RESEARCH PAPER

Determination of CO_2 gas diffusivity in nanofluids: a modeling study

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ABSTRACT

In this study, a three-dimensional model was examined for the evaluation of CO_2 diffusivity in pure water and silicon oxide, aluminum oxide and titanium oxide nanofluids with the concentrations of 0.05, 0.1, and 0.2 wt%, respectively. Different parameters such as temperature and the nanoparticles weight percentage on CO_2 diffusivity in a diffusivity cell were studied in COMSOL software. Next, CO_2 diffusivity was compared with the experimental results. The modeling results showed that water was saturated with gas at 36,000 seconds, and the highest amount of absorbed gas happened at 0.32 m. The CFD results were then validated with the experimental data. Furthermore, temperature was found to have a significant effect on the diffusivity, and it improved by increasing nanofluid concentration until the critical value of 0.1 wt% in all conditions. Moreover, TiO_2 NF was introduced as an appropriate nanofluid for the phenomenon of mass diffusivity.

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1. INTRODUCTION

In recent decades, greenhouse gases emission has created serious environmental problems [1]. The production of CO_2 as an important greenhouse gas has had devastating effects on the climate change [2, 3]. This phenomenon has increased the temperature of the earth, resulting in the melting of polar ice, rising water levels, creating sea storms, the disappearance of some islands, cities, and coastal countries [4]. The concentration of CO_2 has grown significantly since the industrial revolution, and 60% of all greenhouse gases relate to industry and the consumption of fossil fuels [5, 6]. The environmental impacts of CO_2 and its applications in various industries have attracted many researchers to CO_2 removal or reduction [7-9]. Different processes like absorption, chemical and physical absorption, refrigeration separation, and membrane technology have been used for the removal of CO_2 [10]. Amine monoethanolamine (MEA), amine diethanolamine (DEA) and amine N-methyl diethanolamine (MDEA) amines have been utilized for the CO_2 separation [11-13]; however, they had some problems such as

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environmental pollution. Nanofluids (NFs) are one of the methods which have been used by many researchers in recent years [7-9]. In 1995, the nanofluid was introduced by Choi [10]. It caused a great revolution in the field of heat transfer in fluids. In fact, a new perspective for a solid-liquid suspension with particles in the nanoscale was presented. The problems of pressure decay reduced due to the small size of the particles, their corrosion and impurities. In addition, the stability of the fluids improved in contrast to the sedimentation. Some researchers observed that the gas diffusivity increased in the presence of nanoparticles (NPs). This was described as turbulence in the layers around the NPs because of the NPs Brownian motion, which caused a small-scale convective movement, and helped to improve diffusivity [11]. For the first time, Krishnamurthy et al. reported that the diffusivity of color in nanofluids was faster than in water [10].

In a modeling study, Gholami et al. worked on the CO_2 diffusivity and suggested a numerical pressure-decay technique for the measurement of CO_2 mass diffusivity in water [11]. They calculated mass diffusivity from diffusion, the first of the convection (beginning of the second period), and the maximum Sherwood number (beginning of the third period of dissolution). Hajilary et al. analyzed the CO_2 elimination in a hollow fiber membrane by CFD simulation [11]. They used carbon nanotubes (CNTs) and silica nanofluids and compared them with experimental results. They reported an acceptable validation between the model and the experimental data, and confirmed that the CO_2 capture increased by increasing the absorbent. Their findings showed that the removal percentage for CNT and SiO_2 for 0.5 wt.% with 40 L/h liquid flow rate, were 54% and 38% for SiO_2, respectively. Consequently, CNT NF was introduced as a suitable absorbent for the CO_2 separation in HFMC.

