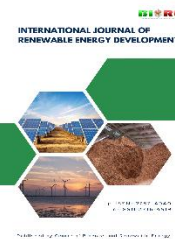




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**International Journal of Renewable Energy Development**Journal homepage: <https://ijred.cbiorc.id>

Research Article

# Development of an isothermal CO<sub>2</sub> absorption process using DMC and PEG400 for carbon capture and storage technology

Ferdiansyah Iqbil Qouli , Iqlima Huda Sahiba , Yuli Rahmawati Dwi Rahayu Ningrum , Rizky Tetrisyanda , Gede Wibawa\* , Wahyudiono, Rendra Panca Anugraha

*Department of Chemical Engineering, Faculty of Industrial and Systems Engineering, Institut Teknologi Sepuluh Nopember, Surabaya, East Java, 60111, Indonesia*

**Abstract.** This study aims to develop and evaluate a green binary solvent system based on dimethyl carbonate (DMC) and polyethylene glycol 400 (PEG400) for physical CO<sub>2</sub> absorption. Efficient and environmentally benign solvents are essential to support large-scale decarbonization efforts. The DMC–PEG400 system was formulated at molar ratios of 1:2, 1:3, and 1:4 to assess its absorption performance. Isothermal solubility experiments were performed at 303.15–323.15 K and 3–7 bar, complemented by Fourier Transform Infrared (FTIR) spectroscopy to elucidate the absorption mechanism. The FTIR spectra showed the emergence of characteristic CO<sub>2</sub> vibrational bands without alterations to the solvent's fingerprint region, confirming that CO<sub>2</sub> uptake proceeds through physical dissolution rather than chemical interaction. The DMC–PEG400 mixtures demonstrated clear temperature and pressure dependencies typical of physical solvents, with solubility decreasing at elevated temperatures and increasing proportionally with pressure. Among the tested formulations, the 1:3 molar ratio exhibited the highest absorption capacity, achieving 0.0606 mole CO<sub>2</sub>/mole solution at 303.15 K and 7 bar. This performance arises from an optimal balance between interaction sites provided by PEG400 and the moderate viscosity needed to facilitate efficient CO<sub>2</sub> diffusion. In contrast, the 1:4 mixture displayed reduced capacity due to excessive viscosity and limited free volume. Overall, the results highlight the promising potential of DMC–PEG400 mixtures, particularly at the 1:3 ratio, as tunable and sustainable physical solvents for CO<sub>2</sub> capture. Their favorable solubility behavior, stability, and benign chemical nature position them as viable candidates for next-generation carbon capture and storage (CCS) technologies.

**Keywords:** Carbon dioxide, Green solvents, Isothermal absorption, Dimethyl carbonate, Polyethylene glycol



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Received: 12<sup>th</sup> Nov 2025; Revised: 26<sup>th</sup> March 2026; Accepted: 4<sup>th</sup> April 2026; Available online: 15<sup>th</sup> April 2026

## 1. Introduction

Global warming due to increasing greenhouse gas emissions has become a problem in recent decades (Ringrose *et al.*, 2024). 71.6% of greenhouse gas emissions are carbon dioxide (CO<sub>2</sub>) gases produced using fossil fuels for various activities such as power generation, industrial processes, and transportation (Leonzio & Shah, 2024; Zhang *et al.*, 2024). If no solutions are implemented, greenhouse gas emissions are projected to increase the Earth's surface temperature up to 6.1°C by 2100 (Leonzio & Shah, 2024). Global efforts to curb climate change are increasingly focused on utilising technologies that can effectively control carbon emissions (Ghazali *et al.*, 2020; Kanniche *et al.*, 2010). Among various initiatives, the Paris Agreement represents a joint commitment by countries worldwide to limit global warming (Guiot & Cramer, 2016). However, the success of achieving these targets depends not only on policy, but also on scientific and industrial innovation that can reduce dependence on fossil fuels and reduce CO<sub>2</sub> emissions into the atmosphere (Rogelj *et al.*, 2016). The impact of CO<sub>2</sub> is not only felt through environmental degradation but also directly on human health. High concentrations of this gas

can trigger respiratory disorders, allergies, and even serious organ damage (Viveiros *et al.*, 2016). The primary challenge is how to manage emissions without hindering economic growth and technological progress that rely on conventional energy sources (Moreaux *et al.*, 2024; Pires *et al.*, 2011).

