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Theoretical Analysis of Mass Transfer with Chemical Reaction Using Absorption of Carbon Dioxide into Phenyl Glycidyl Ether Solution

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ABSTRACT

Theoretical analysis corresponding to the diffusion and reaction kinetics in a chemical reaction between carbon dioxide and phenyl glycidyl ether solution is presented. Analytical expressions pertaining to the concentration of carbon dioxide (CO_2), phenyl glycidyl ether solution (PGE) and flux are obtained in terms of reaction rate constants. In this paper, a powerful analytical method, called the Adomian decomposition method (ADM) is used to obtain approximate analytical solutions for nonlinear differential equations. Furthermore, in this work the numerical simulation of the problem is also reported using Scilab/Matlab program. An agreement between analytical and numerical results is noted.

Keywords: Carbon Dioxide; Phenyl Glycidyl Ether Solution; Nonlinear Differential Equations; Adomian Decomposition Method; Boundary Value Problems

1. Introduction

Carbon dioxide is generally a useful gas that is made up of a carbon atom and two oxygen atoms. It is very important in plant photosynthesis, manufacturing carbonated soft drinks, powering pneumatic systems in robots, used in fire extinguisher, removing caffeine from coffee, etc., Carbon dioxide has the potential to provide a vast and cheap source of carbon. Turning it into useful products would also reduce its environmental impact as a greenhouse gas. Scientists have shown that ionic liquids are selective catalysts for converting carbon dioxide into synthetic intermediates called cyclic carbonates, but it is difficult to separate and recycle the liquid catalyst.

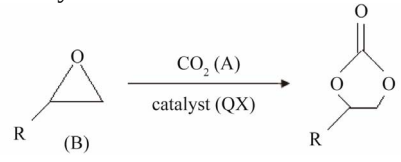
Recently, the chemical fixation of carbon dioxide has become an important research topic [1], because of the danger posed by global warming, and conversion of carbon dioxide into valuable substances is an extremely attractive solution. The reaction with oxiranes leading to five-membered cyclic carbonate (oxirane-reaction) is well-known among many examples [2,3]. These carbonates can be used as aprotic polar solvent and sources for polymer synthesis [4]. In the oxirane-reaction, high pressure (5 - 50 atm) of CO_2 has been thought to be necessary [2]. The oxirane—reactions under atmospheric pressure have been reported [4].

Many organic and inorganic compounds including ammines, phosphines, quaternary ammonium salts, and alkali metal salts are known to catalyze the oxirane-reaction [3]. The kinetics of the reaction between CO_2 and phenyl glycidyl ether (PGE) have been studied using catalyst THA-CP-MS41, The reaction rate constants were obtained using the measured absorption rate of and analyzed with the mass transfer mechanism associated with the chemical reactions.

Park *et al.* [5] investigated the chemical absorption of carbon dioxide and phenyl glycidyl ether solution containing the catalyst THA-CP-MS41 in a heterogeneous system. To our knowledge no analytical solutions of this model have been reported. The purpose of this communication is to derive simple approximate analytical expression for the steady-state concentrations of CO_2, PGE and flux using the Adomian decomposition method.

2. Mathematical Formulation of the Problem and Analysis

Figure 1 shows the schematic representation of the stirred-cell absorber [5]. The overall reaction between CO_2 and phenyl glycidyl ether (PGE) to form the 5—membered cyclic carbonate is as follows:



(1)

*Corresponding author.

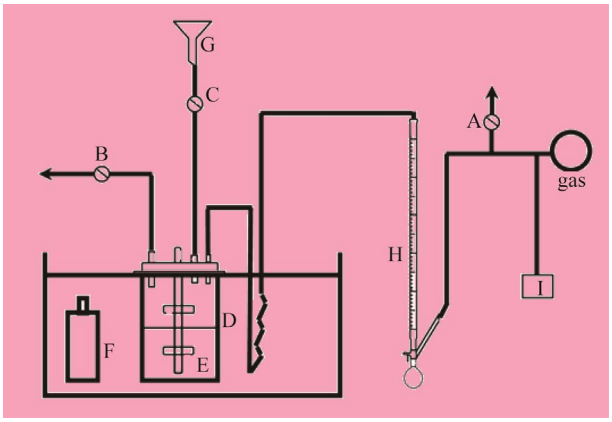


Figure 1. Shows the schematic representation of the stirred-cell absorber [5]. A, B, C: Valve; D: Absorber; E: Impeller; F: Liquid bottle; G: Funnel; H: Soap film meter; I: Gas chromatography.