Mohammaddoost et al. measured the CO_2 elimination through a HFMC [4]. They used the nanofluids containing Al_2O_3, TiO_2, and SiO_2. The study showed that the highest CO_2 removal was 98.9% for Al_2O_3 (40 nm) at the temperature of 25℃ and 40% CO_2 concentration. Azin et al. modeled the CO_2 diffusivity in a saline aquifer [12]. They reported that CO_2 mass diffusivity varied from (3.52-5.98) $\times 10^{-9}$ m^2/s for 5900 KPa to (5.33-6.16) $\times 10^{-9}$ m^2/s for the initial pressure of 6900 KPa at 32-50˚C.

The main goal of this work was to analyze a comprehensive three dimensional (3D) model to evaluate the CO_2 diffusivity in a cell using SiO_2, Al_2O_3, and TiO_2 nanoparticles from Dehghan et al. experimental study [13]. The effects of the temperature and NFs concentration parameters in a diffusion cell are investigated.

2. Research Method

2.1. Governing equations and assumptions

The assumptions considered in this simulation were as follows:

1. The simulation process is 3-dimensional.
2. There is no chemical reaction in the diffusion cell.
3. The system is at unsteady state and isothermal condition.
4. The swelling of NF is negligible which shows that the nanofluid height in the diffusion cell remains constant during the test.
5. Equilibrium concentration of CO_2 in the gas-liquid interface is measured by Henry's law.

By using the assumptions, the continuity equation can be simplified as below:

$$\frac{\partial C_i}{\partial t} = D_{AB}\left[\frac{\partial^2 C_i}{\partial r^2} + \frac{1}{r}\frac{\partial C_i}{\partial r} + \frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2} + \frac{\partial^2 C_i}{\partial z^2}\right] \qquad (1)$$

The initial and boundary conditions are as follows:

$$C(z,0) = 0, \quad C_{gas}(t) = \frac{p(t)}{K_h}, \frac{\partial C(\mathrm{L},\mathrm{t})}{\partial z} = 0$$

where C and D define the gas concentration in the NF (mol/m^3) and gas diffusivity (m^2/s), respectively. t is time (s), x is the distance from the gas-liquid interface (m), and K_h is Henry's constant ($Pa.m^3/kg$).

2.2. Numerical model

In order to investigate the mass transfer diffusivity of CO_2 in nanofluids, the governing equations with suitable initial and boundary conditions were solved in COMSOL Multiphysics software by using the finite element method (FEM) in a 3D dimensional cell. In this work, the experimental data of pressure decay was used. A cylindrical cell with an inner diameter of 3.89 cm and 32 cm height was considered to determine the CO_2 diffusivity in water and NFs.

3. Results and Discussion

Figures 1 and 2 show the concentration of absorbed gas in the pure water at the temperature of 25 and 30 ºC in a diffusion cell. The following contours showed that water was saturated with gas at 36,000 seconds, and the highest amount of absorbed gas occurred at 0.32 m. At the bottom of the cell, the concentration of gas decreased, and the amount of absorbed gas was almost zero. These results showed that this volume of fluid was not needed, and the highest-pressure decay occurred in the early step and reduced until the equilibrium time. Researchers also found that natural convection and diffusion happened for the first and second steps, respectively [14, 15].

