



Experimental and modeling of CO₂ absorption in a bubble column using a water-based nanofluid containing co-doped SiO₂ nanoparticles

Samira Heidari^{1,2,3} · Feridun Esmaeilzadeh^{1,2} · Roozbeh Rafati⁴ · Amin Sharifi Haddad⁴

Received: 3 May 2023 / Accepted: 4 September 2023 / Published online: 16 February 2024
© The Author(s), under exclusive licence to Springer Nature Switzerland AG 2024

Abstract

This study tried to investigate the effect of Co/SiO₂ NPs on CO₂ absorption in a single raising bubble column (20 °C and 1 atm). Co-doped SiO₂ nanoparticles were first synthesized through the chemical vapor deposition (CVD) method, then several nanofluids, including different weight percentages of the synthesized NPs (0.001, 0.01, 0.02, 0.05, and 0.1 wt%) were prepared. Comprehensive experimental studies examined the effect of NPs concentration and nanofluid volume on CO₂ absorption rate. The stability of nanofluids, as an affecting factor on nanofluid efficiency, was investigated over 10 days. It was tried to obtain mass transfer parameters, including Sherwood (*Sh*), and Schmidt (*Sc*) numbers, incorporating the CO₂ diffusivity into the Co/SiO₂ nanofluid. Results showed that increasing NPs concentration from 0.001 to 0.02 caused the CO₂ absorption rate to reach a maximum point followed by a downward trend. Increasing nanofluid volume was not beneficial for increasing gas absorption, which is attributed to the fact that the predominant mechanism of CO₂ absorption was the Brownian motion of NPs. Results confirmed that the prepared nanofluids had acceptable stability over 10 days, and the nanofluid (80 mL), including 0.02 wt% of NPs, had the maximum CO₂ absorption, which was 28% more than the base fluid. Findings indicated that the magnitude of the CO₂ mass transfer coefficient in the nanofluid was 1.953×10^{-4} (m.s⁻¹), which was 1.89 times more than that for the base fluid. Finally, a comprehensive correlation ($R^2=0.99$) was introduced to predict the CO₂ mass transfer coefficient in the Co/SiO₂ nanofluid.

Keywords CO₂ absorption · Nanoparticle · Nanofluid · Bubble column

Introduction

Carbon dioxide (CO₂) absorption refers to the process of capturing and storing carbon dioxide from the atmosphere or industrial processes. It is a crucial component of mitigating climate change, as CO₂ is a potent greenhouse gas that contributes to global warming (Åhlén et al. 2023; Giorgetta et al. 2013; Small et al. 2014). During the last decades, many ways introduced to remove and absorb CO₂ from gas streams like using membranes (Jung, Lee, and Lee 2023; Hamalová et al. 2023; Fu et al. 2023), cryogenics (Kim et al. 2023; He et al. 2023; Meng et al. 2023), absorption (Gautam and Mondal 2023; Huhe, King, and Chuang 2023; Sharif et al. 2023), and adsorption (Skjervold et al. 2023; Al-Absi et al. 2023). Currently, absorption and adsorption methods have been developed to a practical stage but absorption methods are more common (Zhang, Borhani, and Olabi 2020; Ochedi et al. 2021; Fang et al. 2020). The absorption

✉ Samira Heidari
sheidari@unal.edu.co

✉ Feridun Esmaeilzadeh
esmaeil@shirazu.ac.ir

¹ Department of Chemical Engineering, School of Chemical and Petroleum Engineering, Shiraz University, Shiraz, Iran

² Enhanced Oil and Gas Recovery Institute, School of Chemical and Petroleum Engineering, Enhanced Gas Condensate Recovery Research Group, Shiraz University, Shiraz, Iran

³ Research Group on Surface Phenomena — Michael Polanyi, Department of Processes and Energy, Faculty of Mines, National University of Colombia, Sede Medellín, Medellín 050034, Colombia

⁴ School of Engineering, University of Aberdeen, Aberdeen AB24 3UE, UK

methods are divided into physical and chemical types of absorbents. Chemical absorption using amine series solutions is a mature and well-developed technology (Dutcher, Fan, and Russell 2015; Koysoumpa, Bergins, and Kakaras 2018) but enormous costs for energy supply to regenerate solvent is a major drawback of this method (Wang et al. 2015; Raynal et al. 2011). Degradation of amine absorbents, side reactions, and corrosion are some other problems (Ünveren et al. 2017; Wu et al. 2020). Although the physical absorption is a relatively low CO₂ recovery capacity, it is more suitable than the chemical methods for high-pressure systems such as the integrated gasification combined cycle (IGCC) (Ban, Keong, and Mohd Shariff 2014; Zhang, Borhani, and Olabi 2020).

There are two important vital factors for an ideal solvent to be used in CO₂ absorption; high rate of reaction and high CO₂ absorption capacity (Mota-Martinez, Hallett, and Mac Dowell 2017). The presence of nanoparticles (NPs) dispersed homogeneously in a base fluid, typically water or some other liquid, can form a stable colloidal solution namely “Nanofluid”. These nanoparticles can be a metallic, metal oxide, or carbon-based and typically have dimensions in the range of 1 to 100 nanometers. When these nanoparticles are added to the base fluid, they can significantly alter their properties, including their thermal conductivity, viscosity, and absorption characteristics (Tavakoli et al. 2022; Zhang et al. 2018; J.S. Lee, Lee, and Kang 2015). Several attempts have been made to use nanofluids as a suitable candidate for the physical absorption of CO₂ due to the mass transfer enhancement (Mohd Rozaidin and Lau 2022; Zhang et al. 2018; Hussin et al. 2023). The addition of nanoparticles to the base fluid can enhance the absorption of CO₂ due to several properties of the nanoparticles, including their high surface area, high reactivity, and ability to form stable dispersions in the base fluid. Additionally, nanofluids can improve the overall efficiency of the CO₂ absorption process by reducing the energy required to separate CO₂ from other gases.

Over the past decades, many studies have been carried out to improve the mass transfer characteristics of nanofluids. For example, Kim et al. (W.-g. Kim et al. 2008) performed CO₂ absorption experiments in a bubble-type absorber with water-based nanofluids using SiO₂ nanoparticles. It was concluded that the addition of nanoparticles led to an increase in the total CO₂ absorption by 24%. Jiang et al. (Jiang et al. 2013) found that the CO₂ absorption rate could be enhanced by up to 8% with the presence of nanoparticles in comparison to pure monoethanolamine (MEA) solution. Pang et al. (Pang et al. 2012) studied the NH₃/H₂O bubble absorption performance with Ag nanoparticles and found that the absorption rate of a nanofluid including 0.02 wt% Ag NPs were enhanced as high as 55% compared to

the base fluid. Pineda et al. (Pineda et al. 2012) measured CO₂ absorption in a tray column absorber. They reported that the maximum absorption rate enhancements were 9.4% for Al₂O₃ and 9.7% for SiO₂ nanoparticles. Nanoparticles also show a drastic enhancement in low-temperature CO₂ absorption (Zarei and Keshavarz 2023; Lashgarinejad et al. 2023). Amaris et al. (Amaris, Bourouis, and Vallès 2014) studied the effects of carbon nanotubes on the performance of the NH₃/LiNO₃ absorber. They reported that the maximum enhancement in the absorption performance with carbon nanotubes (CNTs) was 1.64 and 1.48 times for cooling water at 40 and 35 °C, respectively. Lee et al. (J.W. Lee et al. 2016) examined a bubble absorber’s CO₂ absorption performance enhancement. They reported that the CO₂ absorption rate was enhanced up to 4.5% at 0.01 vol% of Al₂O₃ nanofluid at 20 °C, and 5.6% at 0.01 vol% of SiO₂ nanofluid at 20 °C. Lee and Kang (J.W. Lee and Kang 2013) investigated enhancement in CO₂ absorption of NaCl aqueous solution-based Al₂O₃ nanofluid. They measured the CO₂ solubility in Al₂O₃/NaCl nanofluid for different Al₂O₃ concentrations and solvent temperatures. The results showed that the CO₂ solubility enhancement ratios at 0.01 vol% of Al₂O₃ nanoparticle concentration, were 11.0% at 30 °C, 12.5% at 20 °C, and 8.7% at 10 °C.