where R is a functional group of $-CH_2-O-C_6H_5$. The overall reaction of Equation (1) consists of two consecutive steps: 1) a reversible reaction between PGE (B) and THA-CP-MS41 (QX) to form an intermediate complex (C_1); 2) an reversible reaction between C_1 and CO_2 (A) to form QX and five-membered cyclic carbonate (C):

$$\mathrm{B}+\mathrm{QX}\underset{k_2}{\overset{k_1}{\leftrightarrow}}\mathrm{C}_1 \tag{2}$$

$$\mathrm{A}+\mathrm{C}_1\overset{k_3}{\rightarrow}\mathrm{C}+\mathrm{QX} \tag{3}$$

At steady state condition, the consecutive chemical reaction rate of CO_2 to form C_1 is given as follows:

$$r_{A,cons}=\frac{C_B S_t}{\frac{1}{k_1}+\frac{1}{K_1k_3C_A}+\frac{C_B}{k_3C_A}} \tag{4}$$

where, S_t is the surface area of catalyst, C_A and C_B are the concentration of CO_2 and PGE respectively. K_1 is the reaction equilibrium constant, k_1 is the forward reaction rate constant in Equation (2) and k_3 is the forward reaction rate constant in Equation (3). The mass balances of CO_2 and PGE, using film theory accompanied by the consecutive chemical reactions are given as follows [5]:

$$D_A\frac{\mathrm{d}^2C_A}{\mathrm{d}z^2}=\frac{C_B S_t}{\frac{1}{k_1}+\frac{1}{K_1k_3C_A}+\frac{C_B}{k_3C_A}} \tag{5}$$

$$D_B\frac{\mathrm{d}^2C_B}{\mathrm{d}z^2}=\frac{C_B S_t}{\frac{1}{k_1}+\frac{1}{K_1k_3C_A}+\frac{C_B}{k_3C_A}} \tag{6}$$

where D_A and D_B are the diffusivity of CO_2 and PGE respectively and z is the distance. The boundary conditions are:

$$\begin{aligned} &C_A=C_{Ai},\ \frac{\mathrm{d}C_B}{\mathrm{d}z}=0 \quad \text{at} \quad z=0\\ &C_A=C_{AL},\ C_B=C_{Bo} \quad \text{at} \quad z=z_L \end{aligned} \tag{7}$$

Equations (5), (6) and the boundary conditions (7) can be normalized by employing the following parameters:

$$a=\frac{C_A}{C_{Ai}};\quad b=\frac{C_B}{C_{Bo}};$$

$$\alpha_1=\frac{z_L^2S_tC_{Bo}K_1k_3}{D_A};\quad \alpha_2=\frac{z_L^2S_tC_{Ai}K_1k_3}{D_B};$$

$$\beta_1=\frac{C_{Ai}K_1k_3}{k_1};\ \beta_2=\frac{C_{Bo}K_1k_1}{k_1};\quad x=\frac{z}{z_L}$$

where, a, is the concentration of CO_2, b is the concentration of PGE, $\alpha_1, \alpha_2, \beta_1, \beta_2$ normalized parameters and x is the dimensionless distance. Now the two nonlinear reaction/diffusion Equations (5), (6) in normalized form becomes as follows:

$$\frac{\mathrm{d}^2a}{\mathrm{d}x^2}=\frac{\alpha_1ab}{1+\beta_1a+\beta_2b} \tag{8}$$

$$\frac{\mathrm{d}^2b}{\mathrm{d}x^2}=\frac{\alpha_2ab}{1+\beta_1a+\beta_2b} \tag{9}$$