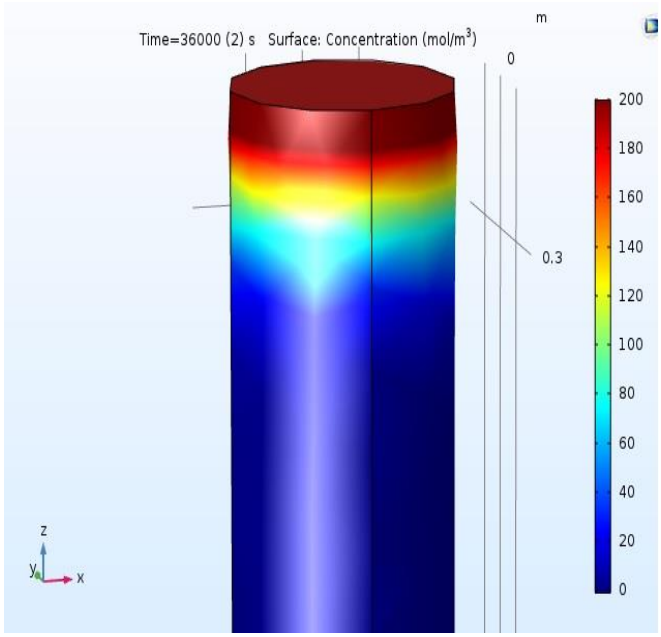

Figure 1. Concentration decay contour of absorbed gas in a diffusion cell at the temperature of 25° C

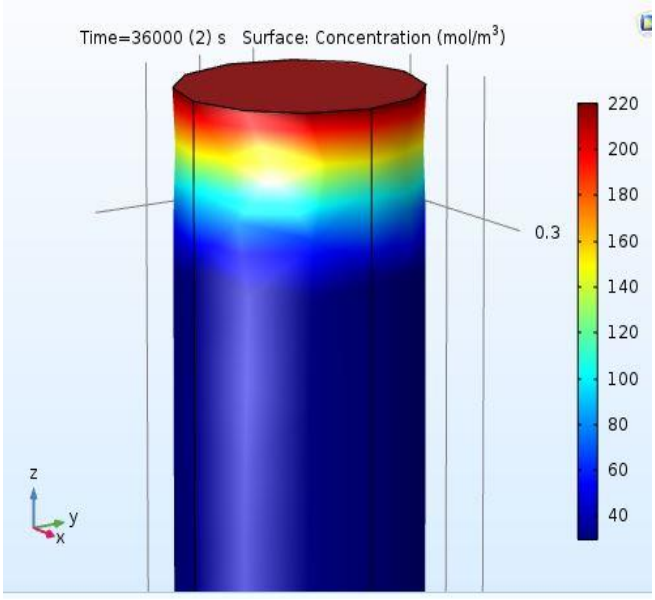

Figure 2. Concentration decay contour of absorbed gas in a diffusion cell at the temperature of 30° C

Figure 3 shows the concentration decay of absorbed gas in a diffusion cell at 35 °C. The findings presented the absorbed gas highest amount in water from the height of 0.32 to 0.26 m, which varied from 212.67 to 0.0 (mol/m^3).

Figure 4 shows the concentration of absorbed gas in pure water at the temperature of 35 °C in a diffusion cell at the height of 0.32 m and a radius of 0.01945 m. The contour shows that water is saturated with gas at 50000 seconds, which proves that the temperature enhances the CO_2 concentration in the nanofluid. The highest amount of gas was absorbed at early stage at the height of 0.32 m which was higher than CO_2 diffusivity at temperatures of 25 and 30 ℃ in the same condition.