Various methods have been developed to address this issue, one of which is Carbon Capture, Utilization, and Storage (CCUS), which can reduce CO<sub>2</sub> emissions by capturing CO<sub>2</sub> for use in industrial processes or storing it for a certain period (Firmansyah *et al.*, 2023). This method has been widely adopted, but using CO<sub>2</sub> in industrial processes increases the use of fossil fuels (Moreaux *et al.*, 2024). Therefore, methods for storing CO<sub>2</sub> in geological storage or Carbon Capture and Storage (CCS) can be an effective solution to this problem (Bose *et al.*, 2024). Efficient CO<sub>2</sub> storage in geological reservoirs is viewed as a key element in supporting global efforts to meet the emission reduction objectives set by the Paris Agreement (Moreaux *et al.*, 2024).

Carbon Capture and Storage (CCS) refers to an integrated process designed to capture carbon dioxide generated from industrial or energy-related operations, transport it to a secure site, and ensure its long-term sequestration from the

\* Corresponding author  
Email: [g.wibawa@its.ac.id](mailto:g.wibawa@its.ac.id) (Gede Wibawa)

atmosphere (Tangparitkul *et al.*, 2025; Tripathi *et al.*, 2023; K. Zhao *et al.*, 2023). The main process begins with CO<sub>2</sub> capture, transportation, and storage (Cuéllar-Franca & Azapagic, 2015). Nevertheless, the carbon capture process remains the most complex and costly step (Kheirnik *et al.*, 2021). The development of energy-efficient, effective, and environmentally friendly systems is a key requirement in this technological innovation (K. Zhao *et al.*, 2023). Depending on how the CO<sub>2</sub> is captured, CCS technologies are broadly categorized into post-combustion, pre-combustion, and oxyfuel-based approaches (Kanniche *et al.*, 2010; Kheirnik *et al.*, 2021).

CO<sub>2</sub> capture through the post-combustion method is the simplest and most widely used method in CO<sub>2</sub> absorption processes, both physically and chemically (Chao *et al.*, 2021). Post-combustion capture is often favored because it can be implemented within existing power plants with relatively minimal modifications to current combustion infrastructure (Kheirnik *et al.*, 2021). However, this advantage comes at the cost of lower overall energy efficiency, since CO<sub>2</sub> separation is highly energy-intensive and can account for approximately 75–80% of the total CCS cost (Davison, 2007; Wang *et al.*, 2011). In physical absorption, CO<sub>2</sub> is dissolved into a solvent following Henry's law, with desorption achieved via heating or depressurization (Gui *et al.*, 2010). This method is most effective when the inlet gas has a high CO<sub>2</sub> partial pressure, as energy consumption mainly stems from gas compression (J. Li *et al.*, 2012; Y. Li *et al.*, 2018). The selection of solvents is the most critical stage in the CO<sub>2</sub> absorption process, particularly in choosing solvents that are environmentally friendly and do not produce toxic compounds (Krishnan *et al.*, 2020).

Kanniche *et al.* (2010) highlighted the important role of green solvents in carbon capture technology based on their efficiency, capacity, and environmental compatibility, emphasizing the need for continuous development of sustainable absorbents. Among the available technologies, amine-based absorption remains the most established due to its high CO<sub>2</sub> capture capacity and stability (Anggraini *et al.*, 2022). However, amines have relatively high corrosion rates and energy consumption due to regeneration at high temperatures (Cuéllar-Franca & Azapagic, 2015). Ionic Liquids (ILs) are highly effective in capturing CO<sub>2</sub> due to their non-volatile nature (Handayani *et al.*, 2017). However, ILs have high viscosity, and some are toxic (Krishnan *et al.*, 2020; Zhang *et al.*, 2024). Similarly, various binary liquid mixtures have been investigated as promising candidates due to their tunable properties, low volatility, and relatively simple preparation methods (Altamash *et al.*, 2020; Krishnan *et al.*, 2020). Therefore, alternative solvents for CO<sub>2</sub> capture must continue to be developed to obtain solvents with the best capacity (Song *et al.*, 2023).

