

## Article

# Modeling and Simulation of the Absorption of CO<sub>2</sub> and NO<sub>2</sub> from a Gas Mixture in a Membrane Contactor

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Received: 9 June 2019; Accepted: 8 July 2019; Published: 11 July 2019



**Abstract:** The removal of undesirable compounds such as CO<sub>2</sub> and NO<sub>2</sub> from incineration and natural gas is essential because of their harmful influence on the atmosphere and on the reduction of natural gas heating value. The use of membrane contactor for the capture of the post-combustion NO<sub>2</sub> and CO<sub>2</sub> had been widely considered in the past decades. In this study, membrane contactor was used for the simultaneous absorption of CO<sub>2</sub> and NO<sub>2</sub> from a mixture of gas (5% CO<sub>2</sub>, 300 ppm NO<sub>2</sub>, balance N<sub>2</sub>) with aqueous sodium hydroxide solution. For the first time, a mathematical model was established for the simultaneous removal of the two undesired gas solutes (CO<sub>2</sub>, NO<sub>2</sub>) from flue gas using membrane contactor. The model considers the reaction rate, and radial and axial diffusion of both compounds. The model was verified and validated with experimental data and found to be in good agreement. The model was used to examine the effect of the flow rate of liquid, gas, and inlet solute mole fraction on the percent removal and molar flux of both impurity species. The results revealed that the effect of the liquid flow rate improves the percent removal of both compounds. A high inlet gas flow rate decreases the percent removal. It was possible to obtain the complete removal of both undesired compounds. The model was confirmed to be a dependable tool for the optimization of such process, and for similar systems.

**Keywords:** global warming; chemical absorption; membrane contactor; removal of NO<sub>2</sub> and CO<sub>2</sub>

## 1. Introduction

Harmful gases are emitted into the atmosphere from industrial plants, because of the increase in the human population and the associated economic development, energy consumption, and the requirement of burning fossil fuels for water desalination and power generation purposes. Nitrogen dioxide (NO<sub>2</sub>) is believed to be one of the gases that contributes to smog and acid rain and which is harmful to human and animal well-being. Accordingly, there is an obligation to capture and eliminate nitrogen dioxide and other harmful gases, such as NO<sub>x</sub>, SO<sub>2</sub>, and CO<sub>2</sub> from industrial emission streams, proceeding to discharge into the atmosphere [1–3]. Various methods have been established for capturing the impurity of compounds such as physical and/or chemical absorption, adsorption, membrane technology, conversion to another compound, and condensation. There are various technologies available to remove CO<sub>2</sub> and NO<sub>x</sub> [3–5]. Physical absorption incorporates mass transport within the phases and mass transfer at the liquid–gas boundary. Operating conditions and gas solubility are the main factors affecting physical absorption. An example of physical absorption is the capture of CO<sub>2</sub> into liquid water using industrial absorption towers or gas–liquid membrane contactors. Chemical absorption is based on a chemical reaction between the absorbed substances and the liquid phase, such as the capture of CO<sub>2</sub> in amine solutions [4,6]. The most widely used commercial and economical method is the chemical absorption technique, used in the conventional