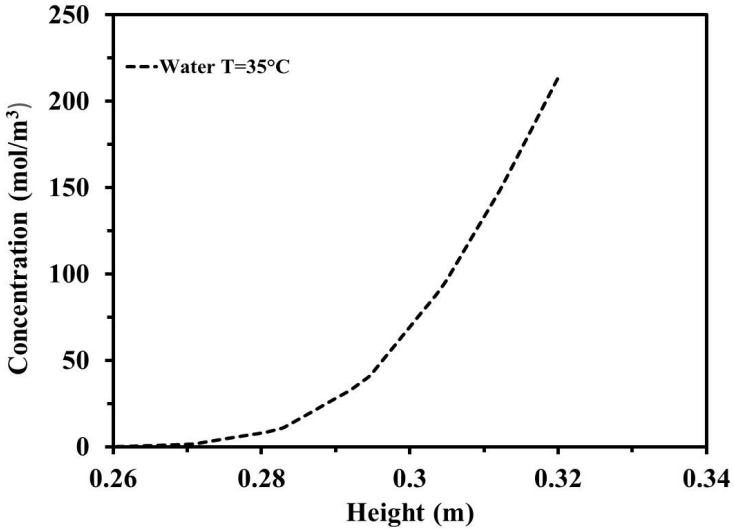

Figure 3. Concentration decay of graphs vs. height of diffusion cell

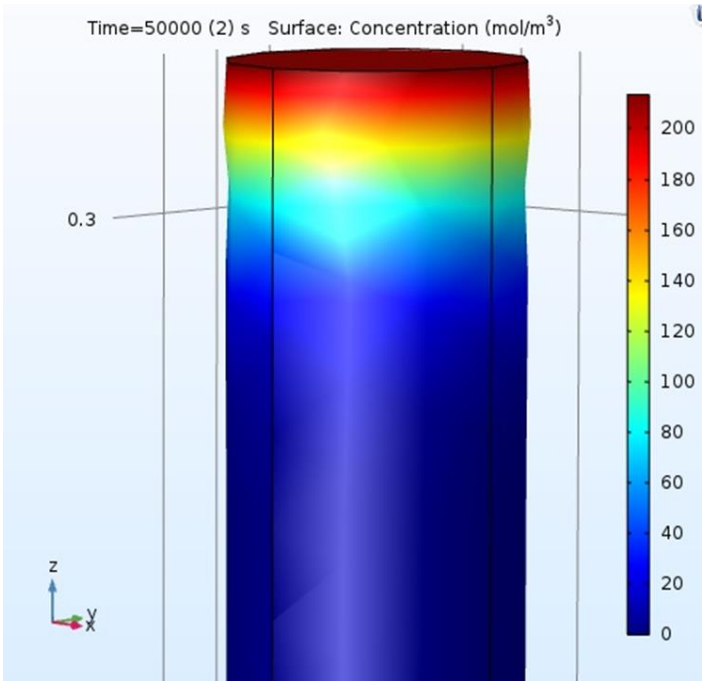

Figure 4. Concentration decay contour of absorbed gas in a diffusion cell at the temperature of 35° C

3.1. Model validation

The CO_2 diffusion coefficient simulation was compared to literature in pure water and different temperatures. As can be found from Figure 5, the results indicate a good validity between the literature and modeling results [16-18].

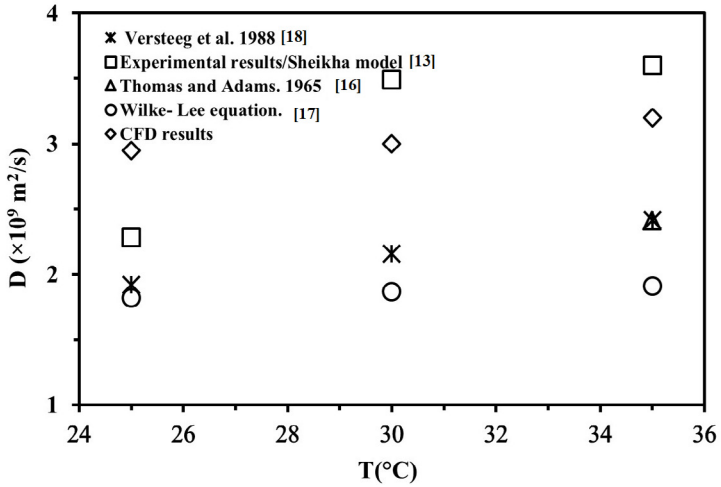

Figure 5. Comparison of CFD results and literature data in pure water

3.2. The temperature effect on CO_2 diffusivity in NFs

Figures (6-8) show a comparison of CO_2 diffusivity in SiO_2, Al_2O_3, and TiO_2 NFs with those in pure water under the same conditions. As can be seen, the diffusion coefficient in NFs is superior to that in pure water owing to the wide surface area per unit volume. The results also show that temperature is effective and can improve the efficiency of CO_2 diffusivity. Increasing the trend of nanofluids is higher than that in pure water and diffusion coefficients of CO_2 in pure water at 25, 30 and 35 ℃ are close to each other. Furthermore, the type of nanoparticle may be a significant factor in the CO_2 gas diffusivity because nanoparticles with different densities show various performance in the diffusivity process.

