Mathematical Model for Extracting Hollow Fiber Membrane Contactors from Carbon dioxide using Adomian decomposition method

P. Jeyabarathi, M. Kannan, L. Rajendran

Abstract: The mathematical model of the carbon dioxide extraction behavior using a hollow fiber membrane contactor where an aqueous bicarbonate ion solution flows. The coupled nonlinear partial differential equations are analytically solved using the Adomian decomposition method, which explains either carbon dioxide absorption or desorption in a membrane contactor. Discuss the effects of the fiber parameter length, initial carbon dioxide concentration, and bicarbonate ion. Our analytical results are compared with the simulation result. The numerical data are found to be in satisfactory agreement with analytical data.

Key words: Mathematical modeling; nonlinear equations; Membrane contactors; Adomian decomposition method; Numerical simulation.

1. INTRODUCTION

In typical gas absorption processes, gas mixtures are normally spread and contacted with liquids using the following device types: a packed tower, a spray tower, a venturi scrubber or a bubble column. The concept of a hollow fiber contactor was developed by Qi and Cussler [1-2] using a hollow fiber membrane to absorb carbon dioxide. Recently, Sirkar updated the processes of gas absorption based on membrane contactors [3]. Karoor and Sirka have extensively investigated the separation of carbon dioxide from nitrogen [4]. Teramoto et al. [5] addressed the transport of carbon dioxide by an aqueous amine solution assisted by a liquid membrane. Experimental absorption experiments with several absorbent liquids using a membrane contactor were reported [3,5]. Nevertheless, it has been stated that few theoretical analyzes identify the membrane contactors in which the essential chemical reaction steps were included without any simplification [6-8]. It is more difficult to analyze theoretically than with other absorbent types. Therefore, in place of microscopic partial differential equations, most researchers applied the macroscopic overall mass transfer coefficients to describe their membrane contactor [9-12]. Recently, Lee et al. [13] uses a quantitative approach to examine carbon dioxide extraction using a hollow fiber membrane contactor. In this paper, the analytical expressions of the concentration of carbon dioxide and bicarbonate ion are obtained by solving the non-linear equation using the Adomian decomposition method.

NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definitions</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_a$</td>
<td>Dimensionless concentration of carbon dioxide</td>
<td>none</td>
</tr>
<tr>
<td>$c_b$</td>
<td>Dimensionless concentration of bicarbonate ion</td>
<td>none</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Dimensionless parameter</td>
<td>none</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Dimensionless parameter</td>
<td>none</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Dimensionless ratio of concentration of carbon dioxide to wall concentration of bicarbonate ions</td>
<td>none</td>
</tr>
<tr>
<td>$L$</td>
<td>Length of fiber</td>
<td>m</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Radial coordinate</td>
<td>m</td>
</tr>
<tr>
<td>$\tau_0$</td>
<td>Dimensionless parameter</td>
<td>none</td>
</tr>
</tbody>
</table>

2. MATHEMATICAL FORMATION OF THE BOUNDARY VALUE PROBLEM

Recently, Lee et al. [13] obtained the carbon dioxide extraction equations using a hollow fiber membrane contactor, which is briefly outlined for completeness in Appendix A. The flow configuration is shown in Fig.1. The dimensionless mass balance equations for the concentration of carbon dioxide ($\bar{C}_A$) and bicarbonate ion ($\bar{C}_B$) are given as follows [13]:

$$\frac{\partial^2 \bar{C}_A}{\partial \tau^2} + \frac{\partial \bar{C}_A}{\partial \tau} \bigg|_{r = 0} = 0$$

$$\frac{\partial \bar{C}_B}{\partial \tau} = 0$$

$$\bar{C}_A = 1, \bar{C}_B = 0$$

where $D_{KB}$ and $r$ are dimensionless parameters and $G$ is the dimensionless ratio of CO$_2$ over HCO$_3^-$ concentration at the wall. The boundary conditions in dimensionless forms are

3. ANALYTICAL EXPRESSION OF THE CONCENTRATION USING THE ADOMIAN DECOMPOSITION METHOD (ADM)

The Adomian decomposition method [14-16] is quantitative rather than qualitative, empirical, involving no linearization or disruption, and continuous without discretion. In this paper, to solve nonlinear differential equations (1) and (2), the Adomian decomposition method is used. The analytical expression of concentrations of carbon dioxide and bicarbonate ion obtained as (Appendix A) are as follows:

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When \( n_{\text{bi}} = 0.1, D_{\text{bi}} = 0.1, D_{\text{so}} = 1, D_{\text{sc}} = 1, \) and \( \gamma = 0.01, \) then \( \alpha = 0.01, 0.05, 0.1, 0.2, 0.5, 0.7, 1 \) and \( \gamma = 0.01, 0.05, 0.1, 0.2, 0.5, 0.7, 1 \).

The key to the plot: (--) Eqn. (5) and (---) numerical simulation of Eqn. (1).

The carbon dioxide and bicarbonate ion concentration at the center of the fiber decreases when rate constants \( \alpha \) and \( \gamma \) are increased.

The concentration of carbon dioxide at the center of the fiber decreases when rate constant \( \alpha \) and initial concentration of absorption \( \tau \) is small. Also the concentration of carbon dioxide increases when \( \tau \) is increases or \( \alpha \) decreases. Also, the concentration is uniform or does not change at the center of the fiber from its bulk value when \( \alpha \) is small and \( \gamma \) is small.