Among the potential candidates, polyethylene glycol (PEG) has attracted considerable attention due to its negligible vapor pressure, chemical and thermal stability, and non-toxic nature, while being more cost-effective than ionic liquids (B. Li *et al.*, 2024; Singh *et al.*, 2018). PEG has high solubility in CO<sub>2</sub> and, as a cosolvent, holds promise for enhancing efficiency in CO<sub>2</sub> capture and reducing energy consumption during regeneration (J. Li *et al.*, 2012). On the other hand, dimethyl carbonate (DMC) has been reported as an effective green physical solvent due to its ability to achieve relatively high CO<sub>2</sub> loading at low temperatures, along with advantages such as low toxicity, chemical stability, and low vapor pressure (Gui *et al.*, 2010; Zhou *et al.*, 2023). Its non-toxic and non-hazardous nature, combined with excellent selectivity toward CO<sub>2</sub>, makes it particularly suitable for sustainable separation processes (Gui *et al.*, 2010). The combination of PEG and carbonate-based solvents has been explored in previous studies, particularly in systems such as dimethyl ether of polyethylene glycol (Selexol), which demonstrate effective CO<sub>2</sub> absorption performance (Im *et al.*, 2015). However, increasing the molecular weight of PEG can enhance CO<sub>2</sub> solubility (J. Li *et al.*, 2012). Therefore, using PEG with a higher molecular weight holds promise for use as a green absorbent for CO<sub>2</sub> capture.

Therefore, in this work the combination of DMC with PEG400 as a binary liquid mixtures to capture CO<sub>2</sub> via physical absorption were studied experimentally. This study provides data on CO<sub>2</sub> solubility and introduces a potential alternative solvent that is more efficient and environmentally friendly, supporting Indonesia's efforts toward Net Zero Emissions (NZE) through the development of Carbon Capture and Storage (CCS) technology.

## 2. Methodology

### 2.1 Materials

Dimethyl Carbonate (DMC) and Polyethylene glycol 400 (PEG400) used in this study were obtained from Sigma-Aldrich for synthesis purposes. The carbon dioxide (CO<sub>2</sub>) used was a product of PT Samator Gas Industri with a purity of ≥99,9%. Information about the materials used is written in Table 1.

### 2.2 Synthesis and characterization of DMC-PEG400

The synthesis process of the DMC and PEG400 mixture is carried out by mixing the volumes of DMC and PEG400 according to the molar ratio shown in Table 2. The two materials were homogeneously mixed. Each mixture was heated to 90°C under continuous stirring using a magnetic stirrer for 2 hours until a clear and homogeneous liquid was

**Table 1**  
Specifications of Materials (from Supplier)

Jenis	MW	CAS Number
Dimethyl carbonate (DMC)	90,08	616-38-6
Polyethylene glycol (PEG400)	380 – 420	25322-68-3
Carbon dioxide (CO <sub>2</sub> )	44,01	124-38-9

**Table 2**  
Variation of DMC-PEG400 Mixtures

Abbreviation	Molar ratio DMC:PEG400	Time
MIX 1	1:2	2 hours
MIX 2	1:3	
MIX 3	1:4	

formed. After the mixtures were fully liquefied, the heating was discontinued, and the samples were allowed to stand at room temperature for 1 to 7 days to ensure stability and complete dissolution. The absence of crystallization or phase separation indicates that a stable and homogeneous binary liquid mixture was successfully obtained. This observation suggests good miscibility between DMC and PEG400 under the studied conditions.

The characterization of the DMC:PEG400 mixture was carried out by performing FTIR testing to determine its effect on the amount of CO<sub>2</sub> absorbed (B. Li *et al.*, 2024; J. Li *et al.*, 2016). The FTIR analysis was conducted at the Laboratory of Water Technology and Industrial Consultation, Department of Chemical Engineering, Faculty of Industrial Technology and Systems Engineering, Institut Teknologi Sepuluh Nopember. The FTIR test was performed to identify the molecular bonds formed within the solvent samples. The analysis was carried out using a UV/Vis spectrometer (Meng *et al.*, 2016). It should be noted that the DMC–PEG400 system in this study is treated as a binary liquid mixture. No thermal characterization, such as Differential Scanning Calorimetry (DSC), was performed to confirm eutectic behavior; therefore, the system is not classified as a deep eutectic solvent.

