Research Paper

Modeling and Simulation of CO₂ Absorption Enhancement in Hollow-Fiber Membrane Contactors using CNT–Water-Based Nanofluids

Nayef Ghasem*

Department of Chemical & Petroleum Engineering, UAE University, Alain City, UAE

Article info
Received 2018-12-23
Revised 2019-05-15
Accepted 2019-05-19
Available online 2019-05-19

Keywords
Membrane contactor
Hollow fiber
Nanofluid
CO₂ absorption
Modeling and simulation
CFD

Highlights
• Modeling of the CO₂ absorption with nanofluids in membrane contactor
• Influence of the wetting in the modeling of nanofluids was considered.
• Results of the modelling were improved by assuming partial wetting mode.
• Modeling predictions were in good agreement with experimental data.

Abstract
Absorption of CO₂ from a gas mixture containing CO₂ and nitrogen by water-based CNT nanofluids in gas–liquid hollow fiber membrane contactor was modeled and solved using COMSOL Multiphysics 5.4. The model assumed partial wetting of the membrane, along with diffusion in the axial and radial directions. In addition, Brownian motion and grazing effects were both considered in the model. The main contribution to the mass transfer resistance for the case of external diffusion-controlled adsorption is the stagnant liquid layer around the particles, despite the layer being very thin. Accordingly, the nanofluid flows in the lumen tube side of the hollow fiber membrane was modeled as a solid-free zone and dense solid phase. The simulations were performed using 7% wetting of the membrane thickness. The results showed a significant increase in CO₂ absorption with increasing concentration of carbon nanotubes (CNT). At a fixed inlet gas flow rate (20 L/h), increasing the CNT concentration from 0.1 wt.% to 0.25 wt.% increased the CO₂ removal from around 20% to 45%. Comparison of the model predictions with experimental data available in the literature confirmed the validity of the developed model.

1. Introduction
Huge amounts of carbon dioxide (CO₂) are being emitted into the atmosphere due to the increase in fossil fuel consumption, the majority of which release carbon dioxide [1]. The carbon dioxide and other pollutants released into the atmosphere act like a blanket, trapping the sun's heat and causing the planet to warm. The resulting weather patterns are making wet areas become wetter and dry areas become drier [2]. Natural gas is generally considered as a cleaner fuel than other fossil fuels, although it contains undesirable compounds such as CO₂ and H₂S. These impurities must be removed to meet the pipeline quality standards and consumer fuel specifications to avoid corrosion of the pipelines and equipment and enhance the calorific value of the natural gas [3].

Absorption processes, such as packed bed or tray columns, are currently used to remove acidic gases from natural gas and flue gas. However, despite the great advantages of conventional gas–liquid absorption columns, these systems have drawbacks including channeling, entrainment, frothing, and liquid overflow [4,5]. Gas–liquid hollow fiber membrane contactors are a promising and efficient technology for removing CO₂ from gas mixtures. The separation process has been extensively investigated and the process has been recommended by many researchers [6-13]. In these systems, the membrane module is comprised of bunches of hollow fiber membranes surrounded by an external metal casing (referred to here as the shell). Usually, the liquid solvent flows through a central distribution tube inside the membrane bundle, while the gas mixture enters from the casing side. However, vice versa is also possible. The large membrane surface area per unit volume is the main advantage of the membrane contactor compared to traditional contacting columns [14-19].

Nanofluids have been used to increase the rate of absorption of the solute gas in membrane contactors. These fluids contain nanoparticle materials such as carbon nanotubes (CNT), SiO₂, Al₂O₃, and Fe₃O₄ in a base fluid, such as distilled or deionized water or amine solutions [20,21]. A schematic diagram...
of a gas–liquid hollow fiber membrane contactor with a nanofluid flowing through the lumen tube side of the hollow fiber membranes is shown in Figure 1. In this case, a CO₂/N₂ gas mixture flows in the shell side of the membrane module.