Although several studies have shown that nanofluids can improve the performance of CO₂ absorption compared to conventional fluids, the use of nanofluids for CO₂ absorption is still in the experimental stage, and more research is needed to fully understand their potential. One advantage of the nanofluids is attributed to the high surface area of the nanoparticles, which provides more contact area between the CO₂ and the fluid. This leads to faster reaction rates and higher CO₂ absorption capacity. Moreover, the presence of nanoparticles can increase the mass transfer coefficient, which is the rate at which CO₂ is transferred from the gas phase to the liquid phase. But nanoparticle concentration, nanoparticle size and shape, nanoparticle surface chemistry, fluid properties, temperature, and pressure are deciding factors in using nanofluids for CO₂ absorption. The effectiveness of nanoparticles can be limited by issues such as aggregation and sedimentation.

Computational models can be used to simulate the absorption of CO₂ using nanofluids. The computational models for simulating CO₂ absorption using nanofluids typically involve solving the mass and energy balances for the system. The equations are solved numerically using a variety of techniques such as finite element analysis, finite difference methods, or computational fluid dynamics. The models can be used to predict the performance of different nanofluids for CO₂ absorption under different conditions such as temperature, pressure, and concentration. The models can also be used to optimize the design and operation of absorption

systems using nanofluids. Some of the key parameters that need to be considered in the computational models for CO₂ absorption using nanofluids include the concentration and size of the nanoparticles, the properties of the base fluid, the temperature and pressure of the system, and the mass transfer coefficient between the gas and liquid phases. Until now, many modeling studies have been accomplished on CO₂ absorption (J.-z. Jiang, Liu, and Sun 2017; Ansarian and Beiki 2022; Sodeifian and Niazi 2021). Jamali et al. (Jamali and Azari 2023), reviewed the numerical simulation of CO₂ absorption columns using the computational fluid dynamics (CFD) strategy and investigated the application of different nanoparticles in various amine-based solutions and the effect of different packings in the packed bed absorption columns. Rashidi et al. (Rashidi and Mamivand 2022), examined the effect of NPs volume fraction, nanofluid flow rate, and temperature on the mass transfer coefficient for CO₂ absorption by Al₂O₃-water nanofluid and concluded that the increase of nanoparticle concentration, temperature, and fluid flow rate favors the mass transfer coefficient. Generally, the modeling of carbon dioxide absorption can suffer from a few weaknesses such as assumptions, incomplete data, simplifications, and model validation, which may lead to inaccurate predictions or results.

In this study, SiO₂ nanoparticles were first synthesized, followed by the doping of Co onto them. Next, their performance on CO₂ absorption was investigated at 20 °C, which was a low and challenging temperature. In this regard, several concentrations of nanoparticles and volumes of the nanofluid were prepared and finally, the nanoparticle dispersion stability was evaluated by measuring the total CO₂ absorption over a period of ten days. It also tried to predict the absorption rate and mass transfer coefficient by presenting a new comprehensive correlation. To the best of our knowledge, this is the first investigation of the absorption rate, molar flux, mass transfer coefficient, and diffusivity coefficient of CO₂ into a Co/SiO₂ water-based nanofluid in a single bubble column through a set of comprehensive experiments and precious correlation.

Experiments

Materials and instrumentations

Tetra epoxy silane (TEOS, 95%) and Bis(cyclopentadienyl) cobalt(II) (Cobaltocene, 98%) were purchased from Merck Company, Germany, and used to synthesize Co/SiO₂ NPs. Deionized water was used to prepare and dilute nanofluids. All chemical materials were used as received without further purification.

To assess the size distribution of dry and dispersed nanoparticles in deionized water, the transmission electron microscopy (TEM) and dynamic light scattering (DLS) were, respectively, performed. The size of nanoparticles and their agglomeration were characterized using TEM images, taken from Hitachi, 9000 NA, Japan (Andrade et al. 2012). To do TEM tests, a dispersed suspension of NPs in ethanol (0.001 wt%) was sonicated using an ultrasonic bath Parsonic 30 S-400 W, 28 kHz, for 20 min, followed by placing on the graphite surface. Then, to remove ethanol from the samples, the samples were placed into a vacuum oven for 4 h. DLS measurements were performed by Malvern, Zeta Sizer Nano ZS, United Kingdom (Xu, Zhang, and Song 2003; Pham, Fullston, and Sagoe-Crentsil 2007). The zeta potential (ξ -potential) tests were accomplished using ELSZ-2000 (Otsuka Electronics Co., Osaka, Japan) to measure the stability and surficial electrostatic charges of NPs (Darvanjooghi and Esfahany 2016). ξ -potential accounts for the electrostatic charges of NPs, leading to repulsive forces among dispersed particles. NPs' stability is known based on the positive and negative high ξ -potential, whereas low ξ -potentials indicate the tendency of NPs to agglomeration (Davoodi et al. 2016). A mass flow controller instrument (MFC, Brooks model, 1-888-554-flow, USA) was employed to inject CO₂ into the nanofluids through the absorption setup. A CO₂ sensor (Testo 535, Germany) was used to measure CO₂ concentration in the outlet gases. To prepare nanofluids, a certain amount of the synthesized Co/SiO₂ NPs were measured using a precise electric balance (TR 120 SNOWREX, Taiwan) and added to the water. The pH of the solutions was measured using a pH meter (PCE-PHD 1, UK). To prevent agglomeration of NPs, an ultrasonic processor (QSONICA-Q700, NY, USA) was utilized. A mechanical ball-mill (YKM-2 L, China) was used to grind the clustered NPs. A magnetic stirrer (IKA-10,038, Germany) was used to stirrer the solutions.

Methods

Synthesis of Co/SiO₂ NPs

The SiO₂ nanoparticles were synthesized through the chemical vapor deposition (CVD) method based on the methodology exposed by Dev et al. (Dev et al. 2021). Tetra epoxy silane was selected as the precursor of SiO₂ nanoparticles. To do so, first, 0.05 g of this reagent was completely dispersed in 50 mL of acetone. Then, to promote CO₂ absorption of SiO₂ NPs, 12.0 wt% of cobaltocene was added to the acetone medium. The prepared solution was then transferred to the tubing furnace (800 °C) with a nitrogen flow rate of 10.0 mL min⁻¹. This process led to Co/SiO₂ NPs with purple color.

Preparation of nanofluid

First, the nanoparticles were placed (4 h) in a ball mill device for the separation of the accumulated NPs. Then, nanofluids were prepared by dispersing a specific amount of the synthesized Co/SiO₂ NPs in 80 mL of deionized water. A vast range of NPs concentrations ranging from 0.001 to 0.1 wt% were examined in this study. Next, the prepared suspensions were stirred at 800 rpm for 5 h. Finally, the sonication process dispersed NPs in the nanofluid through three series of 20 min. the cycle time and amplitude of the sonication process were set on 0.5 s and 70%, respectively.

Experimental setup

The experimental setup was consisted of a bubble absorber column, filled with the synthesized Co/SiO₂ NPs loaded in the nanofluid. A specific volume of N₂ and CO₂ was sequentially injected into the nanofluid in the absorption column. Figure 1 illustrates the schematic diagram of the bubble absorber column which consists of a 170 mm height and 60 mm diameter Poly(methyl methacrylate) tube utilized as a semi-batch device to examine CO₂ absorption by means of the nanofluid. To control the rate of feed gases, two regulators were placed in the outlet of the CO₂ and N₂ accumulators. CO₂ was injected into nanofluids in the absorber column with the constant flow rate of 80 standard cubic centimeters per minute (SCCM) in each experiment. The gas flow rates were measured by two mass flow controllers (MFC) at the inlets of the absorber column. A gas diffuser was embedded at the bottom of the absorber column to produce a minimum bubble size ranged from 6.9 to 7 mm. The rising time of the bubbles was almost 2.3 s. The concentration of CO₂ is accurately measured and recorded by the CO₂ sensor at the outlet of the absorber column in equal time intervals. The temperature of the absorbent was automatically monitored

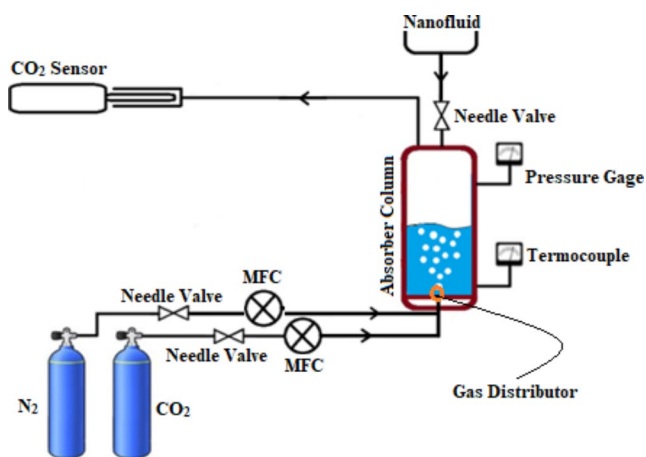


Fig. 1 Schematic diagram of the experimental setup

and controlled during the absorption process using a set of thermocouples and thermostats.