### 2.3 Apparatus and procedures

A stainless apparatus in Figure 1 illustrates a diagram of the equipment used to absorb CO<sub>2</sub>. The main equipment used includes a CO<sub>2</sub> tank (1), a CO<sub>2</sub> buffer tank (2), an equilibrium cell (3) for CO<sub>2</sub> absorption, and a vortex mixer (4). To enhance experimental precision and repeatability, several improvements were incorporated into the system, including an upgraded temperature-controlled heating jacket, reinforced pipeline insulation, and a revised flow pathway intended to minimize pressure fluctuations during gas transfer. Compared with alternative experimental approaches, the constant-volume method was selected due to its simplicity, stability, and proven accuracy in determining vapor–liquid equilibrium (VLE) and solubility data under moderate-pressure conditions. Because the experiments were performed isothermally, all relevant components—from the buffer tank to the equilibrium cell—were equipped with external heaters and thermally insulated to maintain steady-state thermal conditions. Additional temperature indicators were installed at multiple locations to ensure internal temperature homogeneity. All vessels were

constructed from 316 stainless steel to withstand repeated pressurization cycles and to prevent contamination. Before each run, the entire system was purged with CO<sub>2</sub> and rigorously checked for leaks using a soap test and pressure decay method. The experimental temperature was obtained with a temperature controller from Autonics with a precision of ±1°C. The temperature controller used in this study has a precision of ±1°C. Although this is lower than typical high-precision systems, temperature fluctuations during experiments were minimal under steady-state conditions, and the resulting uncertainty is considered to have a limited impact on the calculated solubility data. The experimental pressure measurements were tracked through a digital pressure gauge with a 0–60 MPa range, which provides an accuracy of ±0.2% full-scale.

Before data acquisition, the DMC:PEG400 mixture, prepared according to its designated molar ratio, was loaded into the equilibrium cell and heated to the target temperature. The vortex mixer was activated at a low oscillation speed to promote the uniform distribution of the solvent (J. Li *et al.*, 2012). CO<sub>2</sub> was first introduced into the preheated buffer tank until the target operating pressure was reached. Upon opening the valve between the buffer tank and the equilibrium cell, CO<sub>2</sub> flowed into the solvent phase and began dissolving. Additional CO<sub>2</sub> was injected until the system approached a steady reading. The valve was then closed to isolate the equilibrium cell, allowing the pressure to stabilize. Equilibrium was considered to be reached when the pressure remained constant for at least 10 minutes (Chen *et al.*, 2020; J. Li *et al.*, 2012). This procedure was repeated for each pressure level and for all solvent compositions examined. Identical steps were applied to every solvent mixture to ensure consistency and comparability across the full set of experimental measurements.

### 2.4 Data processing

The absorbed CO<sub>2</sub> can be calculated using the following equation, because of the negligible vapor pressure of solvents:

$$n_{CO_2 \text{ absorbed}} = n_1 - n_2 \quad (1)$$

where  $n_{CO_2 \text{ absorbed}}$  is the amount of gas CO<sub>2</sub> absorbed into the solvent,  $n_1$  is the initial amount of CO<sub>2</sub> gas in the buffer tank,  $n_2$  is the amount of CO<sub>2</sub> gas at equilibrium (J. Li *et al.*, 2012). The