The above Equations (8), (9) are the system of nonlinear differential equations. While no general method of solving these nonlinear problems has been proposed, several vigorous procedure such as Adomian decomposition method [6-10], Homotopy perturbation method [11-15] and Homotopy analysis method [16-21] etc., have been analyzed. Here, Adomian decomposition method is used to solve these nonlinear differential equations. The boundary conditions becomes,

$$\begin{aligned} &a=1,\ \frac{\mathrm{d}b}{\mathrm{d}x}=0 \ \text{ at } \ x=0\\ &a=k,\ b=1 \text{ at } \ x=1 \end{aligned} \tag{10}$$

where, $k=\frac{C_{AL}}{C_{Ai}}$. The enhancement factor of CO_2, defined as the ratio of the flux of CO_2 with chemical reaction to that without chemical reaction is as follows,

$$\beta=-\left(\frac{\mathrm{d}a}{\mathrm{d}x}\right)_{x=0} \tag{11}$$

3. Analytical Solutions of Concentrations of CO_2 and PGE under Steady-State Condition Using the Adomian Decomposition Method

In this paper, the Adomian decomposition method (see Appendix A) is used to solve nonlinear differential equations. The ADM [6-10] yields, without linearization, per-

turbation or transformation, an analytical solution in terms of a rapidly convergent infinite power series with easily computable terms. The basic principle of this method is described in Appendix A and detailed derivation of dimensionless concentration of CO_2 and PGE, from the nonlinear Equations (8) and (9) are described in Appendix B. Using this method (refer Appendix B), we obtain the analytical expression corresponding to the concentrations of CO_2 and PGE as follows:

$$a(x) = (k-1)x + 1 + \frac{\alpha_1 x}{2\beta_1}(x-1) - \frac{\alpha_1(1+\beta_2)}{\beta_1^3(k-1)^2}$$
$$\left[\left(\log\left(1+\beta_2+\beta_1\left((k-1)x+1\right)-1\right)\right)\right.$$
$$\left(1+\beta_2+\beta_1\left((k-1)x+1\right)\right) - x\left(\log\left(1+\beta_2+\beta_1 k\right)-1\right) \quad (12)$$
$$\left.\left(1+\beta_2+\beta_1 k\right)\right] - \frac{\alpha_1(1+\beta_2)}{\beta_1^3(k-1)^2}\left[\log\left(1+\beta_2+\beta_1\right)-1\right]$$
$$\left(1+\beta_2+\beta_1\right)(x-1)$$

$$b(x) = 1 + \frac{\alpha_2}{2\beta_1}\left(x^2-1\right) - \frac{\alpha_2(1+\beta_2)}{\beta_1^3(k-1)^2}$$
$$\left[\left(\log\left(1+\beta_2+\beta_1\left((k-1)x+1\right)-1\right)\right)\right.$$
$$\left(1+\beta_2+\beta_1\left((k-1)x+1\right)\right) - \left(\log\left(1+\beta_2+\beta_1 k\right)-1\right)$$
$$\left.\left(1+\beta_2+\beta_1 k\right)\right] + \frac{\alpha_2(1+\beta_2)(x-1)}{\beta_1^2(k-1)}\log\left(1+\beta_2+\beta_1\right) \quad (13)$$

From Equation (11), we obtain the flux as

$$\beta = 1-k-\frac{\alpha_1(1+\beta_2)}{\beta_1^3(k-1)^2}\left[\left(\log\left(1+\beta_2+\beta_1 k\right)-1\right)\right.$$
$$\left(1+\beta_2+\beta_1 k\right) - \left(\log\left(1+\beta_2+\beta\right)_1 - 1\right)\left(1+\beta_2+\beta_1\right)\left.\right]$$
$$+\frac{\alpha_1(1+\beta_2)}{\beta_1^2(k-1)}\log\left(1+\beta_2+\beta_1\right)+\frac{\alpha_1}{2\beta_1} \quad (14)$$

4. Numerical Simulation

The function pdex4 in Scilab/Matlab software which is a function of solving the initial-boundary value problems for the two reaction/diffusion equations is used to solve Equations (8) and (9). The normalized concentrations of CO_2 and PGE are compared with simulation results in **Figures 1** and **2**. A satisfactory agreement is noted. The Scilab/Matlab program is also given in Appendix C. In **Table 1**, the simulation results compared with ADM results, the maximum error is 0.64%.