Experimental procedure

To measure the CO₂ absorption in the prepared nanofluid, first, pure N₂ was injected into the absorber column for 1 min. Next, 80 mL of the prepared nanofluid was injected to the absorber column. The temperature of the absorber column was adjusted to 19 °C. N₂ was reinjected again for 1 min to purge CO₂ from the nanofluid. CO₂ was injected into the nanofluid at 80 sccm. CO₂ concentration in the outlet gas stream was recorded every 3 s for 27 min.

Results and discussion

Nanofluid characterization

Figure 2 (a & b) illustrate the TEM (a) and DLS (b) images of Co/SiO₂ NPs used for the nanofluid preparation. It was found that the average size of the synthesized nanostructures was 70 nm with a semi-spherical morphology without any special agglomeration (Shi et al. 2008).

The average size of NPs measured by the DLS test was equal to that of the TEM test, affirming no considerable agglomeration during NPs dispersion in the base fluid. Therefore, results confirmed that the method used in this study for NPs dispersion led to a well-dispersion of NPs.

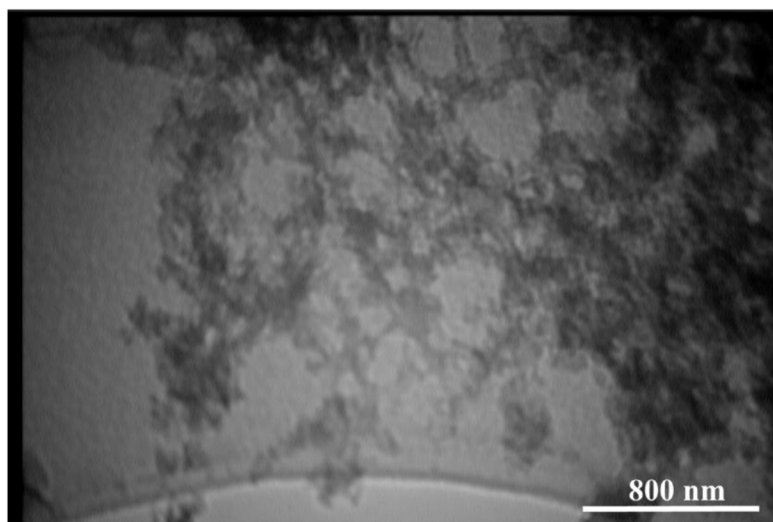
Zeta-potential analysis was accomplished to evaluate the NPs' stability in the nanofluid (áO'Brien 1990). Since the value of the ξ -Potential indicates the magnitude of the electrostatic repulsion among particles with similar charges and the synthesized Co/SiO₂ NPs had a high ξ -Potential value of -98.7 mV. Since the ξ -Potential of the synthesized NPs was lower than -45 mV, it was confirmed that the synthesized NPs benefited from high stability (Faraji et al. 2010).

Absorption

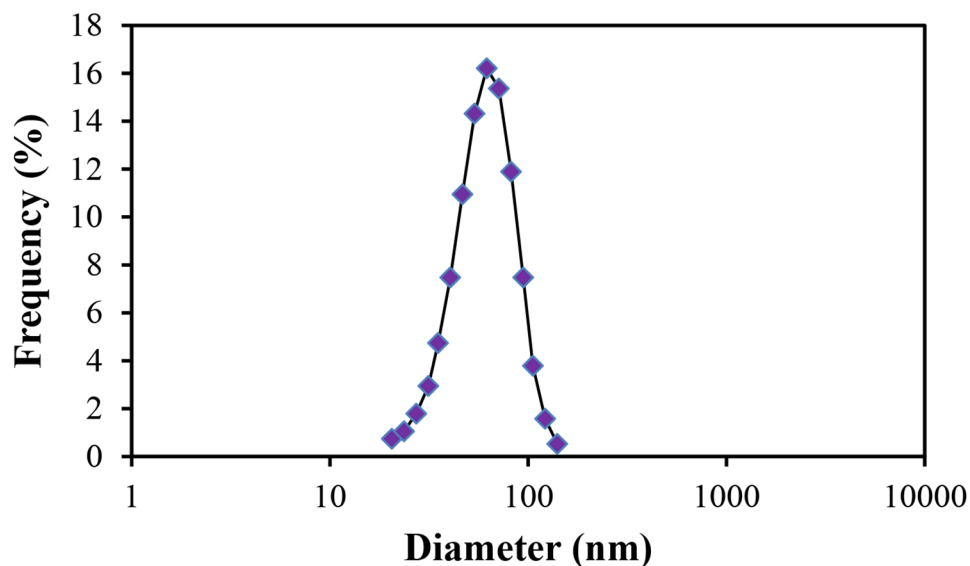
Maximum absorption

Nanofluids were prepared with different NPs concentrations including 0.001, 0.01, 0.02, 0.05, and 0.1 wt.% of NPs. The CO₂ absorption was measured over a 27 min period. The experiments were repeated three times at each volume fraction of the synthesized NPs and the standard deviations were shown as the error bars. Figure 3 (a & b) exhibits the average CO₂ molar flux into the Co/SiO₂ nanofluid. Based on the results presented in Fig. 3 (a & b), the average CO₂ molar flux increased with increasing Co/SiO₂ NPs from 0.001 to 0.02 wt% while the molar flux decreased for higher

Fig. 2 (a) Transmission electron microscopy (TEM) and **(b)** dynamic light scattering (DLS) images of Co/SiO nanoparticles



(a)



(b)

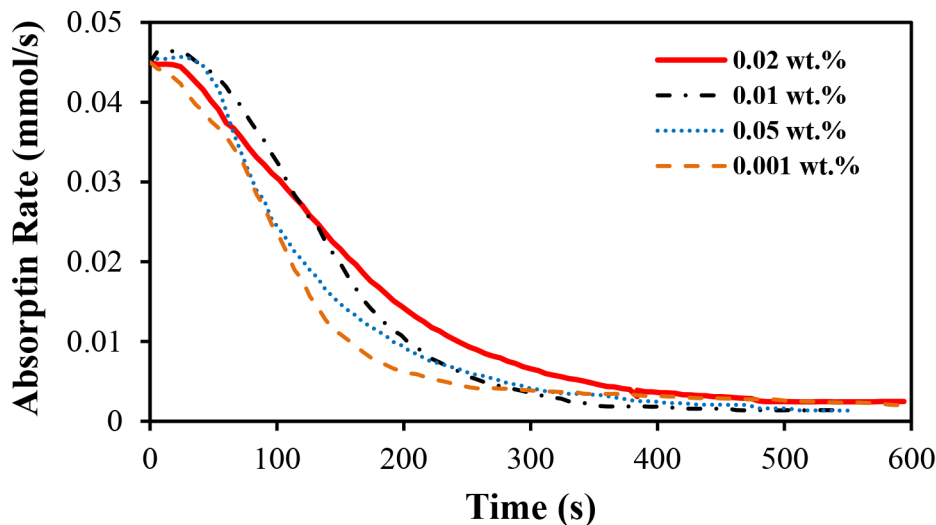
NPs loadings (0.02 to 0.1 wt%). It can be concluded that the absorption molar flux of CO₂ has a maximum value of 0.02 wt% of the synthesized NPs. Besides, it was found that Co/SiO₂ NPs intensified the micro-convections and improved mass transfer rate in comparison with base fluid, thus, the initial increase in the absorption of CO₂ would be reasonable with the aforesaid NPs mass fraction. However, increasing the number of NPs causes the viscosity of nanofluids to increase, thereby dominating the micro-convection impacts of NPs together with reducing the CO₂ absorption within the nanofluid (Esmaeili Faraj et al. 2014; Darvanjoghi and Esfahany 2016).