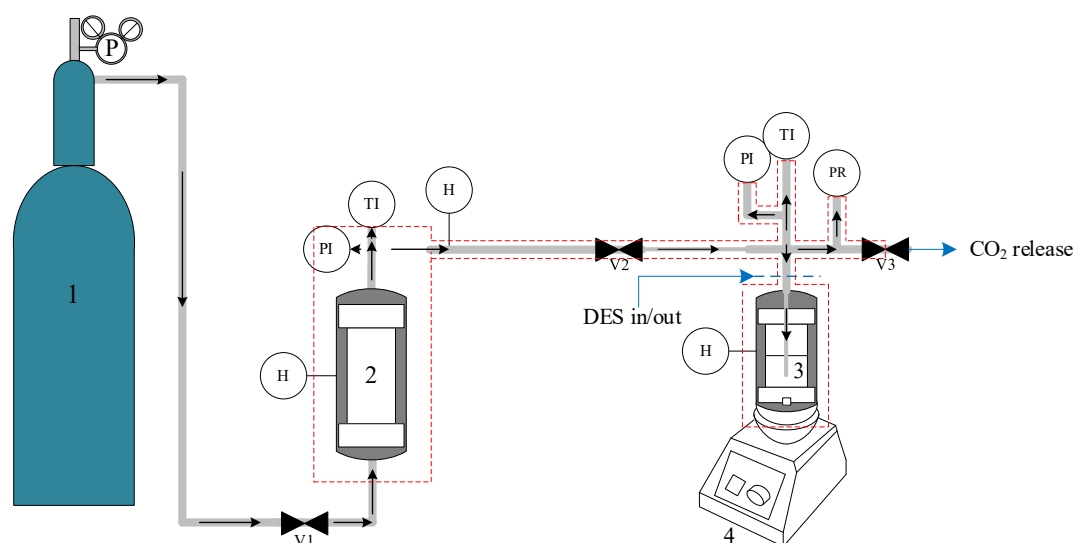


Fig 1. Schematic diagram of CO<sub>2</sub> absorption experiment

absorption capacity of the binary liquid mixture for CO<sub>2</sub> was determined using:

$$n_{CO_2 \text{ absorbed}} = \left( \frac{PV_{\text{void}}}{ZRT} \right)_1 - \left( \frac{PV_{\text{void}}}{ZRT} \right)_2 \quad (2)$$

where  $P$  denotes the system pressure,  $T$  is the system temperature,  $R$  is the universal gas constant,  $Z$  is the compressibility factor, and  $V_{\text{void}}$  is the volume of the void space. To estimate the  $V_{\text{void}}$  occupied by CO<sub>2</sub> gas, the difference between the total system volume ( $V_{\text{total}}$ ) and the volume of the absorbent ( $V_{\text{absorbent}}$ ) is calculated as follows:

$$V_{\text{total}} = \frac{1}{4} \pi l D^2 \quad (3)$$

$$V_{\text{void}} = V_{\text{total}} - V_{\text{absorbent}} \quad (4)$$

where  $l$  is the length of the equilibrium cell and  $D$  is the diameter of the equilibrium cell. In this study, the Peng–Robinson Equation of State (PR-EOS) was used to estimate the compressibility factor ( $Z$ ) of CO<sub>2</sub> for calculating the number of moles in the gas phase. The calculations in this study use the following Peng–Robinson Equation of State (PR-EOS):

$$P = \frac{RT}{V_m - b} - \frac{a}{V_m(V_m + b) + b(V_m - b)} \quad (5)$$

where  $P$  denotes the system pressure,  $T$  is the system temperature,  $R$  is the universal gas constant,  $V_m$  is the molar volume,  $a$  represents the intermolecular attraction parameter, and  $b$  is the van der Waals co-volume parameter accounting for molecular (Peng & Robinson, 1976; Wibawa *et al.*, 2015).

By substituting  $V_m = \frac{zRT}{P}$ , a polynomial expression for the compressibility factor  $Z$  can be derived:

$$Z^3 - (1 - B)Z^2 + \frac{(A - 3B^2 - 2B)Z}{-(AB - B^2 - B^3)} = 0 \quad (6)$$

The mole quantity of solvent  $n_{\text{solvent}}$  can be calculated by the mass weight ( $MW$ ) and the average molar mass of solvents ( $M$ ). So, the solubility of CO<sub>2</sub> in solvents can be obtained using the following equation:

$$x_{CO_2 \text{ absorbed}} = \frac{n_{CO_2}}{n_{\text{total}}} = \frac{n_{CO_2}}{n_{CO_2} + n_{\text{solvent}}} \quad (7)$$

where  $x_{CO_2 \text{ absorbed}}$  is the mole fraction of CO<sub>2</sub> in the solvent (J. Li *et al.*, 2012).