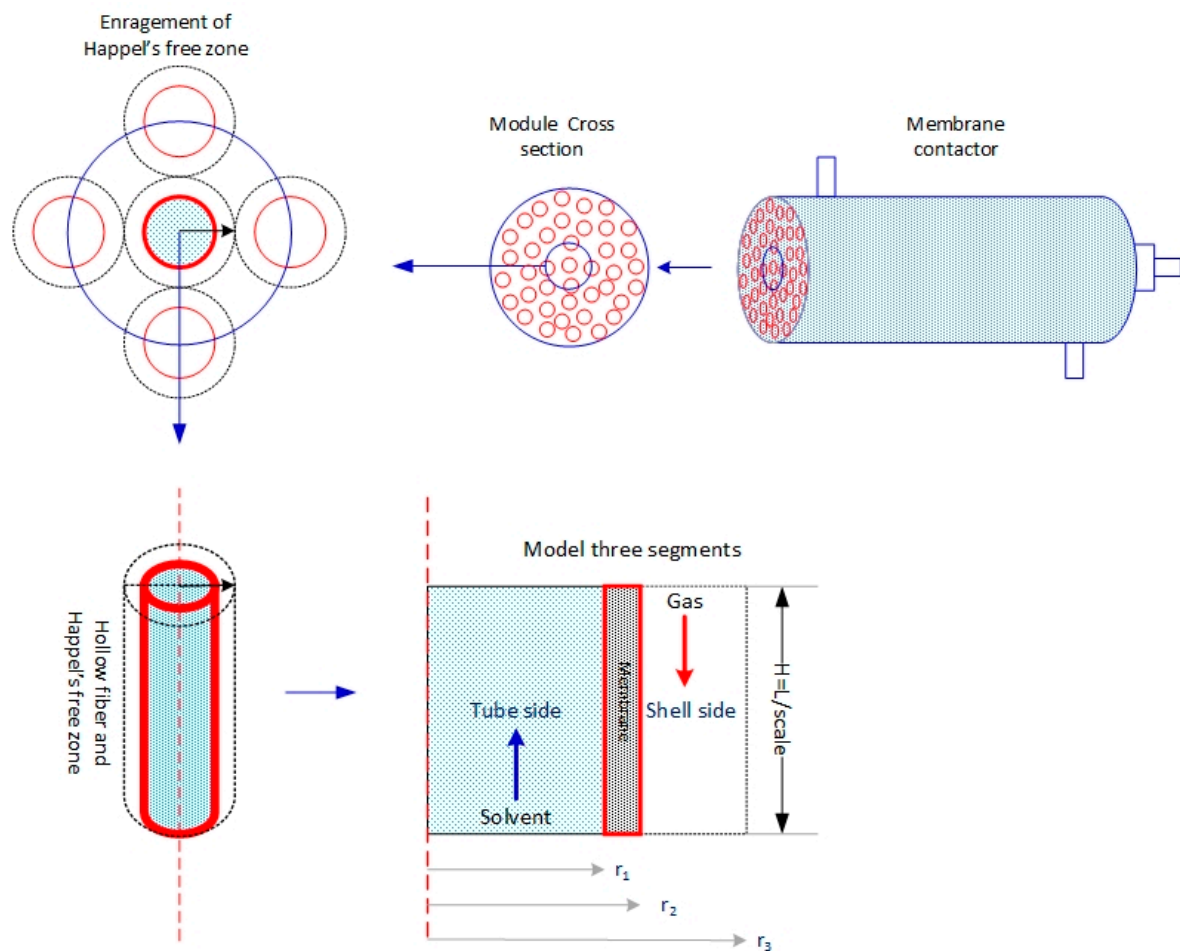
absorption packed bed towers employed in the absorption of  $\text{CO}_2$ ,  $\text{H}_2\text{S}$ , and  $\text{NO}_2$  from chimney gas and natural gas via alkanolamine solutions, where the flue gas and the absorbent liquid are in direct contact. The conventional scrubbing method requires a huge absorption column with excess liquid absorbent and a large cross-sectional area in order to prevent foaming and channeling. The large amount of absorbent liquid utilized in the absorption process (i.e., rich solvent) increases the operating and regeneration cost as more heat is required for the regeneration and pumping of the recycled lean solvent. The main disadvantages of conventional chemical absorption processes are channeling, foaming, corrosion, and a large space area required and hence high operating and capital cost. The idea of using membrane contactor was first proposed for the absorption of carbon dioxide in sodium hydroxide as a liquid absorbent utilizing a non-dispersive microporous membrane where gas and liquid phases are not dispersed in each other [7,8]. A hollow fiber membrane contactor (HFMC) provides a greater surface contact area per unit volume, more than that of a conventional absorption column [9–13]. In most cases of membrane contactor operation, gas flows in the shell side, and liquid absorbent flows in the tube side; vice versa is also possible [14]. The performance of a HFMC declines when the micropores of the membranes are wetted with a liquid solvent [3,11,15–17]. The advantages of membrane processes are as follows: Gas and liquid flow rates are independent, high ratio of surface area per volume, easy scale up and down, and no worry about flooding and channeling [18]. The membrane acts as an obstacle between gas and liquid and delivers an exchange surface zone for the two phases, without the dispersion of the gas phase in the liquid phase. In the non-wetted mode, the membrane pores are filled with gas, and by contrast, in the wetted mode, part of the membrane pores are filled with the liquid absorbent. The pollutant gas compounds' amputation process occurs when the gas filling the membrane micropores diffuses from the gas stream and is absorbed by the liquid absorbent running in the membrane lumen side [1,16,19]. The removal of the contaminant gas compounds from the gas stream depends on the solubility of the acid gas molecules in the absorbent liquid, and on the concentration incline among the gas stream absorbent solution. The interaction between the selected gas solute and the selective absorbent liquid defines the performance of the pollutant gas removal rate [20]. Membrane fouling and membrane wettability are the main drawbacks of the membrane contactor. The wetted portion of the membrane adds an additional mass transfer resistance. Accordingly, in order to avoid membrane wettability, researchers focused on the use of hydrophobic polymeric membranes, such those made from polypropylene (PP), polytetrafluoroethylene (PTFE), polyvinylidene fluoride (PVDF), and polyethylene (PE) [21–24]. The Gas Liquid Hollow Fiber Member Contactor (GLMC) processes were used for the removal of  $\text{CO}_2$  from nitrogen,  $\text{CO}_2$  from natural gas, and the instantaneous removal of  $\text{CO}_2$  and  $\text{SO}_2$  from combustion released gas [17,19,20,25–33]. The experimental simultaneous capture of  $\text{CO}_2$  and  $\text{NO}_2$  from a pretended flue gas mixture containing  $\text{CO}_2/\text{NO}_2/\text{N}_2$  was first investigated using a commercial PTFE membrane by Ghobadi et al. [23]. The effects of the gas and liquid cross-flow velocity on the percent removal of these gasses were investigated. Various mathematical models were developed for the removal of carbon dioxide, sulfur dioxide, and hydrogen sulfide from simulated flue gas and natural gas streams [7,9,15,17,25,32,34–39]. To the extent of the author's knowledge, so far, there is no mathematical model published to designate the synchronized capture of  $\text{CO}_2/\text{NO}_2$  from a mixture of gas consisting of  $\text{CO}_2/\text{NO}_2/\text{N}_2$ .

This study focusses on the development of a numerical model for the capture of  $\text{CO}_2/\text{NO}_2$  from a gas containing: 5%  $\text{CO}_2$ , 300 ppm  $\text{NO}_2$ , and the balance is  $\text{N}_2$ . The principal model equations were solved using COMSOL Multiphysics (Version 5.4, Comsol Inc., Zürich, Switzerland). The developed model was used to predict the influence of various operating parameters on the percent removal and molar flux of the acid gas components. The model was verified and validated with experimental data from literature [23].