5. Results and Discussion

Equations (12) and (13) represent the new closed and simple approximate analytical expressions of the normalized concentrations of CO_2 and PGE for all values of parameters α_1, α_2, β_1, β_2 and k. The current response is given in Equation (14). The concentration profiles of CO_2 and PGE are shown in **Figures 2** and **3**. The concentration of CO_2 increases when the normalized parameter k increases (refer **Figure 2(a)**). The concentration of CO_2 decreases when the parameters β_1 and β_2 increases (refer **Figures 2(b)** and **(c)**). In **Figure 3**, the concentration of PGE decreases when the normalized parameter α_2 or surface area of catalyst increases and diffusivity of PGE decreases. Equation (14) represents the normalized flux. The value of flux increases as the parameters β_1 and β_2 or reaction equilibrium constant increases (refer **Figures 4(a)** and **(b)**). In **Figure 4(c)**, the value of flux decreases as the parameters α_1 or or surface area of catalyst increases and diffusivity of CO_2 decreases.

6. Conclusions

This paper presents a theoretical treatment of carbon dioxide and phenyl glycidyl ether solution in chemical reaction. Also, we have discussed the mathematical models of CO_2 absorption into the PGE solution. We have solved the nonlinear differential equations both analytically and numerically. The approximate analytical expressions for

Table 1. Comparison of normalized substrate concentration of CO_2 ($A(x)$) between Equation (12) and numerical simulation for various values of parameters β_1 when $\alpha_1 = 1$, $\beta_2 = 0.001$, $k = 0.1$.

	$\beta_1 = 0.1$			$\beta_1 = 1$			$\beta_1 = 10$		
x	This work Equation (12)	Numerical simulation	Error %	This work Equation (12)	Numerical simulation	Error %	This work Equation (12)	Numerical simulation	Error %
0.0	1.0000	1.0000	0.0000	1.0000	1.0000	0.0000	1.0000	1.0000	0.0000
0.2	0.7722	0.7754	0.4144	0.7896	0.7906	0.1267	0.8132	0.8132	0.0000
0.4	0.5746	0.5797	0.8876	0.5971	0.5988	0.2847	0.6299	0.6300	0.0159
0.6	0.4011	0.4061	1.2466	0.4202	0.4220	0.4284	0.4501	0.4502	0.0222
0.8	0.2451	0.2482	1.2648	0.2558	0.2569	0.4300	0.2736	0.2737	0.0366
1.0	0.1000	0.1000	0.0000	0.1000	0.1000	0.0000	0.1000	0.1000	0.0000
	Average		0.6356	Average		0.2116	Average		0.0125