### 3. Results and Discussion

#### 3.1 Synthesis of DMC-PEG400

In Figure 2, the wavelength range of 3000–3700 cm<sup>-1</sup>, corresponding to the O–H stretching vibration, exhibits a noticeable broadening and shift toward a lower frequency at the molar ratio of 1:2 (DMC:PEG400). This redshift and band broadening indicate the formation of hydrogen-bonding interactions between the carbonyl oxygen atoms of DMC and the hydroxyl groups of PEG400, resulting in the weakening of the original O–H bonds within PEG400 molecules (Singh *et al.*, 2018). Such a phenomenon is commonly reported in hydrogen-bonded solvent systems, where the interaction between donor and acceptor groups alters electron density distribution, thereby lowering vibrational frequencies (Meng *et al.*, 2016). In the 1800–1500 cm<sup>-1</sup> assigned to C=O stretching vibrations, a

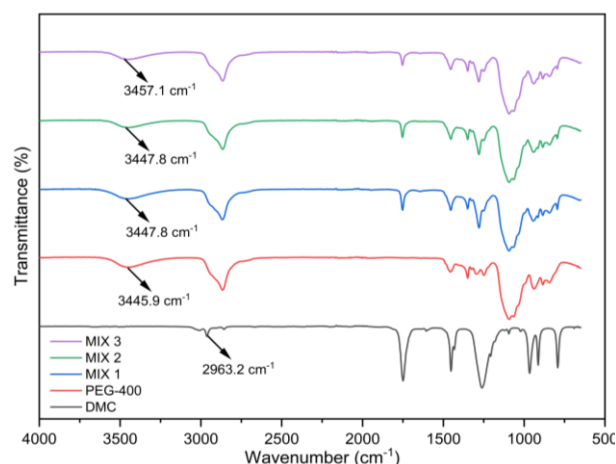


Fig 2. Spectra FTIR of DMC, PEG400, and DMC :PEG400

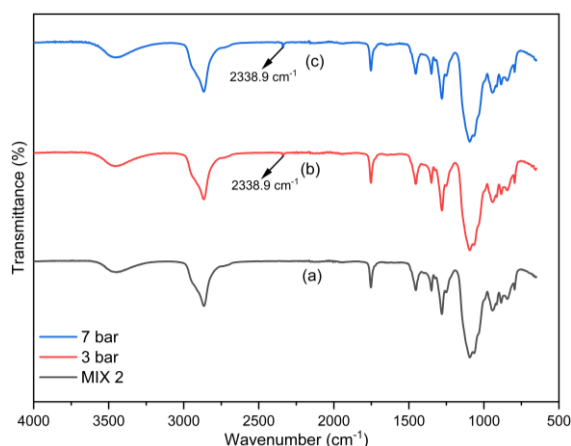
reduction in peak intensity and a slight redshift are evident in the mixed system (green line). This behavior suggests that the carbonyl group of DMC is actively involved in intermolecular interactions, likely forming hydrogen bonds with the hydroxyl groups of PEG400. The partial overlap and intensity decrease in this region confirm the involvement of the carbonyl moieties in non-covalent interactions that modify the local dipole moment of the carbonyl bond (Z. Zhao *et al.*, 2022).

In the fingerprint region (1500–500 cm<sup>-1</sup>), several changes in peak position and intensity are observed, indicating modifications in the molecular environment of the mixture. These changes are associated with C–O and C–C stretching vibrations, suggesting the presence of intermolecular interactions such as hydrogen bonding and dipole–dipole interactions between DMC and PEG400 (Singh *et al.*, 2018). However, no new characteristic peaks corresponding to chemical bond formation are observed, confirming that the interaction between components is physical rather than chemical in nature. There is also a difference in the graphs between the pure compound and the mixture. In MIX 2, the O–H peak is sharper and slightly shifted to the right with higher O–H intensity because PEG-400 is more abundant than in MIX 1. In MIX 3, the O–H peak becomes more like pure PEG-400 due to the higher PEG content compared to previous samples. Z. Zhao *et al.* (2022) also reported that increasing the amount of cosolvent can cause the resulting spectra to resemble those of the pure components.

