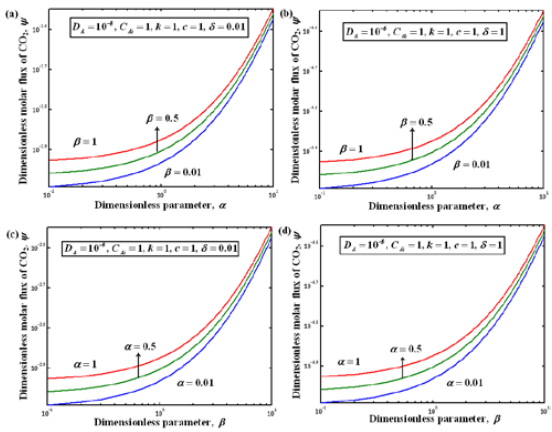

Fig. 4. Plot of the dimensionless molar flux ψ versus dimensionless parameters α and β. The dimensionless molar flux ψ were computed using Eq. (18) when (a) $D_A = 10^{-5},\ C_{Ai} = 1,\ k = 1,\ c = 1,\ \delta = 0.01$ (b) $D_A = 10^{-5},\ C_{Ai} = 1, k = 1, c = 1, \delta = 1$ (c) $D_A = 10^{-5},\ C_{Ai} = 1,\ k = 1,\ c = 1, \delta = 0.01$ and (d) $D_A = 10^{-5},\ C_{Ai} = 1, k = 1, c = 1, \delta = 1$ for various values of dimensionless parameters β and α.

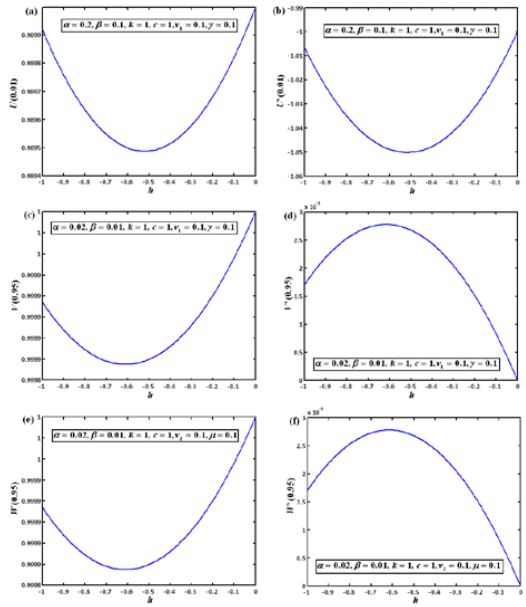

Fig. 5. The h curves to indicate the convergence region for concentration of species j.

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