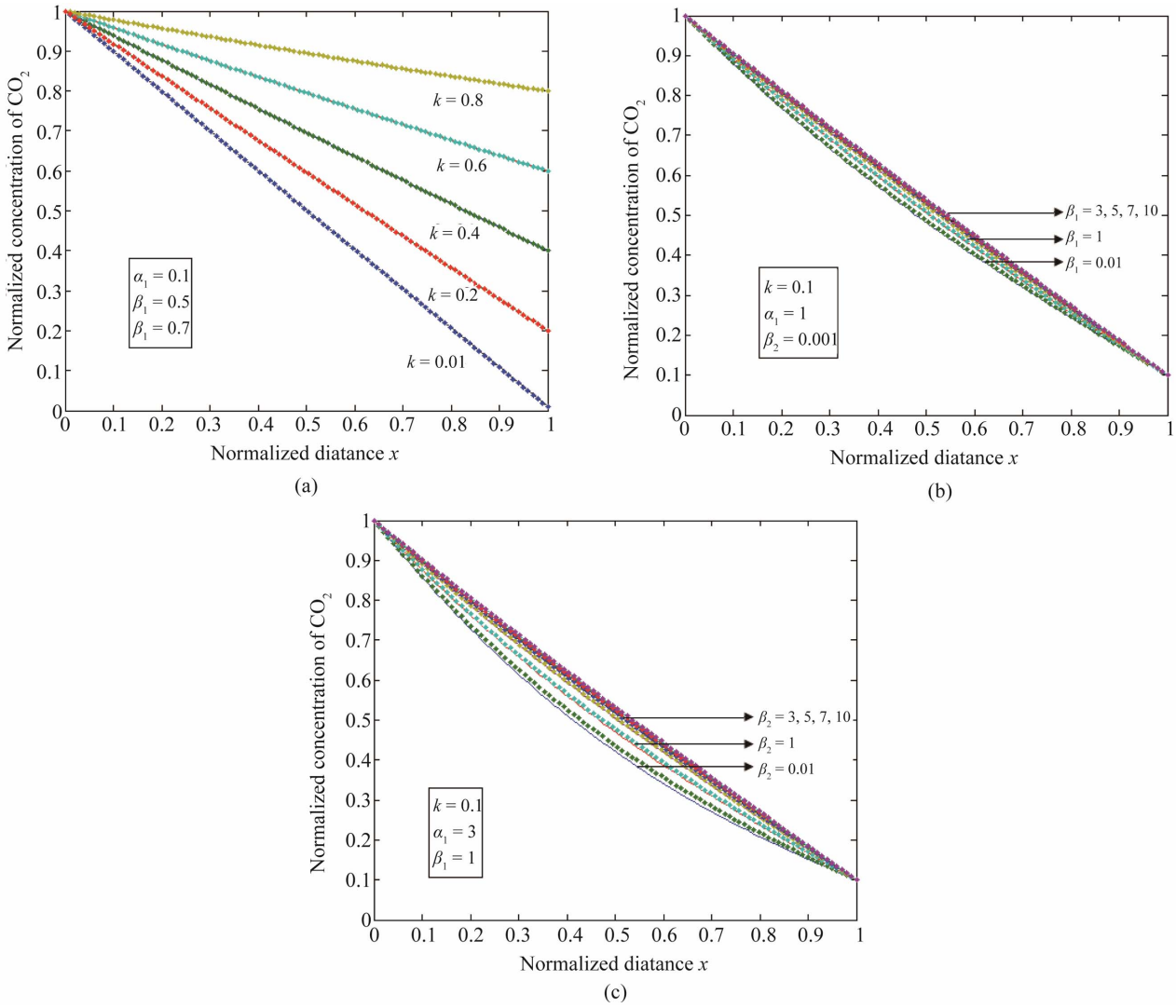


Figure 2. Normalized concentration of CO_2 for various values of parameters is plotted using Equation (12). (a) $\alpha_1 = 0.1$, $\beta_1 = 0.5$, $\beta_2 = 0.7$; (b) $k = 0.1$, $\alpha_1 = 1$, $\beta_2 = 0.001$; (c) $k = 0.1$, $\alpha_1 = 3$, $\beta_1 = 1$. The key to the graph (stacked line) represents the Equation (12) and (dotted line) represents the numerical simulation.

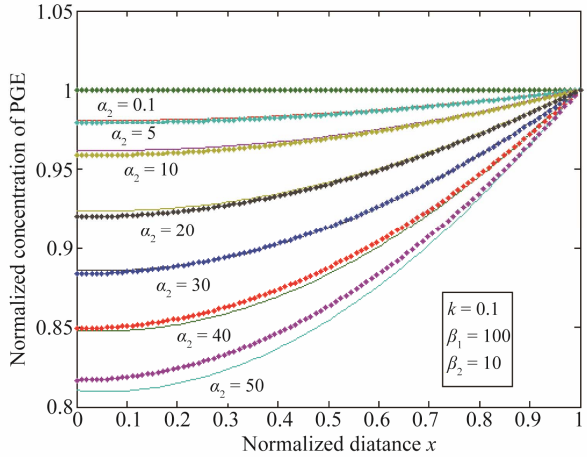


Figure 3. Normalized concentration of PGE for various values of parameters is plotted using Equation (13). The key to the graph (stacked line) represents the Equation (13) and (dotted line) represents the numerical simulation.