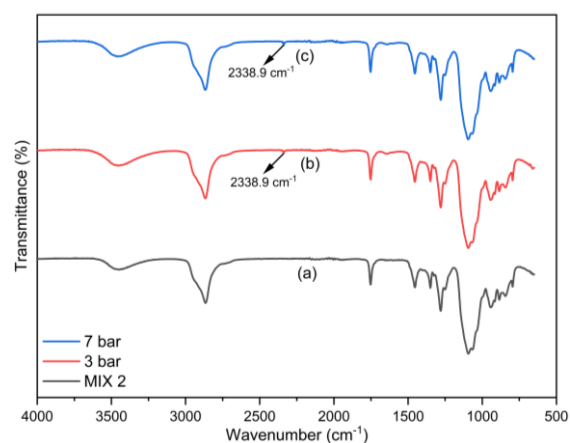
In the region of 1750–1730 cm<sup>-1</sup>, corresponding to the C=O stretching vibration of DMC, a slight shift toward lower wavenumbers (redshift), accompanied by a decrease in peak intensity, is observed in the binary liquid mixture. This shift suggests that the carbonyl group of DMC participates in intermolecular Hydrogen bonding with the hydroxyl groups of PEG400. Such interactions alter the electron density around the carbonyl bond, leading to a weakening of the C=O bond and consequently a reduction in its vibrational frequency. These spectral changes indicate the presence of weak intermolecular interactions between DMC and PEG400 in the mixture (B. Li *et al.*, 2024).

#### 3.2 FTIR results of CO<sub>2</sub> absorption

To ensure that CO<sub>2</sub> is completely dissolved in the solution after the absorption process, further analysis was conducted using FTIR spectroscopy (Haider *et al.*, 2018; J. Li *et al.*, 2016). This test aims to detect the presence of CO<sub>2</sub> in the solution and identify whether CO<sub>2</sub> is physically absorbed or undergoes



**Fig 3.** FTIR test results: (a) before absorption at 303.15 K; (b) after absorption at 303.15 K and 3 bar; (c) after absorption at 303.15 K and 7 bar



**Fig 4.** FTIR test results: (a) before absorption at 323.15 K; (b) after absorption at 323.15 K and 3 bar; (c) after absorption at 323.15 K and 7 bar

chemical interaction with the solvent. FTIR analysis allows for direct identification of characteristic vibrational modes associated with  $\text{CO}_2$  and its potential reaction products, such as carbonates or carbamates, thereby providing molecular-level insight into the absorption mechanism. The following are the FTIR test results of the solvent that has been injected with  $\text{CO}_2$  at pressures of 3 and 7 bar and at temperatures of 303.15 K and 323.15 K.

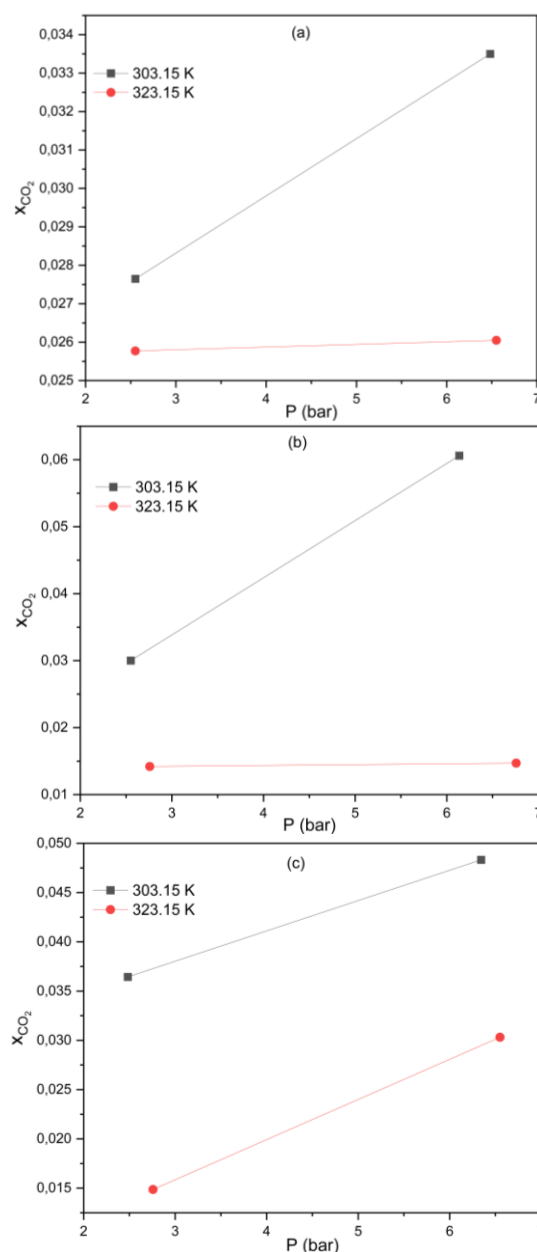
The FTIR results in Figure 3 and Figure 4 show that in the DMC-PEG400 solution, there is an indication of  $\text{CO}_2$ , marked by a peak in the wavelength range of 2330–2350  $\text{cm}^{-1}$ , which was not present in the solution before  $\text{CO}_2$  absorption. This indicates that at that wavelength,  $\text{CO}_2$  is physically dissolved and does not form new compounds, suggesting that the solutions in all three solvents can physically absorb  $\text{CO}_2$  (J. Li *et al.*, 2016). This observation is consistent with previous studies showing that  $\text{CO}_2$  physically solubilized in organic or polymeric solvents exhibits a sharp, symmetric band near 2340  $\text{cm}^{-1}$ .