An increase in the fluid temperature increases the Brownian motion of NPs and the movement of particles, which in turn leads to the momentum transfer. Furthermore, the motion of NPs causes micro convection which enhances mass diffusivity of CO2 in NFs.

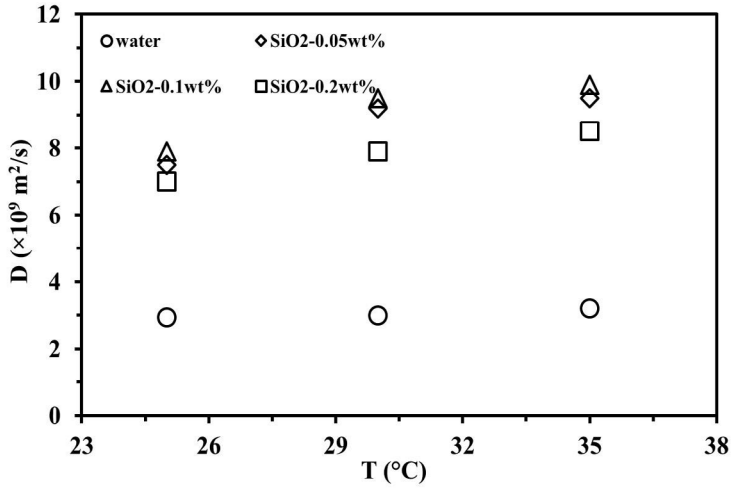

Figure 6. The temperature effect on CO_2 diffusivity in SiO_2 (20-30 nm) NF [13]

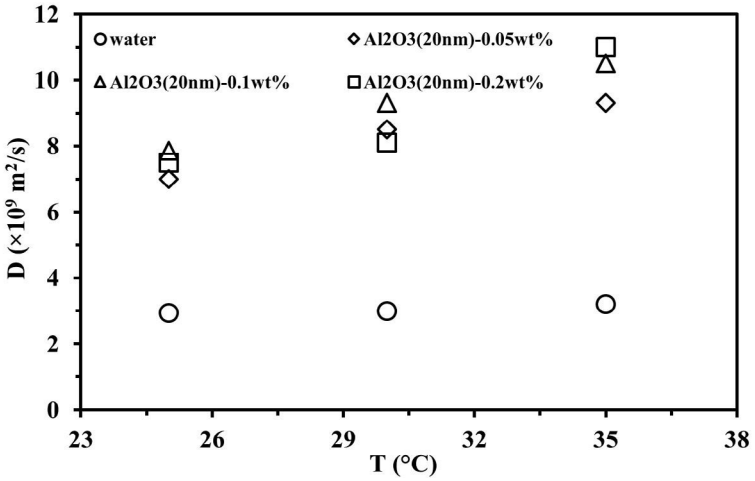

Figure 7. The temperature effect on CO_2 diffusivity in Al_2O_3 (20 nm) NF [13]