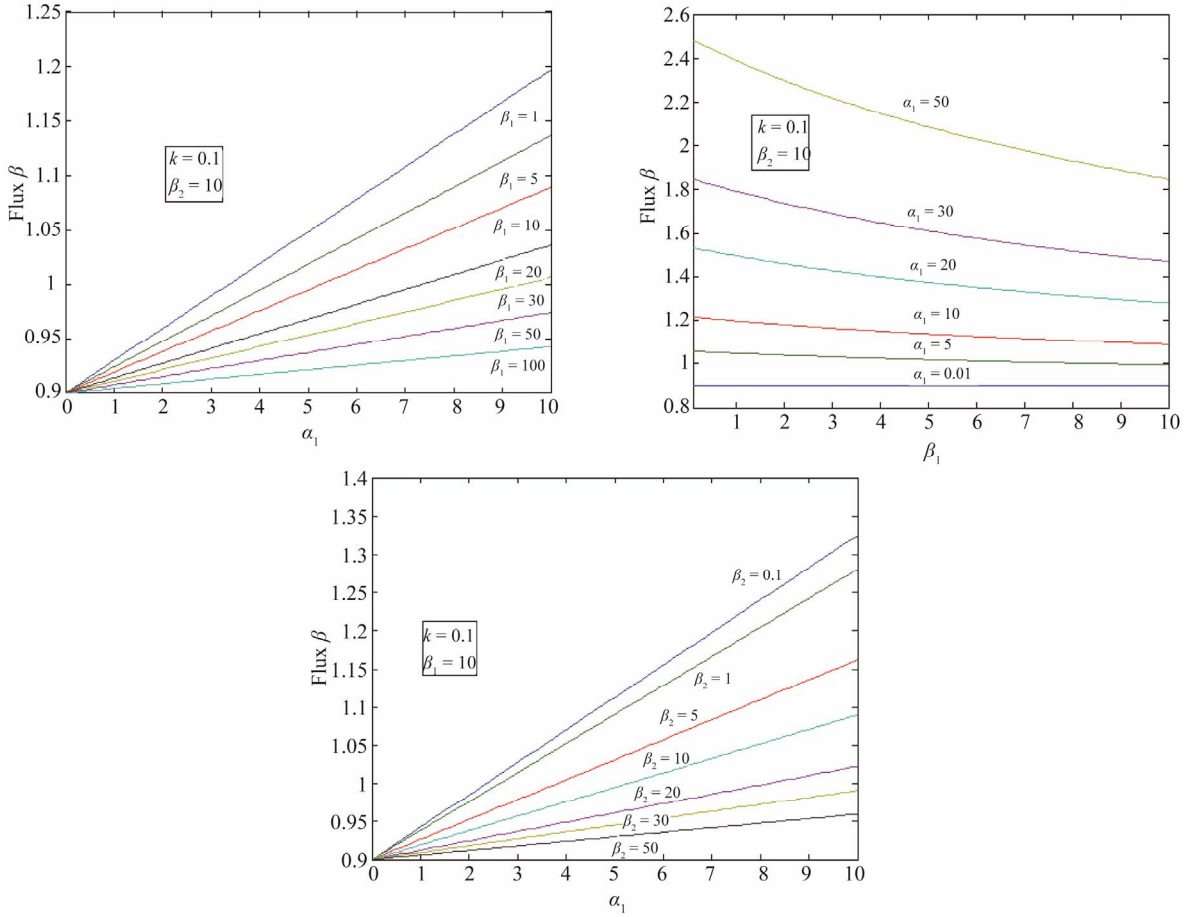


Figure 4. Diagrammatic representation of the normalized flux β for various values of α_1, β_1, β_2 and k.

the steady state concentrations of CO_2 and PGE for all values of parameters using the Adomian decomposition method. These theoretical results are useful to evaluate the overall reaction rate constant and enhancement factor of CO_2. A satisfactory agreement with the numerical result is noted.