## 2. Model Development

The gas-liquid membrane process consists of many hollow fibers assembled in a module, where the liquid solvent flows inside the membrane lumen, and the gas flows in the shell sideways,

or vice versa, in a co-current or countercurrent parallel flow. The pollutant gas compounds diffuse through the fiber walls towards the absorbent membrane–tube interface, as a result of the concentration gradient. Other gases are retained in the membrane pores because of their low diffusivity and low solubility in the liquid solvent. Figure 1 shows a schematic simplified geometry of the model domains representing the HFM module grounded on Happel’s free surface [40]. The model considers the following three separate domains: the liquid phase in the tube side, the non-wetted membrane, and the gas phase in the shell side. The system is steady state, described by cylindrical coordinates, angular concentration gradients are neglected, and an asymmetrical approach is considered.



**Figure 1.** Simplified geometry of membrane module based on Happel’s free surface method.

The sizes of the membrane used in the simulation are presented in Table 1.

**Table 1.** Membrane module dimensions [23].

Property	Value
Inner fiber radius (mm)	0.34
Outer fiber radius (mm)	0.60
Number of fibers	590
Module outer radius (mm)	25.4
Module effective length (mm)	200

As seen from Table 1, the fiber length is 588 times longer than the fiber radius (effective module length is 200 mm and radius are 0.34 mm). Accordingly, the membrane length is scaled up so as to avoid an excessive number of elements and nodes and for a better appearance of the module in the simulation;

therefore, a new scaled length is introduced by dividing the length by 100. The following assumptions were considered:

- The process is at isothermal and steady state conditions;
- Gas phase is an ideal gas, and the liquid phase is incompressible and Newtonian;
- Solubility is based on Henry's law at the liquid-gas interface.

The blended gas (CO<sub>2</sub>, NO<sub>2</sub>, and N<sub>2</sub>) is transported in the shell side by convection and diffusion, whereas, in the membrane section, the only transport mechanism is diffusion. The liquid phase (NaOH + H<sub>2</sub>O) is transported in the lumen by diffusion and convection. The following mass transport equations are formulated to describe the chemical absorption system in the model domains (tube, membrane, and shell). The developed mass transport equations are presented as follows.

### 2.1. Tube Side

The mass balance equations for the gas components of CO<sub>2</sub>, NO<sub>2</sub>, and N<sub>2</sub> in the tube side can be stated, as per Equation (1), as follows:

$$D_{i,t} \frac{1}{r} \left( \frac{\partial}{\partial r} r \left( \frac{\partial C_{i,t}}{\partial r} \right) \right) + D_{i,t} \frac{\partial^2 C_{i,t}}{\partial z^2} = v_{z,t} \left( \frac{\partial C_{i,t}}{\partial z} \right) + R_i \quad (1)$$

The subscripts in the material balance the following equations: *t* refers to tube side, *m* refers to membrane, and *s* refers to shell side, where *C<sub>i,t</sub>* refers to the concentration of component *i* in liquid moving in the tube side, *i* refers to the pollutant gas components: CO<sub>2</sub>, NO<sub>2</sub>, and *R<sub>i</sub>* is the rate of reaction of the species *i*. The length of the fiber is scaled to avoid excessive computation and to make the simulation result in a better profile. The scaling is performed as follows: let  $\xi = z/\text{scale}$ . The scaling factor is substituted in Equation (1). Consequently, the equation becomes Equation (2), as follows:

$$D_{i,t} \frac{1}{r} \left( \frac{\partial}{\partial r} r \left( \frac{\partial C_{i,t}}{\partial r} \right) \right) + \frac{D_{i,t}}{\text{scale}^2} \frac{\partial^2 C_{i,t}}{\partial \xi^2} = \frac{v_{z,t}}{\text{scale}} \left( \frac{\partial C_{i,t}}{\partial \xi} \right) + R_i \quad (2)$$

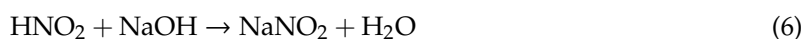
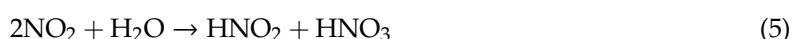
where the velocity of liquid inside the hollow fiber (*v<sub>z,t</sub>*) is described by the following parabolic equation:

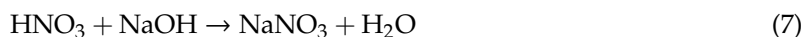
$$v_{z,t} = \frac{2Q_t}{n\pi r_1^2} \left( 1 - \left( \frac{r}{r_1} \right)^2 \right) \quad (3)$$

where *Q<sub>t</sub>* is the volumetric liquid flow rate in the tube side, and *n* is the number of hollow fibers. The appropriate set of boundary conditions are specified as follows:

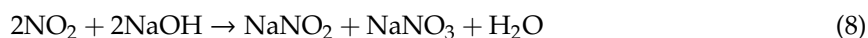
$$\begin{aligned} \text{at } z = 0, \quad C_{i,t} &= 0 & (a) \\ \text{at } z = H, \quad \frac{\partial^2 C_{i,t}}{\partial z^2} &= 0 & (b) \\ \text{at } r = 0, \quad \frac{\partial C_{i,t}}{\partial r} &= 0 & (c) \\ \text{at } r = r_1, \quad C_{i,t} &= m_i C_{i,m} & (d) \end{aligned} \quad (4)$$

where *m<sub>i</sub>* is the dimensionless physical solubility of CO<sub>2</sub> and NO<sub>2</sub> in solvent, 0.82, 0.17, respectively. The values of the dimensionless physical solubility of CO<sub>2</sub> and NO<sub>2</sub> were calculated from Henry's constant (*H*): 0.034 kmol/m<sup>3</sup> atm, 0.007 kmol/m<sup>3</sup> atm [23], respectively, using the relation *m<sub>i</sub>* = *RTxH*. The liquid phase reactions between NO<sub>2</sub> and NaOH took several steps. First, NO<sub>2</sub> dissolved in the aqueous NaOH was reacted with H<sub>2</sub>O, then neutralized with sodium hydroxide [41]. The controlling liquid phase reactions are as follows:





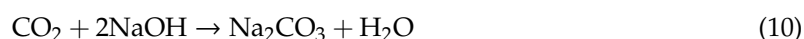
The overall reaction is designated, as per Equation (8), as follows:



The general reaction rate is expressed in Equation (9), as follows:

$$r_{\text{NO}_2-\text{NaOH}} = k_{r,1}[\text{NO}_2][\text{NaOH}] \quad (9)$$

The reaction is the second order with a rate constant,  $k_{r,1}(\text{m}^3 \text{mol}^{-1}\text{s}^{-1}) = 1.0 \times 10^5$ , [1]  
The overall reaction of  $\text{CO}_2$  and  $\text{NaOH}$  is represented by the following reaction [42].



The rate of the reaction is determined, as per Equation (11), as follows:

$$r_{\text{CO}_2-\text{NaOH}} = k_{r,2}[\text{CO}_2][\text{NaOH}] \quad (11)$$

The reaction rate constant (in Equation (11)) is  $k_{r,2} = 8.37 (\text{m}^3 \text{mol}^{-1}\text{s}^{-1})$  [23].

## 2.2. Membrane Side

The transport of the solute gas ( $\text{CO}_2$  and  $\text{NO}_2$ ) components in the membrane section confined between  $r_1$  and  $r_2$  can be described by the steady state material balance equation (Equation (12)), where diffusion is the only transport mechanism in the membrane phase [34], as follows:

$$D_{i,m} \frac{1}{r} \left( \frac{\partial}{\partial r} r \left( \frac{\partial C_{i,m}}{\partial r} \right) \right) + \frac{D_{i,m}}{\text{scale}^2} \frac{\partial^2 C_{i,m}}{\partial \xi^2} = 0 \quad (12)$$

The proper boundary settings are specified, as per Equation (13), as follows:

$$\begin{aligned} \text{at } z = 0, & \quad \frac{\partial C_{i,m}}{\partial z} = 0 & (a) \\ \text{at } z = H, & \quad \frac{\partial C_{i,m}}{\partial z} = 0 & (b) \\ \text{at } r = r_1, & \quad D_{i,m} \frac{\partial C_{i,m}}{\partial r} = D_{i,t} \frac{\partial C_{i,t}}{\partial r} & (c) \\ \text{at } r = r_2 & \quad C_{i,m} = C_{i,s} & (d) \end{aligned} \quad (13)$$

## 2.3. Shell Side

The steady state mass transport of solute gas ( $\text{CO}_2$  and  $\text{NO}_2$ ) components in the shell side (no chemical reaction occurs in the module shell zone) is expressed in Equation (14), as follows:

$$D_{i,s} \frac{1}{r} \left( \frac{\partial}{\partial r} r \left( \frac{\partial C_{i,s}}{\partial r} \right) \right) + \frac{D_{i,s}}{\text{scale}^2} \frac{\partial^2 C_{i,s}}{\partial \xi^2} = \frac{v_{z,s}}{\text{scale}} \left( \frac{\partial C_{i,s}}{\partial \xi} \right) \quad (14)$$

The velocity profile in the shell side is described by Happel's free surface [40] and can be calculated as per Equation (15), as follows:

$$v_{z,s} = v_{z,\max} \left\{ 1 - \left( \frac{r_2}{r_3} \right)^2 \right\} \left\{ \frac{\left( \frac{r}{r_3} \right)^2 - \left( \frac{r_2}{r_3} \right)^2 - 2 \ln \left( \frac{r}{r_2} \right)}{3 + \left( \frac{r_2}{r_3} \right)^4 - 4 \left( \frac{r_2}{r_3} \right)^2 + 4 \ln \left( \frac{r_2}{r_3} \right)} \right\} \quad (15)$$

The applicable boundary conditions are specified as follows:

$$\begin{aligned}
 \text{at } z = H, \quad C_{i,s} &= C_{i,0} & (a) \\
 \text{at } z = 0, \quad \frac{\partial^2 C_{i,s}}{\partial z^2} &= 0 & (b) \\
 \text{at } r = r_2, \quad D_{i,s} \frac{\partial C_{i,s}}{\partial r} &= D_{i,m} \frac{\partial C_{i,m}}{\partial r} & (c) \\
 \text{at } r = r_3, \quad \frac{\partial C_{i,s}}{\partial r} &= 0 & (d)
 \end{aligned} \tag{16}$$

The radius of the free surface ( $r_3$ ) can be determined as per Equation (17), as follows:

$$r_3 = r_2 \left( \frac{1}{1-\varphi} \right)^{0.5} \tag{17}$$

The void fraction of the membrane module ( $\varphi$ ) is calculated as per Equation (18):

$$\varphi = \frac{R^2 - n r_2^2}{R^2} \tag{18}$$

where  $R$  is the module inner radius,  $n$  is the number of fibers  $r_1$ , and  $r_2$  is the fiber outside radius. The parameters used in the model are shown in Table 2.