The absorption of CO₂ in the presence of solid nanoparticles (SiO₂, Al₂O₃, CNT, and Fe₂O₃) in water and amine solutions has been experimentally investigated in a batch process to study the influence of the nanofluids on the enhancement of the absorption of carbon dioxide from gas mixtures [22]. They showed that Fe₂O₃ and CNT nanoparticles showed better CO₂ absorption at lower concentrations, while SiO₂ and Al₂O₃ nanoparticles had better performance at higher concentrations. Simultaneous absorption of CO₂ and H₂S in water using SiO₂ and expandable graphite oxide nanoparticles was experimentally investigated in a bubble column by Esmaeili et al. [23]. They found that synthetic silica nanofluid absorbed both H₂S and CO₂ better than the base fluid owing to hydrogen bonding between the gas molecules and silica groups. A significant increase in the CO₂ removal fraction using Al₂O₃ or SiO₂ nanoparticles in methanol solvent in a bubble type absorber was demonstrated [24]. Absorption of CO₂ from CO₂/air gas mixtures using aqueous nanofluids in a microporous polypropylene membrane module was experimentally investigated [25-30], where a CNT nanofluid showed better separation than a silica nanofluid. The removal fraction of the CNT nanofluid was nearly constant and increased with increasing CO₂ concentration, while that of the silica nanofluid decreased slightly with increasing CO₂ concentration due to saturation. CO₂ removal from N₂ by metal oxide nanofluids in a hollow fiber membrane contactor was experimentally investigated [31], where an aqueous 0.2 wt.% Al₂O₃ nanofluid achieved the maximum CO₂ removal rate. The effect of nanoparticle size of aqueous silica-based nanofluids on CO₂ absorption was investigated, where mass transfer was enhanced with increasing silica particle size [32].

In addition to experimental studies, numerous models have been developed to investigate hollow fiber membrane systems. Modeling of CO₂ and H₂S capture using aqueous monoethanolamine solvent was demonstrated previously as a function of CO₂ concentration across the membrane module [18]. The modeling was performed for gas flows in hollow fiber membranes operated under non-wetted or partially wetted conditions. The absorption of oxygen in the presence of nanoparticles was studied by Nagy et al. [21]. Mathematical models for both homogeneous and heterogeneous modes were developed and analyzed. The absorption rate in the presence of nanosized droplets was measured, and the enhancement of the mass transfer rate was analyzed.

Experimental data were compared to the predicted ones. Mathematical models have been developed to study CO₂ absorption in the presence of nanofluids. For example, experimental and theoretical studies were performed using nano-Al₂O₃ and CNTs in a stirred thermostatic reactor [27]. They found that Brownian motion caused micro-convection and should be considered in the analysis. Their theoretical model considered the absorption enhancement provided by the nanoparticles. Koronaki et al. developed a numerical approach to study the enhancement of CO₂ absorption using CNTs in a batch vessel [28] and observed an increase in absorption over time until an equilibrium point was reached, which is commonly observed for batch systems. Darabi et al. [29] developed a 2D mathematical model to simulate the absorption of CO₂ enhanced by a CNT nanofluid in a hollow fiber membrane contactor under non-wetted conditions. The model considers the fluid flow in the tube side as a highly dilute system; hence, the fluid flow in the lumen side of the fiber is considered a single zone and described by one continuity equation. In this case, the micro-convection effect is not considered as the flow field around the nanoparticles interacts, enhancing diffusion of the absorbed solute. In addition, the enhanced CO₂ absorption by CNT and SiO₂ nanoparticles in distilled water was mathematically modeled and the influence of certain operating parameters on the CO₂ removal rate was studied [30]. The model was developed considering radial and axial diffusion under non-wetting conditions. None of the previous models discussed here considered partial wetting of the membrane.

In the present work, a 2D mathematical model was developed to elucidate the process of enhanced absorption of CO₂ from CO₂/N₂ gas mixtures in the presence of aqueous nanofluids in a hollow fiber membrane contactor under partial wetting of the membrane. Because the resistance to flow is mainly due to the stagnant layer of liquid around the solid nanoparticles, the model divides the membrane contactor module into five segments, two in the tube side (dense and solid free-phase), membrane (wetted zone and dry zone), and shell-side gas-phase region. The influence of the nanoparticle motion is considered in the dense phase of the tube side. Partial wetting of the membrane skin is assumed in the model. Polypropylene hollow fiber membranes wet using various absorbents (deionized water, monoethanolamine (MEA), and methyldiethanolamine (MDEA)) were experimentally investigated by Lv et al. [33]. They observed an increase in mass transfer resistance and a deterioration in CO₂ absorption performance during the membrane gas absorption process for all absorbents. Hence, the equations in the present model considered membrane wetting. The governing equations were solved numerically using the finite element method with COMSOL Multiphysics version 5.4 software. The model predictions were validated by comparison with experimental data reported in the literature. In addition, the effects of the physical characteristics of the nanoparticles and operating parameters of the system on the membrane performance were investigated.
2. Mathematical model