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Appendix A

Basic Concept of the Adomian Decomposition Method (ADM)

Adomian decomposition method [22-27] depends on decomposing the nonlinear differential equation

$$F\left(\chi, y(\chi)\right)=0 \tag{A.1}$$

into the two components

$$L\left(y(\chi)\right)+N\left(y(\chi)\right)=0 \tag{A.2}$$

where L and N are the linear and the nonlinear parts of F respectively. The operator L is assumed to be an invertible operator. Solving for $L(y(\chi))$ leads to

$$L\left(y(\chi)\right)=-N\left(y(\chi)\right) \tag{A.3}$$

Applying the inverse operator L on both sides of Equation (A.3) yields

$$y(\chi)=\varphi\ (\chi)-L^{-1}\ \left[N\left(y(\chi)\right)\right] \tag{A.4}$$

where $\varphi(\chi)$ is a function that satisfies the condition $L\left(\varphi(\chi)\right)=0$. Now assuming that the solution y can be represented as infinite series of the form,

$$\sum_{n=0}^{\infty} y_n(\chi)=\varphi(\chi)-L^{-1}\left(\sum_{n=0}^{\infty} A_n(\chi)\right) \tag{A.5}$$

where

$$\sum_{n=0}^{\infty} y_n(\chi)=y(\chi),$$

$$A_n(\chi)=\frac{1}{n!}\left[\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} N\left(\sum_{i=0}^{\infty}\left[\lambda^i y_i(\chi)\right]\right)\right]_{\lambda=0} \tag{A.6}$$

$$\text{and}\quad \sum_{n=0}^{\infty} A_n(x)=N\left(y(\chi)\right)\quad n\geq 0$$

Then equating the terms in the linear system of Equation (A.5) gives the recurrent relation

$$y_0=\varphi(\chi),\quad y_{n+1}=-L^{-1}\left(A_n\right)\quad n\geq 0 \tag{A.7}$$

However, in practice all the terms of series in Equation (A.5) cannot be determined, and the solution is approximated by the truncated series $\sum_{n=0}^{N} y_n(\chi)$.

Appendix B

Analytical Expression of Concentrations of CO_2 and PGE Using the Adomian Decomposition Method

To solve Equations (8) and (9) using the Adomian decomposition method, we write the Equations (8) and (9) in the operator form,

$$L\left[a(x)\right]=N\left[a(x)\right] \tag{B.1}$$

$$L\left[b(x)\right]=N\left[b(x)\right] \tag{B.2}$$

where

$$L=\frac{\mathrm{d}^2}{\mathrm{d}x^2},\ N\left[a(x)\right]=\left[\frac{\alpha_1 ab}{1+a\beta_1+b\beta_2}\right]$$
$$N\left[b(x)\right]=\left[\frac{\alpha_2 ab}{1+a\beta_1+b\beta_2}\right] \tag{B.3}$$

Applying the inverse operator L^{-1} on both sides of Equation (B.1) and (B.2) yields

$$a(x)=Ax+B+L^{-1}N\left[a(x)\right] \tag{B.4}$$

$$b(x)=Ax+B+L^{-1}N\left[b(x)\right] \tag{B.5}$$

According to the ADM, the solution $a(x)$ and $b(x)$ can be elegantly computed by using the recurrence relation

$$a_0(x)=Ax+B,$$
$$a_{n+1}(x)=L^{-1}N\left[a(x)\right]=L^{-1}A_n(x),\quad n\geq 0 \tag{B.6}$$

$$b_0(x)=Ax+B,$$
$$b_{n+1}(x)=L^{-1}N\left[b(x)\right]=L^{-1}B_n(x),\quad n\geq 0 \tag{B.7}$$

where A_n and B_n are the Adomian polynomials of a_1, $a_2\cdots a_n$ and b_1, $b_2\cdots b_n$ respectively. We can find the first few Adomian polynomial coefficients A_n and B_n using Equation (A.6) as follows:

$$A_0(x)=N(a_0)=\left[\frac{\alpha_1 a_0 b_0}{1+\beta_1 a_0+\beta_2 b_0}\right] \tag{B.8}$$

$$B_0(x)=N(b_0)=\left[\frac{\alpha_2 a_0 b_0}{1+\beta_1 a_0+\beta_2 b_0}\right] \tag{B.9}$$