**Table 2.** Physical properties used in the model.

Physical Property	Value	Reference
Diffusivity of CO <sub>2</sub> in shell, $D_{\text{CO}_2,s}$	$1.855 \times 10^{-5} \text{ m}^2/\text{s}$	[9]
Diffusivity of CO <sub>2</sub> in tube, $D_{\text{CO}_2,t}$	$1.92 \times 10^{-9} \text{ m}^2/\text{s}$	[19]
Diffusivity of CO <sub>2</sub> in membrane, $D_{\text{CO}_2,m}$	$D_{\text{CO}_2,s} \times \varepsilon/\tau$	[37]
Diffusivity of NO <sub>2</sub> in shell, $D_{\text{NO}_2,s}$	$1.54 \times 10^{-5} \text{ m}^2/\text{s}$	[43]
Diffusivity of NO <sub>2</sub> in tube, $D_{\text{NO}_2,t}$	$1.4 \times 10^{-9} \text{ m}^2/\text{s}$	[43]
Diffusivity of solvent in tube, $D_{s,t}$	$0.5 \times D_{\text{CO}_2,t}$	Estimated
Diffusivity of NO <sub>2</sub> in membrane, $D_{\text{NO}_2,m}$	$D_{\text{NO}_2,s} \times \varepsilon/\tau$	[37]
Porosity, $\varepsilon$	0.52	[23]
Tortuosity, $\tau$	$(2-\varepsilon)^2/\varepsilon$	[9]

### 3. Numerical Solution

The model governing the partial differential and algebraic equations was solved simultaneously using COMSOL software version 5.4. The software uses a finite element method to solve the model equations.

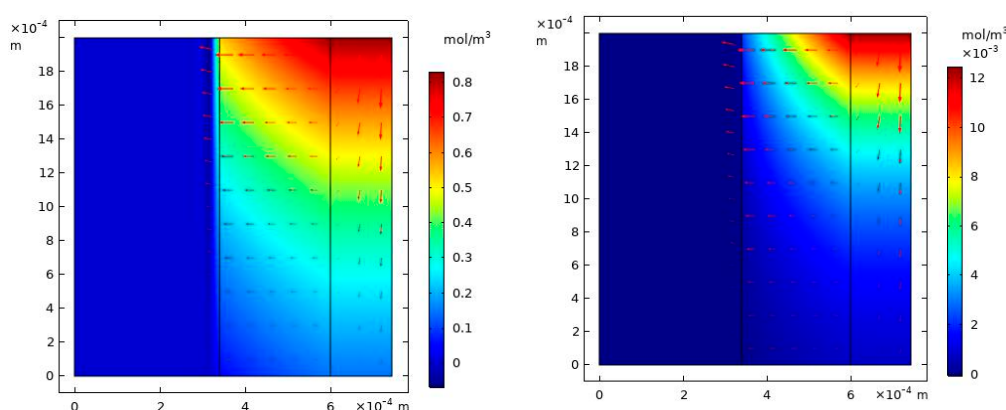
### 4. Results and Discussion

The accuracy of the mathematical model was checked prior to using the model for studying the effect of the various operating parameters on the percent deletion of CO<sub>2</sub> and NO<sub>2</sub> from the imitated flue gas. The model was authenticated with experimental data for the simultaneous absorption of an NO<sub>2</sub> and CO<sub>2</sub> from gas mixture in a PTFE polymeric gas–liquid hollow fiber membrane [23]. The percent removal of CO<sub>2</sub> and NO<sub>2</sub> was calculated as per Equation (19), as follows:

$$\% \text{Removal} = \frac{F_{g,in} C_{i,in} - F_{g,out} C_{i,out}}{F_{g,in} C_{i,in}} \times 100 \tag{19}$$

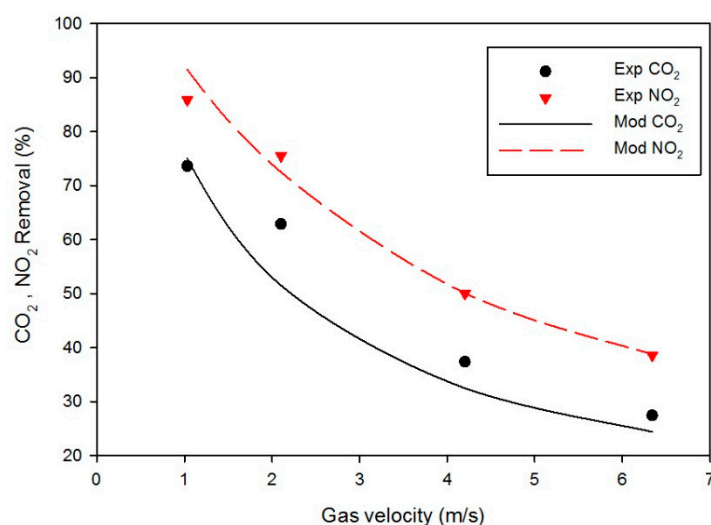
where  $F_{g,in}$ ,  $F_{g,out}$ ,  $C_{i,in}$ , and  $C_{i,out}$  are the inlet gas flow rate, outlet gas flow rate, inlet gas concentration of component  $i$ , and outlet gas concentration of component  $i$ , respectively. The 2D surface plot of the CO<sub>2</sub> and NO<sub>2</sub> concentration profile throughout the model domains are shown in Figure 2. The figure reveals that, even though the solubility of CO<sub>2</sub> (0.75) is higher than NO<sub>2</sub> (0.17) in the aqueous NaOH solution, the removal rate of nitrogen dioxide is much higher than that of carbon dioxide, which is attributed to the high reaction rate of NO<sub>2</sub>-NaOH.