From the figures, it is inferred that the concentration of bicarbonate ion at the center of the fiber decreases when rate constants \( \alpha \) and \( \gamma \) are increased.
increases whereas the concentration of bicarbonate ion decrease when the initial concentration of \( \alpha \) increases.

6. CONCLUSION

Using the Adomian decomposition method the nonlinear differential equation method for extracting carbon dioxide using solution flows of bicarbonate ion in hollow fiber membrane contactors is solved. A simple analytical expression of the concentration of carbon dioxide and bicarbonate ion solution is obtained for all values of a parameter. The analytical result is compared with the simulation result (Matlab program) for all possible values of operating parameters. With numerical simulation results, a satisfactory agreement is noted.

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7. Appendix A

Analytical solution of non-linear reactions Eqns. (1) and (2) using the Adomian decomposition method [18]. In this Appendix, we derive the general solution of nonlinear Eqn. (1) and (2) by using the Adomian decomposition method. We write the equations (1) and (2) in the operator form as

\[ \mathcal{L}(x_{i}(t)) = D_{x_{i}} \left( t + \frac{\alpha t}{\alpha} \right) \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.1)

\[ \mathcal{L}(x_{i}(t)) = -G \frac{\alpha t}{\alpha} \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.2)

\[ \mathcal{L}(x_{i}(t)) = -G \frac{\alpha t}{\alpha} \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.3)

\[ \mathcal{L}(x_{i}(t)) = -G \frac{\alpha t}{\alpha} \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.4)

Applying the inverse operator \( \mathcal{L}^{-1}(\cdot) = \sum_{i=0}^{\infty} \frac{B_{i} \mathcal{L}^{-1} \left( x_{i} \right)}{\alpha} \) on both sides of the equation (A.1) to (A.4) yield.

\[ \mathcal{L}(x_{i}(t)) = A + B + D_{x_{i}} \]  

(A.5)

\[ \mathcal{L}(x_{i}(t)) = C + D - G_{x_{i}} \]  

(A.6)

Where \( A, B, C, D, G_{x_{i}}, \) and \( G \) are constants of integration. Let

\[ \mathcal{L}(x_{i}(t)) = A + B + D_{x_{i}} \]  

(A.7)

\[ \mathcal{L}(x_{i}(t)) = C + D - G_{x_{i}} \]  

(A.8)

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.9)

where

\[ \mathcal{L}(x_{i}(t)) = D_{x_{i}} \left( t + \frac{\alpha t}{\alpha} \right) \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.10)

\[ \mathcal{L}(x_{i}(t)) = -G \frac{\alpha t}{\alpha} \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.11)

In view of Eqn. (C.7), (C.9) gives

\[ \mathcal{L}(x_{i}(t)) = A + B + D_{x_{i}} \]  

(A.12)

the zero element is defined as

\[ \mathcal{L}(x_{i}(t)) = A + B \]  

(A.12)

and the remaining components as the recurrence relation

\[ \mathcal{L}(x_{i}(t)) = D_{x_{i}} \]  

(A.13)

\[ \mathcal{L}(x_{i}(t)) = -G \frac{\alpha t}{\alpha} \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.14)

\[ \mathcal{L}(x_{i}(t)) = -G \frac{\alpha t}{\alpha} \left( x_{i} + \frac{1}{x_{i}} \right) \]  

(A.15)

The remaining polynomials can be easily generated and so on \( \mathcal{L}(x_{i}(t)) \) gives

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.16)

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.17)

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.18)

Adding (A.16) to (A.18) we get the Eqn. (5). In view of Eqns. (A.8),(A.10) gives

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.19)

the zero element is defined as

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.20)

and the remaining components as the recurrence relation

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.21)

where \( \alpha \) are Adomian polynomials of \( \mathcal{L}(x_{i}(t)) \). We can find \( \alpha \) as follows:

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.22)

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.23)

The remaining polynomials can be easily generated and so on \( \mathcal{L}(x_{i}(t)) \) gives

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.24)

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.25)

\[ \mathcal{L}(x_{i}(t)) = \sum_{i=0}^{\infty} A_{i} \]  

(A.26)

Adding (A.24) to (A.26) we get the Eqn. (6) in the text.

I. Matlab program for Equations (1) and (2) numerical solution.

function pde4
m = 1;
x = linspace(0,1);
t=linspace(0,10);
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,1)')
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;
F1 = Dka * ((1 + a*((y-u(2))/u(2)))*(u(1)-(g*u(1)*u(1)/(y-u(2)))))
F2 = Dkb * (1 + a*((y-u(2))/u(2)))*(u(1)-(g*u(1)*u(1)/(y-u(2))));
s=[F1; F2];
%---------------------------------------------------------------------
function u0 = pdex4ic(x)
%create a initial conditions
u0 = [1; 1];
%---------------------------------------------------------------------
function [pl,ql,pr,qr]=pdex4bc(xl,u1,xr,ur,t)
%create a boundary conditions
pl = [u1(1); u1(2)];
ql = [1; 1];
pr = [ur(1)-1; ur(2)-1];
qr = [0; 0];

REFERENCES
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