The mathematical model describes the bunch of hollow fiber membranes packed in the membrane module. Modeling of the membrane contactor module considering a cylindrical coordinate system resulted in a set of partial differential and algebraic equations that defined the material balance of the physical absorption of CO$_2$ using a nanofluid solvent composed of distilled water and CNTs. The membrane contactor consisted of three parts: tube, membrane, and shell section. The tube side where the nanofluid flows is modeled as a solid-free zone and dense phase. The membrane section is divided into wetted and non-wetted segments. The CO$_2$/N$_2$ gas mixture flows outside the hollow fiber membranes, while the nanofluid flows through the lumen of the hollow fiber membrane tubes in a counter-current manner, as described in Figure 2. The CO$_2$/N$_2$ gas mixture enters the membrane module from the top side (at $z = L$), while the nanofluid enters the lumen of the hollow fibers from the bottom side (at $z = 0$) in the case of vertical operation of the membrane module. Carbon dioxide diffuses from the gas mixture through the membrane pores to the nanofluid. The ability of N$_2$ to dissolve in an aqueous solvent is insignificant compared to that of CO$_2$. Hence, some of the CO$_2$ dissolved in the nanofluid is adsorbed on the solid nanoparticles. The CO$_2$ removal rate depends on the morphology of the polymeric membrane, distribution factor of CO$_2$, type of aqueous solvent, absorbent and nanoparticle concentrations, liquid and gas flow rates, and operating conditions.

The fluid flow is incompressible and Newtonian, concentration of CNT nanoparticles are considered homogeneous and uniformly distributed in the interface layer [27]. The fluid flow in the tube side is assumed to be fully developed neglecting end effects and the influence of the nanoparticles due to low concentration. The gas velocity in the shell side follows the Happel’s free surface model.

Based on Happel’s free surface [34], the tubes are bounded by a laminar gas flow in the opposite direction to that of the liquid. At the Happel’s hypothetical free surface of the fiber ($r = r_f$), symmetry is assumed. The steady state model assumed constant solvent properties, an ideal gas, and that the nanoparticles are spherical and homogeneous. The mathematical equations that describe the system behavior are developed for the tube side (solid and liquid phase), microporous membrane (wetted and non-wetted zones), and shell side. Accordingly, the continuity equations for CO$_2$ absorption are described in the following sections.

2.1. Tube Side: ($0 \leq r \leq r_f$)

The nanofluid contains nanoparticles suspended in a base fluid. In the model developed here, the nanoparticles are CNTs and the base fluid is water. The CNTs are black tubular nanostructures with an outer diameter of 8 nm, inner diameter of 2–5 nm, and length of 10 µm [26]. The nanofluid flowing in the lumen of the hollow fiber membranes removes CO$_2$ in the gas stream by absorption by the water and adsorption by the nanoparticles. The concentration of CO$_2$ in the solution free of solid particles ($C_D$) is written as follows:

$$D \frac{\partial^2 C_D}{\partial z^2} + \frac{1}{L} \frac{\partial C_D}{\partial z} + \frac{u_{z,s} \partial C_D}{L} = 0$$

(1)

The concentration of CO$_2$ in the dense phase ($C_{AD}$) is:

$$D \frac{\partial^2 C_{AD}}{\partial z^2} + \frac{1}{L} \frac{\partial C_{AD}}{\partial z} + \frac{u_{z,s} \partial C_{AD}}{L} = -R_d$$

(2)