**Figure 2.** The 2D surface plot for the concentration profile of CO<sub>2</sub> (left) and NO<sub>2</sub> (right) at other fixed parameters (velocity of gas: 1.05 m/s; liquid rate: 0.02 m/s; 2% CO<sub>2</sub>; 300 ppm NO<sub>2</sub>; the balance is N<sub>2</sub>, initial concentration of CO<sub>2</sub> and NO<sub>2</sub>, 0.832 mol/m<sup>3</sup>, 0.0125 mol/m<sup>3</sup>, respectively).

Figure 3. illustrates the association of this model's predictions relative to the experimental results for the effect cross-flow velocity of the feed gas on the simultaneous percent removal of CO<sub>2</sub> and NO<sub>2</sub> with fixed other parameters. A comparison of the percent removal of NO<sub>2</sub> and the experimental data obtained from the literature was in good agreement; by contrast, there is a slight variance in the case of CO<sub>2</sub>. The removal flux decreased with the increased inlet gas velocity, attributable to the low residence time.



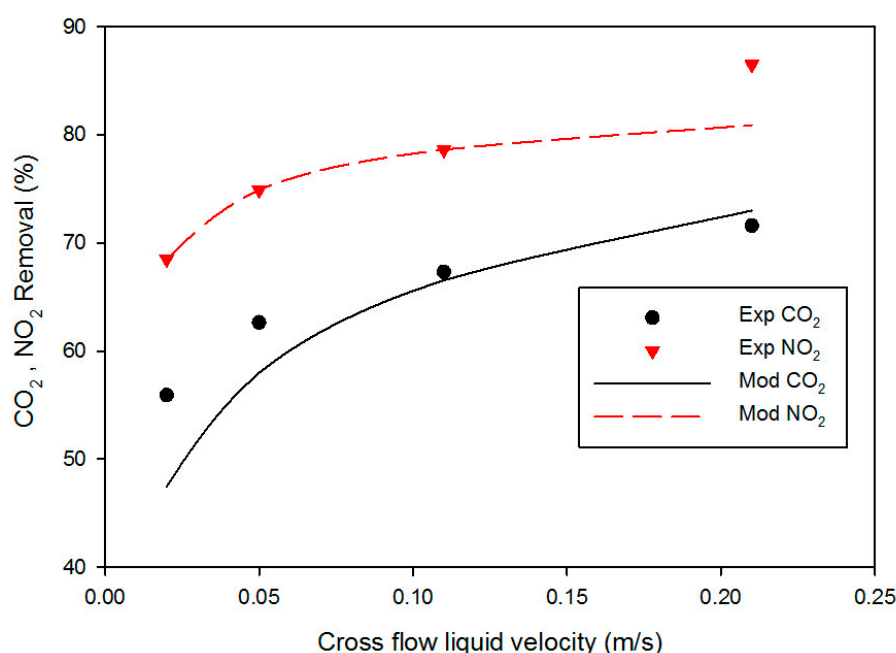
**Figure 3.** A comparison of this model's predictions and experimental data [23] for the influence of the inlet gas velocity on the simultaneous percent removal of CO<sub>2</sub> and NO<sub>2</sub> (velocity of liquid: 0.05 m/s; solvent concentration: 0.5 M NaOH; inlet gas composition: 2% CO<sub>2</sub>; 300 ppm NO<sub>2</sub>; the balance is N<sub>2</sub>).

The predicted results were also authenticated with the experimental investigations for the case of the effects of the variable liquid velocities on the percent removal of NO<sub>2</sub> and CO<sub>2</sub> (Figure 4) at a fixed gas cross-flow velocity of 2.11 m/s, 0.5 M NaOH, 2% CO<sub>2</sub>, 300 ppm NO<sub>2</sub>, and the balance was nitrogen. The simulation results matched the experimental data, to a certain extent [23]. The results revealed that the increase in solvent velocity increased the percent removal of CO<sub>2</sub> and NO<sub>2</sub> sharply at low liquid velocities (below 0.05 m/s); as the liquid velocity increased further, there was a slight increase in the percent simultaneous removal of CO<sub>2</sub> and NO<sub>2</sub> from the gas mixture. The insignificant increase in

liquid velocity higher than 0.05 m/s was attributed to a decrease in the residence time. The removal flux was calculated as per Equation (20):

$$J_i = \frac{(y_{i,in}Q_{in} - y_{i,out}Q_{out}) \times 273.15 \times 1000}{22.4 \times T_g \times A} \quad (20)$$