Furthermore, Fig. 4 affirms the higher amount of CO₂ absorption in nanofluids with different mass loadings of NPs than in deionized water. It was found that the maximum CO₂ absorption enhancement in comparison to pure water is 28% at the nanofluid including 0.02 wt% of Co/SiO₂ NPs.

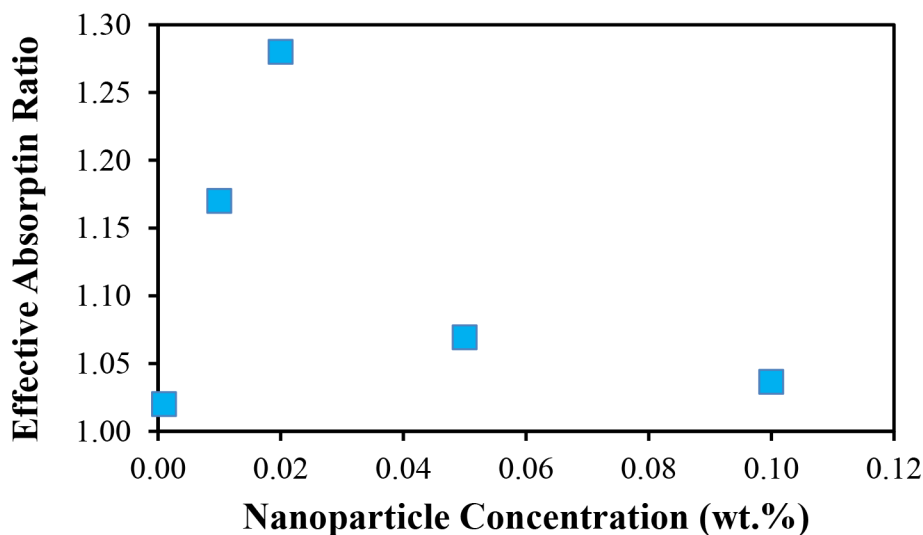
Probing the rate of mass transfer

To find out the effect of absorbent volume on the CO₂ absorption rate, 4 different volumes (80, 100, 120, and 150 mL) of the nanofluid were prepared while the concentration of the synthesized NPs was kept at the optimum mass fraction of 0.02 wt% at the temperature of 25 °C. Findings

Fig. 3 Effective absorption ratio of CO₂ versus mass fraction of Co/SiO₂ NPs



(a)



(b)

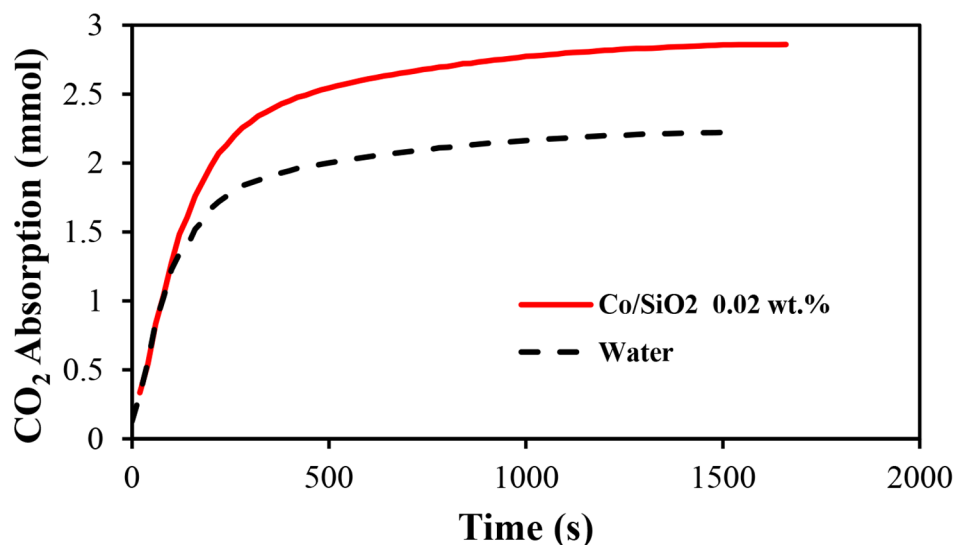
(Fig. 5) revealed that the absorption rate and mass transfer flux decreased with the enhancement in the volume loading of nanofluid. It can be attributed to the high height of absorbent in the vessel at a higher volume of nanofluid. Due to the forced and natural convection of the nanofluid under the specified geometry of the vessel, there is a wider diffusion regime at a higher height of absorbent than the smaller one. Since the Brownian motion of NPs and CO₂/water mixing flow are two important factors affecting CO₂ absorption, it was found that the effect of nanoparticles becomes weaker by forced or natural convection in a good mixing condition. As a result, the effect of the Brownian motion of NPs is in the reverse relationship with the height of absorbent, which

is in good agreement with other findings (Samadi, Haghshenasfard, and Moheb 2014).

Absorption stability

The stability of nanofluid suspension is an important parameter, in determining the success of the absorption process. NPs suspended in the adsorbent are under the influence of the intermolecular repulsive force caused by the Coulomb force and the attractive force originating from the van der Waals force. [3]. Under this condition, nanoparticles may agglomerate, grow in size, and form greater clusters. It is highly likely that heavy clusters sediment due to gravitational force. Since the main reason for the mass transfer

Fig. 4 Cumulative absorption amount in comparison to base water



enhancement of nanofluid is the presence of NPs, their sedimentation causes the absorption efficiency to reduce. In this study, to evaluate the stability of Co/SiO₂ nanofluid, a nanofluid was prepared based on the optimum condition (80 mL of nanofluid, 0.02 wt% of NPs, and 20 °C of absorbent temperature). After a 5 min sonication of the nanofluid, its stability (the rate of CO₂ absorption over time) was tested over 10 days. Results were shown in Fig. 6. Since the rate of CO₂ absorption versus time decreases with a completely uniform slope, which is related to the saturation of the nanofluid with CO₂, no agglomeration process has occurred inside the nanofluid for 10 days. Therefore, it can be concluded that the prepared Co/SiO₂ nanofluid is an acceptably stable absorbent.

Mass transfer coefficient

To calculate the mass transfer coefficient, different volumes of CO₂ gas (20, 25, 30, 35, 40, 45, and 50 mL) were separately injected into the absorber column and then CO₂ concentration and its molar flux were measured. Figure 7 illustrates the average molar flux versus the dissolved concentration of CO₂ in the liquid bulk. Results confirmed the reduction of average molar flux by increasing CO₂ bulk concentration, attributing to the decrease of mass transfer driving force. Besides, this observation followed a linear behavior. To evaluate this linear trend, the principal mass transfer equation (Eq. 1) was utilized and the experimental values were fitted to it.

$$N_{avg} = K_l (C_{CO_2}^* - C_{CO_2}) \quad (1)$$

where K_l represents the mass transfer coefficient ($m \cdot s^{-1}$) at the liquid phase. C_{CO_2} ($mol \cdot m^{-3}$) and $C_{CO_2}^*$ ($mol \cdot m^{-3}$)