The remaining polynomials $A_i(x)$ and $B_i(x)$ can be generated easily, using Equation (A.6). Applying the following boundary conditions

$$a_0(0)=1,\ a_0(1)=k$$
$$\text{and } a_i(0)=0,\ a_i(1)=0 \tag{B.10}$$
$$\text{for } i\geq 1$$

$$b_0'(0)=0,\ b_0(1)=1$$
$$\text{and } b_i'(0)=0,\ b_i(1)=0 \tag{B.11}$$
$$\text{for } i\geq 1$$

From Equations (B.6) and (B.7) using the above conditions we obtain the following results:

$$a_0(x)=(k-1)x+1 \tag{B.12}$$

$$a_1(x) = \frac{\alpha_1 x}{2\beta_1}(x-1) - \frac{\alpha_1(1+\beta_2)}{\beta_1^3(k-1)^2} \left[\left(\log\left(1+\beta_2+\beta_1\left((k-1)x+1\right)-1\right)\right)\left(1+\beta_2+\beta_1\left((k-1)x+1\right)\right) - x\left(\log(1+\beta_2+\beta_1 k)-1\right)\left(1+\beta_2+\beta_1 k\right)\right] - \frac{\alpha_1(1+\beta_2)}{\beta_1^3(k-1)^2}\left[\log(1+\beta_2+\beta_1)-1\right](1+\beta_2+\beta)_1(x-1) \quad \text{(B.13)}$$

$$b_0(x) = 1 \quad \text{(B.14)}$$

$$b_1(x) = \frac{\alpha_2}{2\beta_1}(x^2-1) - \frac{\alpha_2(1+\beta_2)}{\beta_1^3(k-1)^2} \left[\left(\log\left(1+\beta_2+\beta_1\left((k-1)x+1\right)-1\right)\right)\left(1+\beta_2+\beta_1\left((k-1)x+1\right)\right) - \left(\log(1+\beta_2+\beta_1 k)-1\right)\left(1+\beta_2+\beta_1 k\right)\right] + \frac{\alpha_2(1+\beta_2)(x-1)}{\beta_1^2(k-1)}\log(1+\beta_2+\beta_1) \quad \text{(B.15)}$$

Adding Equations (B.12) and (B.13), (B.14) and (B.15), we get the concentration of CO_2 and PGE (Equations (12) and (13)) in the text.

Appendix C

Scilab/Matlap program for the numerical solution of the system of nonlinear Equations (8) and (9)

```
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;
a=0.001;
b=10;
M=10;
N=0.01;
F=-(a*u(1)*u(2))/(1+(M*u(1))+(N*u(2)));
F1=-(b*u(1)*u(2))/(1+(M*u(1))+(N*u(2)));
s=[F; F1];
function u0 = pdex4ic(x);
u0 = [1; 1];
function [pl,ql,pr,qr]=pdex4bc(xl,ul,xr,ur,t)
pl = [ul(1)-1;0];
ql = [0; 1];
pr = [ur(1)-0.1; ur(2)-1];
qr = [0; 0];
```

Appendix D

Nomenclature

Symbols

C_A: Concentration of CO_2 (M)
C_B: Concentration of PGE (M)
D_A: Diffusivity of CO_2 (m^2/s)
D_B: Diffusivity of PGE (m^2/s)
K_1: Reaction equilibrium constant (1/M)
k_1: Forward reaction rate constant in reaction Equation (2) ($1/m^2s$)
k_2: Backward reaction rate constant in reaction Equation (2) (M/m^2s)
k_3: Forward reaction rate constant in reaction Equation (3) ($1/m^2s$)
$r_{A,cons}$: Reaction rate of CO_2 in consecutive reaction model (M/s)
S_t: Surface area of catalyst (m^2)
z: Distance (m)
z_L: Film thickness (m)
a: Normalized concentration of CO_2 (Dimensionless)
b: Normalized concentration of PGE (Dimensionless)
$\alpha_1, \alpha_2, \beta_1, \beta_2$ and k : Normalized parameters (Dimensionless)
β : Flux of CO_2 (Dimensionless)

Subscripts

A: CO_2
B: PGE
L: Bulk solution
o: Feed or solvent