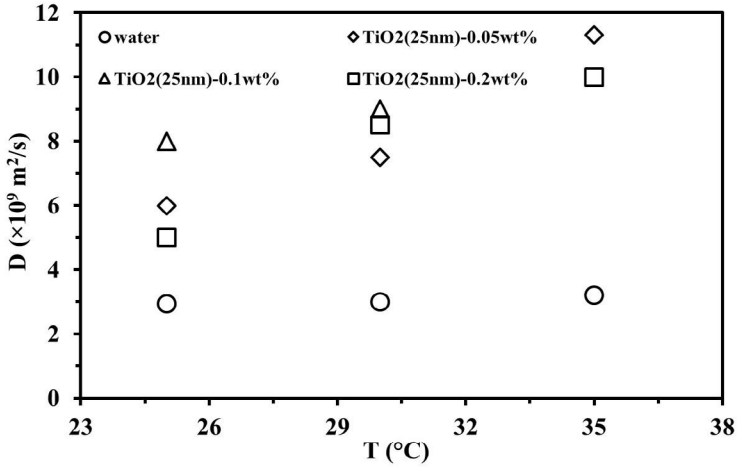

Figure 8. The effect of temperature on CO_2 diffusivity in TiO_2 (25 nm) NF [13]

The gas molecules are absorbed at the gas-liquid interface and enter the mass transfer layer and bulk liquid [19-21].

3.3. The NF concentration effect on CO_2 diffusivity

Another parameter that enhances mass diffusivity is the NFs concentration. Figures (9-11) show the modeling results of the role of NFs concentration in the CO_2 diffusivity. This improved by increasing the NFs concentration to the optimum concentration value of 0.1 wt% because an increase in the NP concentration leads to increasing the rate of nanoparticles at the surface. As a result, CO_2 mass diffusivity is enhanced. Similar results were also found in the literature [22].

However, by adding more NPs to the base fluid, the CO_2 mass diffusivity decreased. Therefore, there was an optimum weight fraction of NPs for the enhancement of diffusivity. Increasing the NF concentration causes an increase in the NFs viscosity and the NP becomes too dense in the liquid owing to the decrease in Brownian motion and gas diffusivity [10, 23, 24]. Viscosity, intermolecular forces, and surface tension have reduced the mass diffusivity by adding NPs to the base fluid [25-27].

Figures (12-14) display types of nanofluid, nanofluid concentration, and temperature influence on the CO_2 diffusivity. The highest diffusivity at 35 ℃ for nanofluid concentrations of 0.05. 0.1, and 0.2 wt.% was obtained for TiO_2 (25 nm), Al_2O_3 (20 nm), Al_2O_3 (20 nm), respectively.