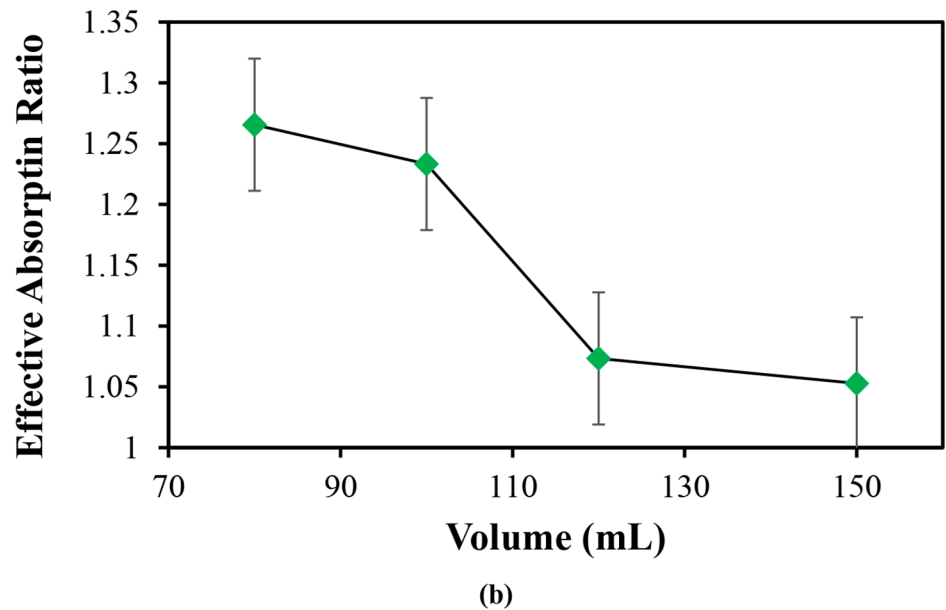
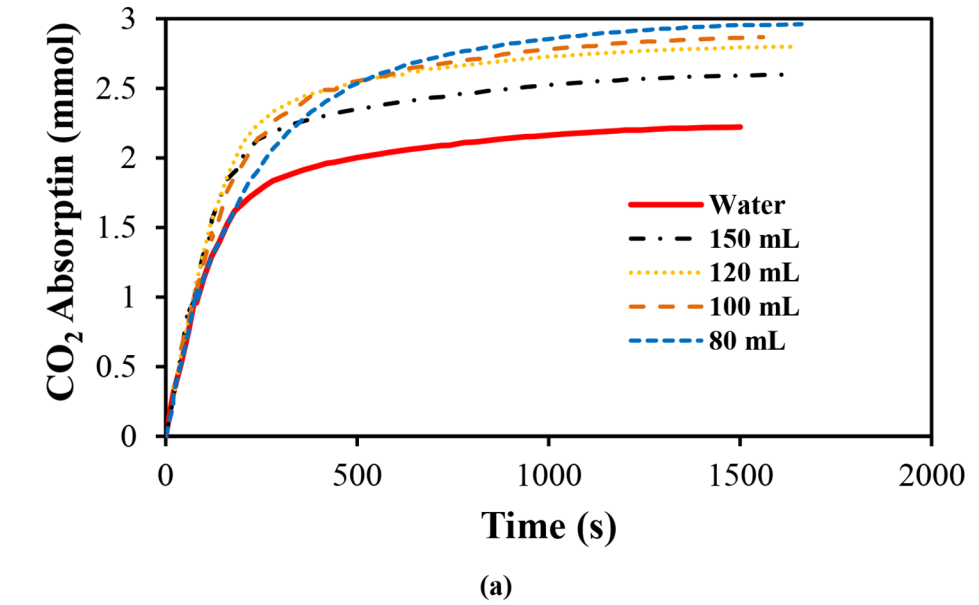
show the bulk and gas-liquid interface concentration of CO₂, respectively. It is worth mentioning that the observed CO₂ concentration in the interface was accounted for by extrapolating the line fitted on the obtained experimental data. It raises from the assumption of linear pattern for gas concentration and molar flux. Results (Fig. 7) showed that the suggested model was acceptably fitted to the experimental data with an R^2 value of 0.9855, confirming the high accuracy of the regression and low deviation of the model from the experimental data.

It can be concluded that the dashed line diagram (vertical plot) represents the observed concentration of CO₂ at the liquid-bubble interface. Besides, the average molar flux diagram versus the bulk concentration of CO₂ (diagonal plot) shows the gas absorption operating line. According to the slope of the operating line in Fig. 7, the relative mass transfer coefficient for CO₂ absorption (K_l) using Co/SiO₂ nanofluid was found to be $1.953 \cdot 10^{-4}$ ($m \cdot s^{-1}$), which was 1.89 times more than that for the water alone (relative mass transfer coefficient). The CO₂ absorption using nanofluid indicated higher values for relative gas concentration and relative mass transfer coefficient at the liquid-bubble interface.

Diffusivity Coefficient

Generally, the diffusivity of gases into a liquid has a significant impact on both the rate of gas absorption and the magnitude of the mass transfer coefficient. In this study, it was tried to benefit from Eq. 2 to obtain CO₂ diffusivity into the Co/SiO₂ nanofluid. Equation 2 presents raising a single bubble within a fluid according to Dankwert's theory (Esmacili-Faraj and Nasr Esfahany 2016; Zhao et al. 2003).

Fig. 5 Average molar flux of CO₂ versus volume of nanofluid



$$N_{ave} = \frac{D \sinh(\delta \sqrt{\frac{s}{D}}) + D r_0 \sqrt{\frac{s}{D}} \cosh(\delta \sqrt{\frac{s}{D}})}{r_0 \sinh(\delta \sqrt{\frac{s}{D}})} (C_{CO_2,i} - C_{CO_2}) \quad (2)$$

$$K_l = \frac{D \sinh(\delta \sqrt{\frac{s}{D}}) + D r_0 \sqrt{\frac{s}{D}} \cosh(\delta \sqrt{\frac{s}{D}})}{r_0 \sinh(\delta \sqrt{\frac{s}{D}})} \quad (3)$$

where the main factors of the model affecting the rate of mass transfer are the diffusivity of gas within a liquid (*D*), the thickness of the diffusion layer (δ), the radius of bubbles (r_0), and the rate of surface renewal (*s*). N_{ave} represents the CO₂ molar flux (mol.m⁻²s⁻¹) while C_{CO_2} and $C_{CO_2,i}$ are the CO₂ concentration through the liquid bulk and at the interface of liquid-bubble (mol.m⁻³), respectively.

Comparing Eqs. 1 and 2 results in Eq. 3, showing the mass transfer coefficient of a gas within a liquid based on a single bubble model:

In this study, Eq. 3 was used to estimate the CO₂ diffusivity through the nanofluid. Based on Darvanjooghi et al. report, impressive factors of Eq. 3 like *D*, *s*, and δ violently depend on the size of NPs in the nanofluid (Darvanjooghi, Esfahany, and Esmacili-Faraj 2018). They mentioned that the range of NPs' size was between 50 and 70 nm, the rate of surface renewal (*s*) was 6.85 mm.s⁻¹, and the thickness of the diffusion layer was 0.201 mm. In this study, on the one hand, the average size of nanoparticles was 70 nm, and on the other hand, the values of *s* and δ were assumed to be

Fig. 6 Cumulative absorption of CO₂ over time

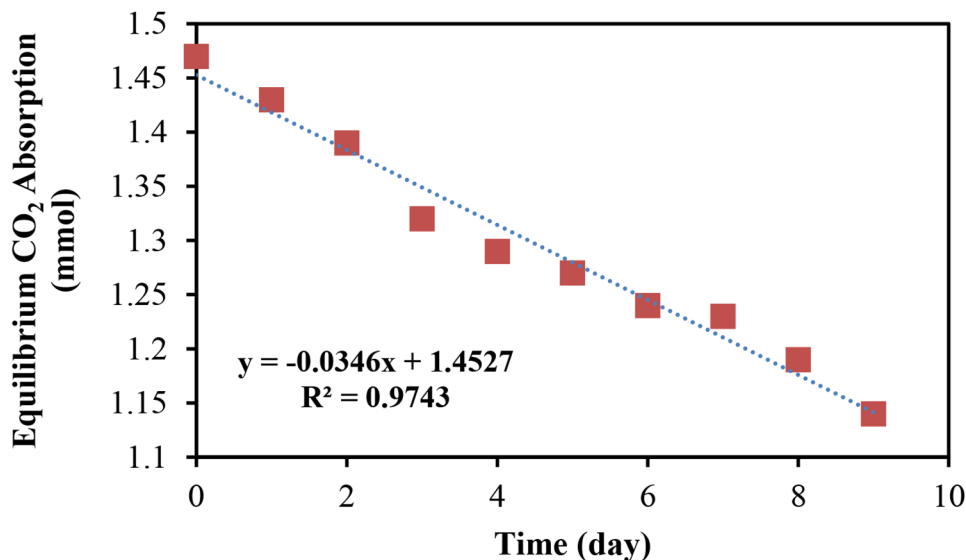
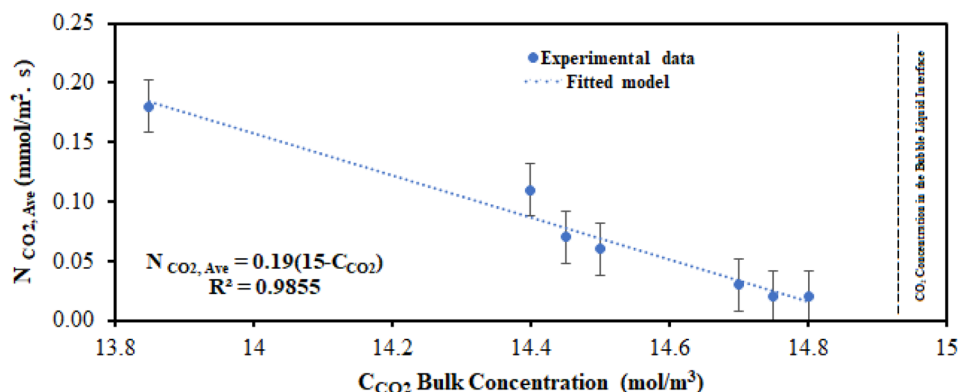