The dimensionless parameters used in Eq. (1) and Eq. (2) are $\xi = z/L$ and $\xi = r/r_f$, where $D$ is the diffusion coefficient of CO$_2$ in the solid free zone and $D_{AD}$ is the diffusion coefficient of CO$_2$ in the dense solid phase. The diffusion coefficient of CO$_2$ in the dense phase liquid film around the nanoparticles can be written as follows [21]:

$$D_{n,s} = D \left(1 + 640 \text{Re}^{-1.7} \text{Sc}^3 \phi \right)$$

(3)

Here, $\phi$ is the solid volume fraction, and the Reynolds number, Re, of the nanoparticles under Brownian motion is:

$$\text{Re} = \frac{18 k T \rho P}{\pi d_p \rho_p \mu^2}$$

(4)

where $k$ is Boltzmann’s constant ($1.38 \times 10^{-23} \text{ J/K}$), $T$ is the temperature (K), $\rho$ is the liquid density, $d_p$ is the particle diameter, $\rho_p$ is the particle density, and $\mu$ is the viscosity of the liquid. The Schmidt number Sc is written as:

$$\text{Sc} = \frac{\mu}{\rho D}$$

(5)

The adsorption rate $R_d$ is written as:

$$R_d = k_p a_p (C_{AD} - C_{AS})$$

(6)

where $k_p$ is the solid–liquid mass transfer coefficient (m s$^{-1}$), $a_p$ is the solid–liquid interfacial area (m$^2$ m$^{-3}$), $C_{AD}$ is the solute concentration in the suspension (mol m$^{-3}$), and $C_{AS}$ is the solute concentration at the interface of the particles (mol m$^{-3}$). The amount of CO$_2$ absorbed on the solid per unit mass of particles, $q$ (mol kg$^{-1}$) can be given by:

$$\phi \rho_p \frac{v_{z,s} \partial q}{L} = k_p a_p (C_{AD} - C_{AS})$$

(7)
The adsorption of the solute CO$_2$ on the particles is described by:

$$q = q_{_{\text{wm}}} \frac{k_d C_{_{\text{AS}}} }{1 + k_d C_{_{\text{AS}}}}$$

(8)

where, $q_{_{\text{wm}}}$ is the highest quantity of adsorbed gas solute, and $k_d$ (m$^{-1}$ mol$^{-1}$) is the adsorption coefficient of the solute. The velocity distribution in the tube side ($v_{_{\text{zc}}}$) is assumed to follow Newtonian laminar flow.

$$v_{_{\text{zc}}} = \frac{2Q_x}{\pi r_t^4} \left( 1 - \left( \frac{r}{r_t} \right)^2 \right)$$

(9)

The boundary conditions of the tube side are given as:

Solvent inlet side: $z = 0$ (fresh solvent)

Solvent exit side: $z = L$ (convective flux)

Tube center: $r = 0$ (axial symmetry)

Inner radius: $r = r_1$ (solubility of CO$_2$ in solvent)

2.2. Skin layer of the hollow fiber membrane $r_1 \leq r \leq r_2$

2.2.1. Wetted section of membrane ($r_1 \leq r \leq r_w$)

The steady-state material balance for CO$_2$ transport inside the wetted portion of the membrane is shown in Equation (14); there is no convection term as only diffusion is taking place in the wetted membrane.

$$\frac{\partial}{\partial z} \left( D_{_{\text{wm}}} \frac{\partial C_{_{\text{wm}}} }{\partial z} \right) + \frac{\partial}{\partial \xi} \left( D_{_{\text{wm}}} \frac{\partial C_{_{\text{wm}}} }{\partial \xi} \right) = 0$$

(14)

The boundary conditions in this zone are given as:

Tube–wetted-membrane interface: $r = r_1$

Wet–dry membrane interface: $r = r_2$

Membrane inlet end: $z = 0$

Membrane exit side $z = L$

2.2.2. Non-wetting section of the membrane ($r_w \leq r \leq r_2$)

The steady state material balance for the transport of CO$_2$, inside the membrane ($C_{_{\text{Ag}}}$), no convection term, only diffusion is taking place in membrane.

$$\frac{\partial}{\partial z} \left( D_{_{\text{m}}} \frac{\partial C_{_{\text{m}}} }{\partial z} \right) + \frac{\partial}{\partial \xi} \left( D_{_{\text{m}}} \frac{\partial C_{_{\text{m}}} }{\partial \xi} \right) = 0$$

(19)