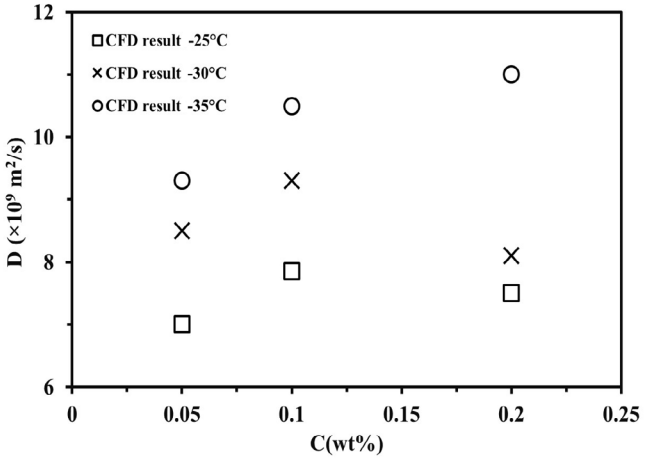

Figure 9. The effect of SiO_2 (20-30 nm) NF concentration on CO_2 diffusivity

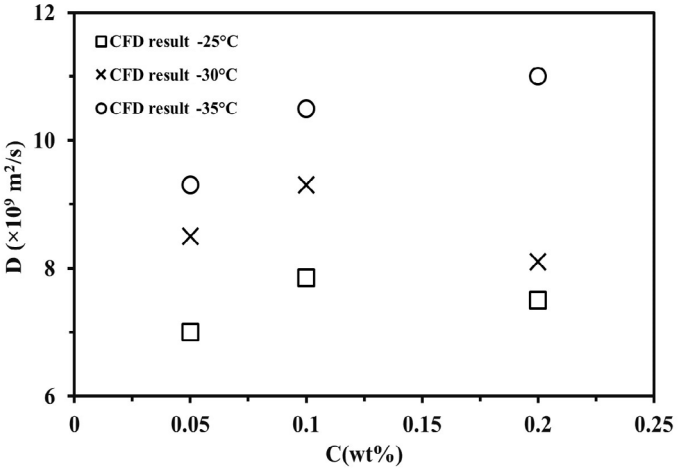

Figure 10. The effect of Al_2O_3 (20 nm) NF concentration on CO_2 diffusivity

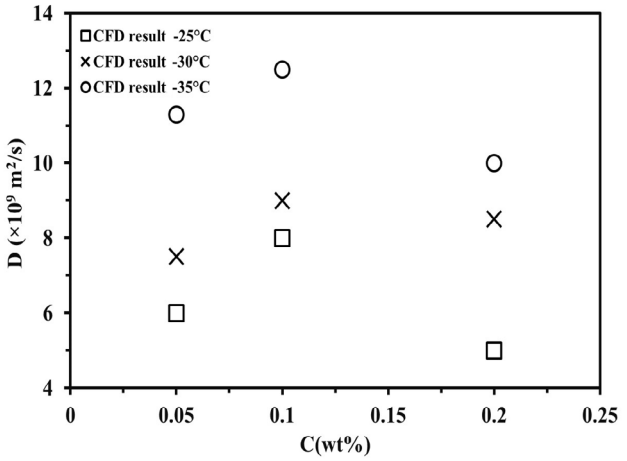

Figure 11. The effect of TiO_2 (25 nm) NF concentration on CO_2 diffusivity

Therefore, NF concentration had a key role in diffusivity and NFs showed a variety of behaviors in different conditions. Two approaches exist here. First, the presence of solid particles in water molecules causes the tortuosity of the water molecules to increase. Second, the particles cause the joining of water molecules which have a lower mass diffusivity than free molecules [19, 20].