Fig. 7 Average molar flux versus CO₂ bulk concentration



constant during the CO₂ absorption, depending on only the mean diameter of NPs. Besides, the mass transfer coefficient of CO₂ within the nanofluid was previously calculated. Therefore, Eq. 3 can be simplified to Eq. 4 as follows:

$$F(s, \delta, D) = \exp\left(2\delta\sqrt{\frac{s}{D}}\right) \pm \frac{D - r_0\sqrt{s.D} - r_0K_l}{r_0\sqrt{s.D} - r_0K_l} = 0 \quad (4)$$

where s and δ were considered to be 6.85 and 0.201, respectively (Darvanjooghi, Esfahany, and Esmacili-Faraj 2018). Equation 4 was solved according to the Newton-Raphson method as follows:

$$D_{n+1} = D_n - \frac{F(s, \delta, D_n)}{\frac{\partial F(s, \delta, D_n)}{\partial D_n}} \quad n = 0, 1, 2, \dots \quad (5)$$

where $\frac{\partial F(s, \delta, D_n)}{\partial D_n}$ can be calculated based on the partial derivation of Eq. 4. Besides, the initial value of D_0 was considered to be 10^{-10} .

Results illustrated that the diffusion values of CO₂ into Co/SiO₂ nanofluid and base fluid were 5.86×10^{-9} and $2.12 \times 10^{-9} \text{ m}^2 \cdot \text{s}^{-1}$, respectively.

Previous studies confirmed that only Brownian micro-convection and grazing effect are predominate mechanism for gas absorption into a nanofluid (Darvanjooghi, Esfahany, and Esmacili-Faraj 2018; Esmacili-Faraj and Nasr Esfahany 2016; Ashrafmansouri and Nasr Esfahany 2016; Ullah et al. 2023; Koo and Kleinstreuer 2005). In this study, it was found that Brownian mechanism serves an important role for the CO₂ absorption into Co/SiO₂ nanofluid. It is because CO₂ molecules have not a strong polar structure and asymmetric molecular configuration to generate considerable molecular charges (O=C=O) to be absorbed on surface charge of nanoparticles. Therefore, increasing volume of nanofluid is not in the favor of more CO₂ absorption because of lower micro-convections. It is worth mentioning that since Co/SiO₂ NPs have a high magnitude of surface charge (Darvanjooghi and Esfahany 2016), attributing to the silanol bond formation (Si-O-H), the grazing effect could be another affecting mechanism with a low-intensity.

Table 1 Diffusion coefficient, Reynolds (*Re*), Sherwood (*Sh*), and Schmidt (*Sc*) numbers for CO₂ absorption into Co/SiO₂ nanofluid

Absorbent	<i>v</i> (m.s ⁻¹)	<i>Re</i>	<i>Sh</i>	<i>Sc</i>
Nanofluid	8.88 * 10 ⁻⁷	1300	243	146
Basefluid	8.9 * 10 ⁻⁷	1298	316	420

Correlation

Equation 6 calculates the mass transfer of a single bubble in a fluid (Vasconcelos, Orvalho, and Alves 2002). Equation 6 has been accepted as a precious correlation to predict gas absorptions into a vast range of liquids using a single bubble absorber column (Calderbank and Lochiel 1964).

$$Sh = 0.6 Re^{\frac{1}{2}} Sc^{\frac{1}{3}} \tag{6}$$

To use Eq. 6 for the estimation of *Sh* number for the CO₂ absorption into a nanofluid, some other physical properties are needed to obtain like kinematic viscosity, dynamic viscosity, and density of Co/SiO₂ nanofluid (Mishra et al. 2014). These physical properties can be calculated according to Eq. 7 to 9 as follow:

$$\rho_{nanofluid} = \phi \rho_p + (1 - \phi) \rho_{basefluid} \tag{7}$$

$$\mu_{nanofluid} = \mu_{basefluid} (1 - \phi)^{2.5} \tag{8}$$

$$\nu_{nanofluid} = \frac{\mu_{nanofluid}}{\rho_{nanofluid}} \tag{9}$$

where ϕ is the volume fraction of Co/SiO₂ NPs in the base fluid and can be calculated from Eq. 10. $\mu_{nanofluid}$ and $\mu_{basefluid}$ are dynamic viscosities of the nanofluid and base fluid, respectively. ρ_p and $\rho_{basefluid}$ present the bulk density of NPs

(2.196 kg.m⁻³) and density of the base fluid (1000 kg.m⁻³), respectively.

$$S\phi (vol.\%) = \frac{w (wt.\%)}{w (wt.\%) + \frac{\rho_p}{\rho_{basefluid}} (100 - w (wt.\%))} \tag{10}$$

Re, *Sh*, and *Sc* numbers were calculated from Eq. 11 to 13, respectively.

$$Re_b = \frac{U_b d_b}{\nu_{nanofluid}} \tag{11}$$

$$Sh_{nanofluid} = \frac{k_{l,nanofluid} \cdot d_b}{D_{nanofluid}} \tag{12}$$

$$Sc_{nanofluid} = \frac{\nu_{nanofluid}}{D_{nanofluid}} \tag{13}$$

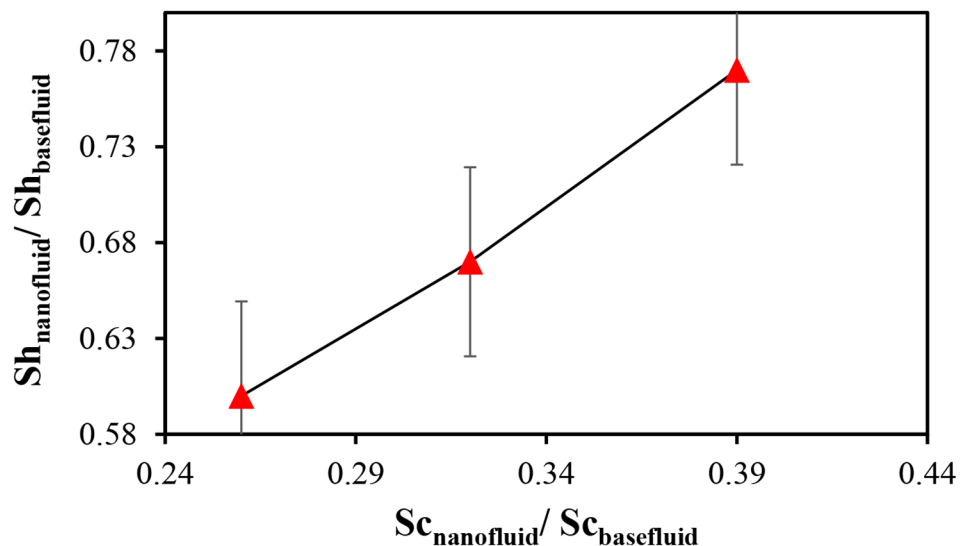
In these Equations, *U_b* is the rising velocity of the bubbles in the absorber column, which was considered to be 0.21 m.s⁻¹. Besides, *d_b* means the diameter of the bubbles, which was measured at almost 7 mm.

Table 1 shows the physical properties of CO₂ absorption into Co/SiO₂ nanofluid and base fluid.