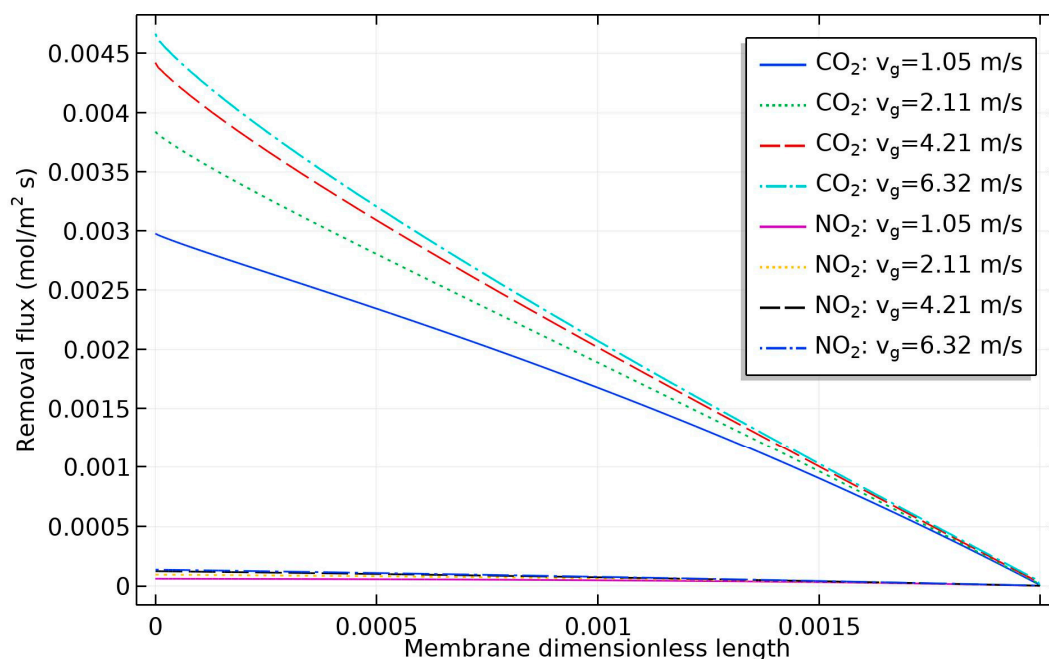
where  $J_i$  is the removal molar flux of component  $i$  ( $\text{mol/m}^2\cdot\text{s}$ ),  $y_{i,in}$ ,  $y_{i,out}$  are the inlet and outlet molar fraction of component  $i$  in the gas phase,  $Q_{in}$ ,  $Q_{out}$  are the inlet and outlet gas volumetric flow rate ( $\text{m}^3/\text{s}$ ), respectively, in gas molar volume (liter/mol) at standard conditions (1 atm and 0 °C) is 22.4;  $A$  is the membrane surface area ( $\text{m}^2$ ); 1000 is the conversion factor ( $\text{liter/m}^3$ );  $T_g$  is the gas temperature in K. The 273.15 is the temperature at 0 °C (273.15 K).



**Figure 4.** Effect of flow rate of absorbent on the percent removal of undesired gas (gas flow rate = 2.11 m/s, solvent concentration: 0.5 M NaOH; inlet gas composition: 2% CO<sub>2</sub>; 300 ppm NO<sub>2</sub>; the balance is N<sub>2</sub>).

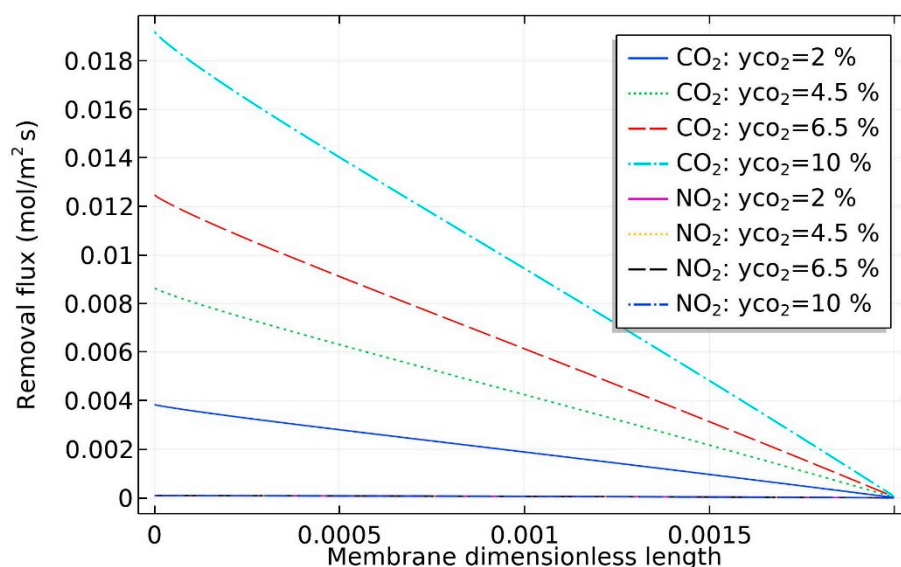
The influence of the speed of the gas on the molar flux of CO<sub>2</sub> and NO<sub>2</sub> is illustrated in Figure 5. The figure reveals that there was noticeable increase in the removal flux of CO<sub>2</sub> with the gas velocity; by contrast, the removal flux of NO<sub>2</sub> was insignificant because of its lower inlet concentration in the gas stream (300 ppm), compared with the CO<sub>2</sub> inlet concentration (2%). When the velocity of gas was increased from 1.05 m/s to 2.11 m/s, the removal flux increased from 0.003 to 0.0038  $\text{mol/m}^2\cdot\text{s}$ ; at a high gas velocity, the increase was insignificant, from example, with the increase in gas velocity from 4.21 to 6.32 m/s, the increase in molar flux was very small. This was attributed to a decrease in residence time, as well as the insufficient amount of solvent available for the excess amount of CO<sub>2</sub> and NO<sub>2</sub> components associated with the increase in gas stream volumetric feed rate.