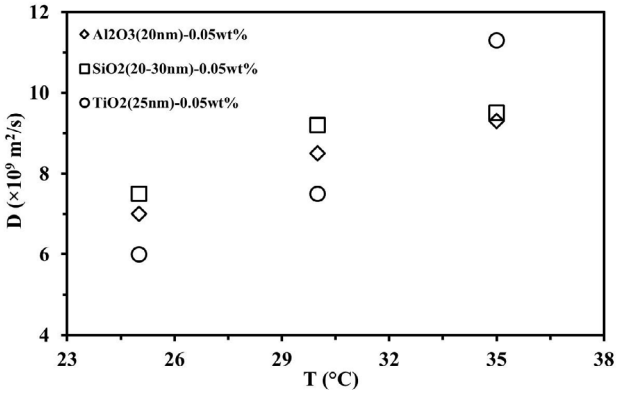

Figure 12. CO_2 diffusivity for 0.05 wt% of NFs vs. various temperature

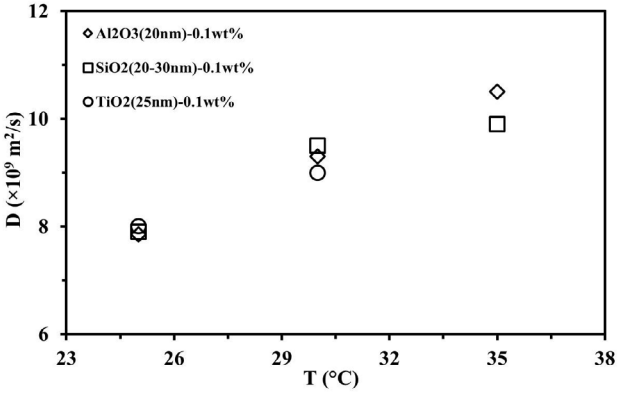

Figure 13. CO_2 diffusivity for 0.1 wt% of NFs vs. various temperature

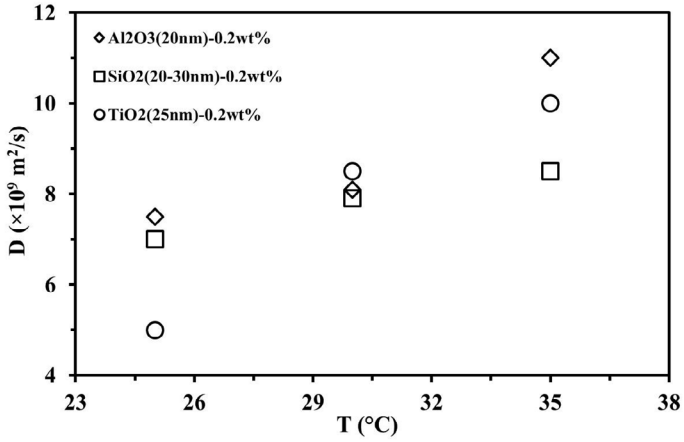

Figure 14. CO_2 diffusivity 0.2 wt% of NFs vs. various temperature

4. Conclusion

In this paper, the modeling of CO_2 diffusivity in pure water based- SiO_2, Al_2O_3, and TiO_2 NFs was evaluated for the concentrations of 0.05, 0.1 and 0.2 wt%. It was found that the CO_2 diffusivity improved to 9.9×10^{-9}, 11×10^{-9}, and 12.5×10^{-9} (m^2/s) at 35ºC for 0.1,0.2, and 0.1 wt% of SiO_2, Al_2O_3, and TiO_2 NFs, respectively. It is essential to note that the temperature, weight fraction and types of NPs are significant parameters for the enhancement of diffusion coefficient. The increase in the temperature had a positive effect, and there was an optimum concentration of o.1 wt% in all conditions. Therefore, micro-convection and grazing effect are controlling mechanisms for the mass transfer. Consequently, the results suggest that TiO_2 NFs can be an appropriate candidate for the phenomenon of mass diffusivity. Also, modeling results were compatible with sheikha's model.

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مقاله تحقیقاتی

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چکیده

پیش‌بینی پارامترهای الاستیک مانند نسبت پواسون و مدول یانگ دریک مدل سه بعدی برای ارزیابی نفوذ گاز دی اکسید کربن در آب خالص و نانوسیالات اکسید سیلیکون، اکسید آلومینیوم و اکسید تیتانیوم با غلظت‌های ۰/۰۵، ۰/۱ و ۰/۲ درصد وزنی بررسی شده است. پارامترهای مختلف مانند دما و درصد وزنی نانوذرات بر روی نفوذ گاز دی اکسید کربن در یک سلول نفوذ در نرم افزار کامسول مورد مطالعه قرار گرفته و ضریب نفوذ دی اکسید کربن با نتایج آزمایشگاهی مقایسه شده است. نتایج مدل سازی گزارش می دهد که آب در ۳۶۰۰۰ ثانیه با گاز اشباع می شود و بیشترین مقدار گاز جذب شده در ۰/۳۲ متر اتفاق می افتد و نتایج DFC با داده های آزمایشگاهی تطابق قابل قبولی دارد. علاوه بر این، دما تأثیر مثبتی بر ضریب نفوذ دارد و نفوذپذیری با افزایش غلظت نانوسیال تا مقدار بحرانی ۰/۱ درصد وزنی در همه شرایط افزایش می یابد. همچنین نانوسیال تیتانیوم اکسید به عنوان یک نانوسیال مناسب برای پدیده نفوذ جرمی معرفی شده است..

نحوه استناد به این مقاله:

Dehghan P, Mohammaddoost H, Azari A., Determination of CO2 gas diffusivity in nanofluids: a modeling study, Journal of Oil, Gas and Petrochemical Technology, 2023; 10(1): 60-69. DOI:10.22034/jogpt.2023.385081.1110.