Based on the summarized values in Table 1 and Eq. 11, there were no significant changes in *Re* number in the nanofluid or base fluid within the absorption i.e., $\nu_{nanofluid} \approx \nu_{basefluid}$. Therefore, it can be concluded that *Re* did not have a significant effect on the *Sc* number and followed a relative function according to below:

$$\frac{Sh_{nanofluid}}{Sh_{basefluid}} = K \left(\frac{Sc_{nanofluid}}{Sc_{basefluid}} \right)^m \tag{14}$$

Fig. 8 The effect of relative *Sc* number on relative experimental *Sh* number



m and K were accounted for using a two-dimensional regression analysis upon the experimental data illustrated in Fig. 8. Based on the results, Eq. 15 was introduced for the physical parameters with $R^2 = 0.99$. the following Equation can predict the Sh number for CO_2 absorption into a nanofluid at $Re_b \sim 1300$.

$$\frac{Sh_{nanofluid}}{Sh_{basefluid}} = 1.34 \left(\frac{Sc_{nanofluid}}{Sc_{basefluid}} \right)^{0.53} \quad (15)$$

Conclusions

In this research, Co-doped SiO_2 nanoparticles were synthesized and used to enhance CO_2 absorption in a single bubble column at $20^\circ C$ and 1 atm. Results confirmed that the prepared nanofluid had high stability with the ζ -potential lower than -45 mV. TEM and DLS analyses represented the average size of the synthesized NPs was 70 nm. The results also confirmed that the NPs' weight% and the volume of the nanofluid served important roles in the CO_2 absorption rate in such a way that the optimum condition was achieved for 80 mL of the nanofluid including 0.02 wt% of NPs. Increasing NPs concentration from 0.001 to 0.02 favors CO_2 absorption while the higher increase caused the absorption rate to decrease. Besides, CO_2 molecules showed a better absorption rate in lower volumes of nanofluids. Indeed, it was found that although both the grazing effect and the Brownian motion of NPs served a crucial role in increasing CO_2 absorption, the Brownian motion of NPs was the predominant mechanism. Moreover, mass transfer parameters affecting CO_2 diffusivity into the Co/ SiO_2 nanofluid like Sherwood (Sh) and Schmidt (Sc) numbers were calculated. Finally, a new correlation was introduced to predict the Sh number over the Sc number in a gas-nanofluid column ($Re \sim 1300$) with a high accuracy of $R^2 = 0.99$.

Supplementary Information The online version contains supplementary material available at <https://doi.org/10.1007/s40808-023-01869-1>.

Acknowledgments The authors are grateful to Shiraz University for supporting this research.

Declarations

Conflict of interest The authors declare no conflict of interest.

Competing interests This research received no external funding.

References

- Åhlén M, Zhou Y, Hedbom D, Cho HS, Strømme M, Terasaki O, and Ocean Cheung (2023). Selective capture/separation of potent greenhouse gases with gallium-and vanadium-based metal-organic frameworks
- Al-Absi, Akram A, Axelle Domin M, Mohamedali AM, Benneker, Nader Mahinpey (2023) CO_2 capture using in-situ polymerized amines into pore-expanded-SBA-15: performance evaluation, kinetics, and adsorption isotherms. *Fuel* 333:126401
- Amaris C, Bourouis M, Manel, Vallès (2014) Passive intensification of the ammonia absorption process with $NH_3/LiNO_3$ using carbon nanotubes and advanced surfaces in a tubular bubble absorber. *Energy* 68:519–528
- Andrade Angela L, José D, Fabris JD, Ardisson, Manuel A, Valente, José MFF (2012) “Effect of tetramethylammonium hydroxide on nucleation, surface modification and growth of magnetic nanoparticles.” *Journal of Nanomaterials* 2012
- Ansarian O, Beiki H (2022) Nanofluids application to promote CO_2 absorption inside a bubble column: ANFIS and experimental study. *Int J Environ Sci Technol* 19(10):9979–9990
- áO'Brien RW (1990) Electroacoustic studies of moderately concentrated colloidal suspensions. *Faraday Discuss Chem Soc* 90:301–312
- Ashrafmansouri S-S, Mohsen Nasr Esfahany (2016) Mass transfer into/from nanofluid drops in a spray liquid-liquid extraction column. *AIChE J* 62(3):852–860
- Ban ZH, Keong LK, Azmi Mohd Shariff (2014) Physical absorption of CO_2 capture: a review. *Adv Mater Res* 917:134–143
- Calderbank PH, Lochiel AC (1964) Mass transfer coefficients, velocities and shapes of carbon dioxide bubbles in free rise through distilled water. *Chem Eng Sci* 19(7):485–503
- Darvanjooghi MHossein K, Mohsen Nasr Esfahany (2016) Experimental investigation of the effect of nanoparticle size on thermal conductivity of in-situ prepared silica-ethanol nanofluid. *Int Commun Heat Mass Transfer* 77:148–154
- Darvanjooghi MH, Karimi MN, Esfahany, Seyyed Hamid Esmaili-Faraj (2018) Investigation of the effects of nanoparticle size on CO_2 absorption by silica-water nanofluid. *Sep Purif Technol* 195:208–215
- Davoodi S, Mohammadreza M, Sadeghi M, Naghsh, Ahmad Moheb (2016) Olefin-paraffin separation performance of polyimide Matrimid®/silica nanocomposite membranes. *RSC Adv* 6(28):23746–23759
- Dev A, Sardoiwala MN, Karmakar S (2021) Silica nanoparticles: methods of fabrication and multidisciplinary applications. *Functionalized Nanomaterials II*. CRC Press, pp 189–206
- Dutcher B, Maohong Fan, and, Armistead G, Russell (2015) Amine-based CO_2 capture technology development from the beginning of 2013 a review. *ACS Appl Mater Interfaces* 7(4):2137–2148
- Esmaili Faraj S, Hamid MN, Esfahany M, Jafari-Asl, Nasrin Etesami (2014) Hydrogen sulfide bubble absorption enhancement in water-based nanofluids. *Ind Eng Chem Res* 53(43):16851–16858
- Esmaili-Faraj S, Hamid, Mohsen Nasr Esfahany (2016) Absorption of hydrogen sulfide and carbon dioxide in water based nanofluids. *Ind Eng Chem Res* 55(16):4682–4690
- Fang M, Yi N, Di W, Wang T, Qinhui Wang (2020) Emission and control of flue gas pollutants in CO_2 chemical absorption system—A review. *Int J Greenhouse Gas Control* 93:102904
- Faraji M, Yamini Y, Rezaee MJ JotCS (2010) Magnetic nanoparticles: synthesis, stabilization, functionalization, characterization, and applications. *J Iran Chem Soc* 7:1–37
- Fu H, Xue K, Li Z, Zhang H, Gao D, Chen H (2023) Study on the performance of CO_2 capture from flue gas with ceramic and PTFE membrane contactors. *Energy* 263:125677