The boundary conditions are given as:

Interface of membrane-tube: $r = r_w$

Membrane-shell interface: $r = r_2$

Dry membrane inlet end: $z = 0$

Dry membrane exit side $z = L$

The diffusivity of CO$_2$ in the non-wetted membrane section, $D_{_{\text{m}}} = D_{_{\text{g}}} \xi^2 / \ell$. The material balance of the gas solute in the shell side at steady state ($C_{_{\text{Ag}}}$) is:

$$\frac{\partial}{\partial z} \left( D_{_{\text{g}}} \frac{\partial C_{_{\text{g}}} }{\partial z} \right) + \frac{\partial}{\partial \xi} \left( D_{_{\text{g}}} \frac{\partial C_{_{\text{g}}} }{\partial \xi} \right) + v_{_{\text{zc}}} \frac{\partial C_{_{\text{Ag}}}}{\partial \xi} = 0$$

(24)

The boundary conditions:

Gas inlet side: $z = L$ (inlet concentration)

Gas exit side: $z = 0$ (convective flux)

Free surface: $r = r_3$ (symmetry)

Shell-membrane interface: $r = r_2$

Assuming Happel’s free surface model [34], the axial velocity in the shell side is expressed as:

$$v_{_{\text{zc}}} = \frac{2Q_x}{\pi (r_t^2 - r_3^2) \ln \left( \frac{r_t}{r_3} \right)} \left[ \frac{r_3^2 - r_2^2}{r_2^4 - r_3^4} \ln \left( \frac{r_2}{r_3} \right) \right]$$

(29)

Table 1 contains the parameters used in the simulation. The COMSOL Multiphysics 5.4 software package was used to solve the set of partial differential equations that described the separation process.
Table 1
Characteristics of the polypropylene membrane module and operating parameters used in the model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner fiber tube diameter (m)</td>
<td>0.32×10^{-2}</td>
<td>[26]</td>
</tr>
<tr>
<td>Outer fiber tube diameter (m)</td>
<td>0.45×10^{-2}</td>
<td>[26]</td>
</tr>
<tr>
<td>Inner module diameter(m)</td>
<td>2×10^{-2}</td>
<td>[26]</td>
</tr>
<tr>
<td>Module length (m)</td>
<td>40×10^{-2}</td>
<td>[26]</td>
</tr>
<tr>
<td>Total number of tubes</td>
<td>400</td>
<td>[26]</td>
</tr>
<tr>
<td>Membrane contact area (m²)</td>
<td>0.16</td>
<td>[26]</td>
</tr>
<tr>
<td>CNT true density (g/cm³)</td>
<td>2.2</td>
<td></td>
</tr>
<tr>
<td>CNT absorption capacity (mol/g)</td>
<td>1.57×10^{-2}</td>
<td>[26]</td>
</tr>
<tr>
<td>$D_{ax} (m^2/s)$</td>
<td>2.35×10^{-6} e^{2199/ \tau}</td>
<td>[35]</td>
</tr>
<tr>
<td>$D_{ap} (m^2/s)$</td>
<td>1.85×10^{-6}</td>
<td>[36]</td>
</tr>
<tr>
<td>$D_{am} (m^2/s)$</td>
<td>$D_{ap}/\tau$</td>
<td>Calculated</td>
</tr>
<tr>
<td>$D_{e excl} (m^2/s)$</td>
<td>0.5D_{ax}</td>
<td>Calculated</td>
</tr>
<tr>
<td>$m = 1/H$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H = 2.82×10^4 \exp\left( \frac{-2046}{T}\right)/RT$</td>
<td>[35]</td>
<td></td>
</tr>
<tr>
<td>Porosity, $\varepsilon$</td>
<td>0.50</td>
<td>[35]</td>
</tr>
<tr>
<td>Tortuosity, $\tau$</td>
<td>$(2-\varepsilon)^2/\varepsilon$</td>
<td>[37]</td>
</tr>
</tbody>
</table>

3. Results and discussion

3.1. Model validation

The modeled surface plot of CO₂ concentration across the membrane module (tube, wet and dry membrane zones, and shell sides) is presented in Figure 3. An initial feed concentration of CO₂ of 0.5 mol·m⁻³ was selected to match the conditions used to generate experimental data [26] later used to validate the current mathematical model. The surface plot shows that the CO₂ concentration was much lower on the shell side than within the membrane and tube. This lower CO₂ concentration is attributed to absorption of the diffused CO₂ by the solvent. The arrows in Figure 3 represent the total CO₂ diffusion fluxes, where the smaller arrows in the membrane area are due to the slow diffusion flux through the membrane micropores.