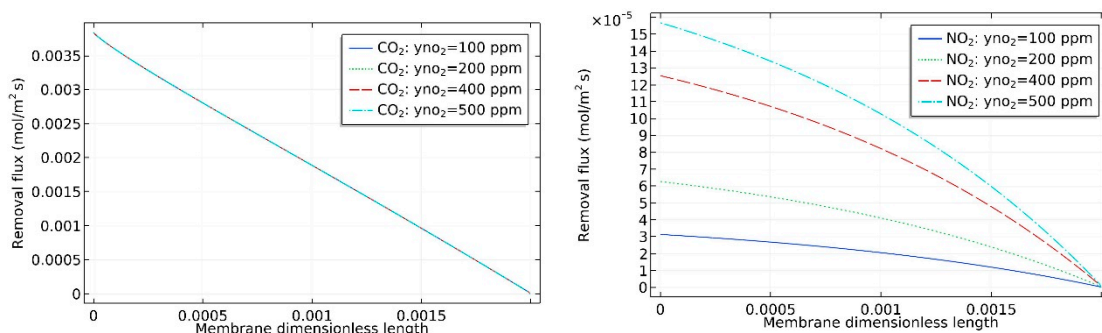
**Figure 5.** Effect of the variable gas velocities on the NO<sub>2</sub> and CO<sub>2</sub> removal flux along the membrane length with fixed other parameters (concentration of NaOH: 0.5 M; velocity of solvent: 0.05 m/s; gas composition: 2% CO<sub>2</sub>; 300 ppm NO<sub>2</sub>; the balance is N<sub>2</sub>).

Figure 6 demonstrates the effect of the change in the inlet CO<sub>2</sub> mole fraction at a fixed inlet concentration of NO<sub>2</sub> (300 ppm) on the component's molar flux. The CO<sub>2</sub> molar flux increased significantly when its concentration increased, which was expected, because as the amount of CO<sub>2</sub> increased in the inlet gas stream, more CO<sub>2</sub> was being absorbed, and hence the CO<sub>2</sub> removal molar flux increased (molar flux: moles gas removed per area per time). By contrast, because of the fixed low concentration of NO<sub>2</sub> in the feed stream, its removal flux was insignificant compared to that of CO<sub>2</sub>.



**Figure 6.** Impact of the inlet CO<sub>2</sub> feed concentration on the NO<sub>2</sub> and CO<sub>2</sub> capture flux along the membrane length at other fixed parameters (aqueous NaOH: 0.5 M; velocity of solvent: 0.05 m/s; gas velocity: 2.11 m/s; gas composition: (2% to 10%) CO<sub>2</sub>; 300 ppm NO<sub>2</sub>; the balance is N<sub>2</sub>).

Figure 7 explains the effect of change in the inlet  $\text{NO}_2$  mole fraction in the feed gas stream at a fixed concentration of  $\text{CO}_2$  (2%) on the removal flux of  $\text{CO}_2$  and  $\text{NO}_2$ . The predicted results are in the range of the experimental data [23] under the same conditions. The effect of change in the inlet mole fraction of  $\text{NO}_2$  on the  $\text{CO}_2$  removal flux was insignificant, the  $\text{CO}_2$  removal flux was kept around  $0.004 \text{ mol/m}^2\cdot\text{s}$  and was not influenced by the change of the  $\text{NO}_2$  inlet mole fraction. By contrast, there was a slight increase in the removal flux of  $\text{NO}_2$  which caused an increase from  $3 \times 10^{-5}$  to  $15 \times 10^{-5} \text{ mol/m}^2\cdot\text{s}$ . This was attributed to the low inlet concentration of  $\text{NO}_2$  (in ppm) compared with the  $\text{CO}_2$  inlet concentration (2%), and consequently, the amount absorbed from  $\text{CO}_2$  and  $\text{NO}_2$  did not change significantly.



**Figure 7.** Effect of  $\text{NO}_2$  mole fraction in the feed gas stream on the removal molar flux of  $\text{CO}_2$  (left) and  $\text{NO}_2$  (right) at other fixed parameters (liquid velocity:  $0.05 \text{ m/s}$ ; gas velocity:  $2.11 \text{ m/s}$ ;  $0.5 \text{ M NaOH}$ ; 100 to 500 ppm  $\text{NO}_2$ ; 2%  $\text{CO}_2$ ; the balance is  $\text{N}_2$ ).

## 5. Conclusions

Model equations based on material balance were utilized to describe and study the simultaneous detention of  $\text{NO}_2$  and  $\text{CO}_2$  with aqueous  $\text{NaOH}$  solution in a membrane module. The hollow fiber membranes were fabricated from PTFE polymer. The model equations were solved, and the model predicted results were compared with data from experimental investigation available in literature. The model was found to be in good agreement with the experimental findings. The mathematical model was then employed to study the influence of the inlet flow rate of gas and liquid, concentration of  $\text{CO}_2$  and  $\text{NO}_2$  in the feed stream on their percent removal and molar flux. The results revealed that the increase in  $\text{CO}_2$  inlet mole fraction and gas cross-flow velocity shows a strong impact on the molar flux. By contrast, the change in the  $\text{NO}_2$  inlet concentration showed insignificant influence on the  $\text{CO}_2$  removal flux.

**Conflicts of Interest:** The author declare no conflict of interest.

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