- Gautam A, Monoj Kumar Mondal (2023) Review of recent trends and various techniques for CO₂ capture: special emphasis on biphasic amine solvents. *Fuel* 334:126616
- Giorgetta MA, Johann Jungclaus CH, Reick S, Legutke J, Bader M, Böttinger V, Brovkin T, Crueger M, Esch, Fieg K (2013) Climate and carbon cycle changes from 1850 to 2100 in MPI-ESM simulations for the coupled model Intercomparison Project phase 5. *J Adv Model Earth Syst* 5(3):572–597
- Hamalová K, Neubertová V, Vostiňáková M, V Fila, and Z Kolská (2023) Amine-doped PEBA membrane for CO₂ capture. *Mater Lett* 333:133695
- He T, Liu Z, Son H, Gundersen T, Wensheng Lin (2023) Comparative analysis of cryogenic distillation and chemical absorption for carbon capture in integrated natural gas liquefaction processes. *J Clean Prod* 383:135264
- Huhe FNU, Jaelynn King, Steven SCC (2023) Amine-based sorbents for CO₂ capture from air and flue gas—a short review and perspective. *Res Chem Intermed* : 1–27
- Hussin F, Aroua MK, Saidur R, Zaim Nor Rashid Zainol Nor Rashid (2023) Nanofluids for CO₂ capture. *Nanomaterials for Carbon Dioxide capture and Conversion Technologies*. Elsevier, pp 89–135
- Jamali M, Ahmad Azari (2023) A review on computational Fluid Dynamics Simulations of Industrial Amine Absorber Columns for CO₂ capture. *ChemBioEng Reviews* 10(1):6–21
- Jiang J, Zhao B, Cao M, Wang S, Zhuo Y (2013) Chemical absorption kinetics in MEA solution with nano-particles. *Energy Procedia* 37:518–524
- Jiang Jia-zong, Liu L, Bao-min Sun (2017) Model study of CO₂ absorption in aqueous amine solution enhanced by nanoparticles. *Int J Greenhouse Gas Control* 60:51–58
- Jung W, Lee J, Jong Suk Lee (2023) New facile process evaluation for membrane-based CO₂ capture: apparent selectivity model. *Chem Eng J* 460:141624
- Kim Wun-gwi, Kang HU, Jung Kang-min, and Sung Hyun Kim (2008) Synthesis of silica nanofluid and application to CO₂ absorption. *Sep Sci Technol* 43(11–12):3036–3055
- Kim Y, Lee J, Cho H, Kim J (2023) Novel cryogenic carbon dioxide capture and storage process using LNG cold energy in a natural gas combined cycle power plant. *Chem Eng J* 456:140980
- Koo J, and Clement Kleinstreuer (2005) Impact analysis of nanoparticle motion mechanisms on the thermal conductivity of nanofluids. *Int Commun Heat Mass Transfer* 32(9):1111–1118
- Koytsoumpa E, Ioanna C, Bergins, Emmanouil Kakaras (2018) The CO₂ economy: review of CO₂ capture and reuse technologies. *J Supercrit Fluids* 132:3–16
- Lashgarinejad A, Hosseini SS, Irani V, Mohammad H, Ghasemi R, Mohammadpour, Ahmad Tavasoli (2023) Enhancement of CO₂ absorption and heat transfer properties using amine functionalized magnetic graphene oxide/MDEA nanofluid. *J Iran Chem Soc* : 1–14
- Lee JW, Yong Tae Kang (2013) CO₂ absorption enhancement by Al₂O₃ nanoparticles in NaCl aqueous solution. *Energy* 53:206–211
- Lee JS, Lee JW, Yong Tae Kang (2015) CO₂ absorption/regeneration enhancement in DI water with suspended nanoparticles for energy conversion application. *Appl Energy* 143:119–129
- Lee J, Won IT, Pineda JH, Lee, Yong Tae Kang (2016) Combined CO₂ absorption/regeneration performance enhancement by using nanoabsorbents. *Appl Energy* 178:164–176
- Meng Y, Chen L, Yang X, Yang H, Mao Z, Chen S, and Yu Hou (2023) Spontaneous desublimation of carbon dioxide in turbo-expander applied for cryogenic carbon capture. *Int Commun Heat Mass Transfer* 140:106528
- Mishra P, Chandra S, Mukherjee SK, Nayak, Arabind Panda (2014) A brief review on viscosity of nanofluids. *Int nano Lett* 4:109–120
- Mota-Martinez, Maria T, Jason P, Hallett, Niall Mac Dowell (2017) Solvent selection and design for CO₂ capture—how we might have been missing the point. *Sustainable Energy & Fuels* 1(10):2078–2090
- Ochedi FO, Yu JYuH, Liu Y, Hussain A (2021) Carbon dioxide capture using liquid absorption methods: a review. *Environ Chem Lett* 19:77–109
- Pang C, Wu W, Sheng W, Zhang H, Yong Tae Kang (2012) Mass transfer enhancement by binary nanofluids (NH₃/H₂O + ag nanoparticles) for bubble absorption process. *Int J Refrig* 35(8):2240–2247
- Pham KN, Damian, Fullston, Sagoe-Crentsil K (2007) Surface charge modification of nano-sized silica colloid. *Aust J Chem* 60(9):662–666
- Pineda I, Torres JW, Lee I, Jung, Yong Tae Kang (2012) CO₂ absorption enhancement by methanol-based Al₂O₃ and SiO₂ nanofluids in a tray column absorber. *Int J Refrig* 35(5):1402–1409
- Rashidi H, and Sajad Mamivand (2022) Experimental and numerical mass transfer study of carbon dioxide absorption using Al₂O₃/water nanofluid in wetted wall column. *Energy* 238:121670
- Raynal L, Bouillon P-A, Gomez A, Broutin P (2011) From MEA to demixing solvents and future steps, a roadmap for lowering the cost of post-combustion carbon capture. *Chem Eng J* 171(3):742–752
- Rozaiddin M, Aishah S, Kok Keong Lau (2022) “A review on enhancing solvent regeneration in CO₂ absorption process using nanoparticles.” *Sustainability* 14 (8): 4750
- Samadi Z, Haghshenasfard M, Ahmad Moheb (2014) CO₂ absorption using nanofluids in a wetted-wall column with external magnetic field. *Chem Eng Technol* 37(3):462–470
- Sharif M, Wu HFanX, Yu Y, Zhang T, Zhang Z (2023) Assessment of novel solvent system for CO₂ capture applications. *Fuel* 337:127218
- Shi H, Liu F, Yang L, Han E (2008) Characterization of protective performance of epoxy reinforced with nanometer-sized TiO₂ and SiO₂. *Prog Org Coat* 62(4):359–368
- Skjervold VT, Giorgia Mondino L, Riboldi, Lars ON (2023) “Investigation of control strategies for adsorption-based CO₂ capture from a thermal power plant under variable load operation.” *Energy*: 126728
- Small R, Justin J, Bacmeister D, Bailey A, Baker S, Bishop F, Bryan J, Caron J, Dennis P, Gent, Hsiao-ming Hsu (2014) A new synoptic scale resolving global climate simulation using the Community Earth System Model. *J Adv Model Earth Syst* 6(4):1065–1094
- Sodeifian G, and Zahra Niazi (2021) Prediction of CO₂ absorption by nanofluids using artificial neural network modeling. *Int Commun Heat Mass Transfer* 123:105193
- Tavakoli A, Rahimi K, Saghandali F, Scott J, Emma Lovell (2022) Nanofluid preparation, stability and performance for CO₂ absorption and desorption enhancement: a review. *J Environ Manage* 313:114955
- Ullah H, Shoaib M, Khan RA, Nisar KS, Muhammad Asif Zahoor Raja, and, Islam S (2023) “Soft computing paradigm for heat and mass transfer characteristics of nanofluid in magnetohydrodynamic (MHD) boundary layer over a vertical cone under the convective boundary condition.” *International Journal of Modeling and Simulation*: 1–25
- Ünveren E, Erdal Bahar Özmen Monkul, Şerife Sarioğlan, Nesrin Karademir, and Erdoğan Alper. 2017. Solid amine sorbents for CO₂ capture by chemical adsorption: a review. *Petroleum* 3 (1): 37–50
- Vasconcelos JMT, Sandra P, Orvalho, Sebastião S, Alves (2002) Gas-liquid mass transfer to single bubbles: effect of surface contamination. *AIChE J* 48(6):1145–1154
- Wang M, Joel AS, Ramshaw C, Eimer D, Nuhu MM (2015) Process intensification for post-combustion CO₂ capture with chemical absorption: a critical review. *Appl Energy* 158:275–291

- Wu Y, Xu J, Mumford K, Stevens GW, Fei W, Wang Y (2020) Recent advances in carbon dioxide capture and utilization with amines and ionic liquids. *Green Chem Eng* 1(1):16–32
- Xu G, Zhang J, Guangzhi Song (2003) Effect of complexation on the zeta potential of silica powder. *Powder Technol* 134(3):218–222
- Zarei F, Keshavarz P “Enhanced Co2 Absorption and Reduced Regeneration Energy Consumption Using Modified Magnetic Nanoparticles.” *Available at SSRN 4376289*
- Zhang Z, Cai J, Chen F, Li H, Zhang W, Wenjie Qi (2018) Progress in enhancement of CO2 absorption by nanofluids: a mini review of mechanisms and current status. *Renewable Energy* 118:527–535
- Zhang Z, Tohid N, Borhani, Abdul GO (2020) Status and perspective of CO2 absorption process. *Energy* 205:118057
- Zhao B, Wang J, Yang W, Jin Y (2003) Gas–liquid mass transfer in slurry bubble systems: I. Mathematical modeling based on a single bubble mechanism. *Chem Eng J* 96(1–3):23–27

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.