The effect of inlet gas flow rate on the CO₂ removal rate along the gas-membrane interface is shown in Figure 4. The CO₂/N₂ gas mixture enters the membrane shell opposite to the solvent inlet port. The CO₂ is at its maximum initial feed concentration at the inlet port ($z = L$); hence, the removal rate is zero. As the gas mixture flows downward through the membrane shell side, CO₂ diffuses through the membrane to the nanofluid liquid solvent flowing in the lumen of the hollow fibers in the opposite direction, where the CO₂ is dissolved and consumed, resulting in a decrease in CO₂ concentration (increase in removal rate) as it travels through the shell side. The CO₂ removal rate decreases with increasing gas flow rate due to a reduction in the residence time of the gas inside the membrane module.

The differences between the predicted results and the experimental data were quantified using the root mean square error (RMSE), as follows:

$$\text{RMSE} = \left( \frac{\sum (\varepsilon_{ij})^2}{n} \right)^{0.5}$$

(30)

where $n$ is the sum of the investigated data points and $\varepsilon_{ij}^2$ is the square of the error between the predicted and experimental data point. The relative error ($\varepsilon_{rel}$) is as follows:

$$\varepsilon_{rel} = \frac{y_{\text{exp}} - y_{\text{mod}}}{y_{\text{exp}}}$$

(31)

where $y_{\text{exp}}$ and $y_{\text{mod}}$ are the experimental and predicted data points. The RMSE values of the distilled water and CNT/water systems were 0.074 and 0.057, respectively, indicating that the present model accurately predicts...
Experimental membrane behavior. The results showed that, even though the CO$_2$ removal rate decreases with increasing gas flow rate, the mass transfer coefficient increases with increasing flow rate of the gas mixture [29].

Further comparison of the predicted results from the present model with those from another model that did not consider the wetting and dense phase resistance to mass transfer [29] showed that the results of the present model better matched the experimental data, as shown in Figure 6. This confirms that polypropylene polymeric membranes operate under partially wetted conditions when under the influence of pressure [31].

Figure 7 shows that the enhancement factor as a function of inlet gas flow rate predicted by the present model agrees well with experimental data from the literature [26]. In addition, for a fixed nanoparticle concentration, the inlet gas flow rate did not significantly affect the enhancement factor; as the nanoparticles are saturated, increasing the flow rate does not result in further improvements. Similarly, the effect of nanoparticle volume fraction on the enhancement factor is shown in Figure 8 for the present predictions and the experimental data [26], where good agreement between the two was observed. The nanoparticle volume fraction did not significantly affect the enhancement factor, although, increasing the nanoparticle concentration theoretically increases CO$_2$ removal, and hence the enhancement factor, increasing the nanoparticle concentration can also result in particle agglomeration on the membrane surface. This can block the membrane pores, resulting in a decrease in the gas–liquid interface area and lower removal rate. In addition, the nanoparticle concentration affects the stability of the nanofluid, which can reduce the absorption efficiency of the hollow fiber membrane contactor.

To further validate the model, we demonstrated that the effect of nanofluid flow rate on the CO$_2$ removal rate predicted by the model and determined experimentally [25] were in good agreement, as shown in Figure 9. The figure indicates that the CO$_2$ removal rate increases with increasing liquid flow rate, while the CO$_2$ deduction proficiency increases with increasing liquid flow rate due to a reduction in the thickness of the resistance mass transfer film [29].

The effect of the diameter of the solid nanoparticles on the CO$_2$ removal rate is shown in Figure 10. There is a sharp decrease in the CO$_2$ removal rate for particle sizes between 10 to 200 nm, while further increase in particle size did not significantly affect the removal rate. The decrease in the removal rate with increasing particle size is attributed to the lower liquid–solid interface area, as observed by Koronaki et al. [28].

The effect of inlet gas solute mole fraction on the CO$_2$ removal flux is shown in Figure 11, where it can be seen that the removal flux increases with increasing CO$_2$ concentration. This is attributed to the further CO$_2$ molecules...
diffusing toward the membrane for higher CO₂ concentrations. The more CO₂ absorbed, the higher the removal flux. This can be ascribed to an increase in the mass-transfer driving force. In contrast, there is only a slight effect of the inlet CO₂ mole fraction on the CO₂ removal rate, as shown in Figure 12. The figure shows that the model predictions and experimental data [26] agree well; hence, the model is suitable for studying parameters other than those experimentally investigated.

4. Conclusions

A compressive mathematical model was developed to represent the CO₂ absorption enhanced by aqueous CNT nanofluids considering the partially wetted mode of a hollow fiber membrane contactor system. The model divides the membrane absorption process into five zones, where the nanofluid in the tube side is modeled as a solid-free phase and dense phase where Brownian motion and grazing effects took place. The membrane side is divided into two zones; partially wetted and non-wetted segments. The shell side through which gas flows is considered as one zone. The present model predictions were in good agreement with experimental data reported in literature and showed better results than those of a similar model that did not consider the wetting and dense phase resistance to mass transfer. This model offers a viable method for exploring the mechanisms of CO₂ capture in the existence of nanoparticles, which is a promising method for enhancing CO₂ absorption and the performance of gas-liquid hollow fiber membrane contactors. The simulation results revealed that the liquid flow rate and CNT weight fraction in the nanofluid significant affect the CO₂ removal rate. For example, at an inlet gas flow rate of 20 l h⁻¹, around 20% CO₂ removal is achieved with 0.1 wt.% CNT, and approximately 45% of the CO₂ is removed using 0.25 wt.% CNT in a water-based nanofluid.

Acknowledgement

The author would like to acknowledge UAE University for the financial support (UPAR grant number: 31N374).

Nomenclature

- $T$: Total membrane area, m²
- $A$: Inlet gas concentration, mol·m⁻³
- $C_{in}$: Outlet gas concentration, mol·m⁻³
- $C_{i}$: Concentration of component $i$; 1: CO₂, 2: N₂
- $C_{m}$: Concentration of component $i$ in the membrane section, mol·m⁻³
- $C_{w}$: Concentration of component $i$ in the wetted membrane section, mol·m⁻³
- $C_{i,m}$: Concentration of component $i$ in the shell section, mol·m⁻³
- $C_{t}$: Concentration of component $i$ in the tube section, mol·m⁻³
- $C_{L,m}$: Inlet liquid concentration, mol·m⁻³
- $C_{L}$: Outlet liquid concentration, mol·m⁻³
- $CO_{2}$: Inlet CO₂ concentration, mol·m⁻³
Diffusion coefficient of component i, m²/s

Diffusivity of CO₂ in liquid solvent at the tube side, m²/s

Diffusivity of CO₂ in gas phase at the shell side, m²/s

Diffusivity of CO₂ in membrane pores, m²/s

Diffusivity of CO₂ in solvent, m²/s

Inner diameter of hollow fiber diameter, m

Outer diameter of hollow fiber diameter, m

Henry’s constant

Length of hollow fiber membrane, m

Distribution factor

Pressure, Pa

Absorbed amount of solute, mol kg⁻¹

Maximum amount of adsorption by nanoparticles, mol kg⁻¹

Inlet gas flow rate, m³/s

Inlet liquid flow rate, m³/s

Universal gas constant, 8.314 J mol⁻¹·K⁻¹

Inlet gas temperature, K

Fluid density, kg m⁻³

Absorbed amount of solute, mol kg⁻¹

Membrane porosity

Dimensionless module radius, r/R

Dimensionless module length, z/L

Velocity of fluid inside the module in the z-direction, m s⁻¹

Velocity of gas in the shell side, m s⁻¹

Velocity of liquid in the tube side, m s⁻¹

Average velocity, m s⁻¹

Axial distance, m

Greek letters

Fluid density, kg m⁻³

Solid particle density, kg m⁻³

Volume fraction

Membrane porosity

Dimensionless module radius, r/R

Dimensionless module length, z/L

References