When  $\text{CO}_2$  is in the gas phase or physically dissolved in a solvent, it will appear and produce a sharp absorption band in the range of 2330–2350  $\text{cm}^{-1}$ . In the FTIR results above, all samples show a peak around the wavelength of 2338  $\text{cm}^{-1}$ , indicating that  $\text{CO}_2$  is present in the system in a dissolved or absorbed state and has not undergone chemical reactions, as no new groups such as carbonates have formed. In the study by

Haider *et al.*, a comparison of graphs before and after  $\text{CO}_2$  absorption was made, showing a new peak at a wavelength of 2340  $\text{cm}^{-1}$ , consistent with the FTIR results from the previous study (Haider *et al.*, 2018). The absence of additional peaks in the 1300–1600  $\text{cm}^{-1}$  region, which would correspond to carbonate ( $\text{CO}_3^{2-}$ ) or carbamate ( $-\text{NHCOO}^-$ ) groups, further supports the conclusion that the dissolution process is purely physical in nature. This differs from amine-based solvents, which form new compounds due to  $\text{CO}_2$  being chemically bound and exhibit changes in the fingerprint region (Haider *et al.*, 2018; Robinson *et al.*, 2012). The consistent spectral profile across different pressures and temperatures further implies that temperature primarily influences solubility and peak intensity rather than inducing chemical transformation.

### 3.3 Gas solubilities in DMC-PEG400 mixtures

The solubility of  $\text{CO}_2$  in DMC-PEG400 at Fig 5 yields results that are consistent with the literature, specifically that the  $\text{CO}_2$



**Fig 5.**  $\text{CO}_2$  solubility results in solvents: (a) MIX 1; (b) MIX 2; and (c) MIX 3

absorption capacity decreases with increasing temperature and increases with increasing pressure (Y. Li *et al.*, 2018). Based on Figure 5, the maximum CO<sub>2</sub> absorption capacity using DMC:PEG400 (1:3), was achieved at a pressure of 7 bar, with values of 0.0606 mole CO<sub>2</sub>/mole solution at 303.15 K, which indicates a strong affinity between CO<sub>2</sub> molecules and the solvent matrix under moderate temperature and elevated pressure conditions.

At higher temperatures, 323.15 K, the CO<sub>2</sub> absorption capacity for all molar ratios tends to be lower than at 303.15 K. This is due to the increase in kinetic energy of CO<sub>2</sub> molecules at high temperatures, causing molecular movement to become faster and more random, thereby easily breaking the hydrogen bonds initially formed between the solvent molecules, reducing the tendency of CO<sub>2</sub> gas molecules to remain in the solvent. As temperature increases, the hydrogen-bonding network between PEG400's hydroxyl groups and the carbonyl oxygen of DMC becomes less stable, reducing the solvent's ability to retain dissolved CO<sub>2</sub>. Consequently, CO<sub>2</sub> molecules are more easily released from the solvent phase, resulting in lower solubility values. As a result, CO<sub>2</sub> molecules become easier to release from the solvent and can reduce the amount of gas dissolved in the solvent (Haider *et al.*, 2018).

Conversely, increased pressure has a positive effect on CO<sub>2</sub> solubility. The higher the pressure, the greater of driving force forcing CO<sub>2</sub> molecules into the solvent (Haider *et al.*, 2018; Pan *et al.*, 2022). As pressure increases, the molecular driving force that pushes CO<sub>2</sub> molecules into the solvent intensifies, enhancing the gas-liquid contact and reducing the gas-phase volume according to Henry's Law. Higher pressure facilitates greater molecular interaction between CO<sub>2</sub> and the polar functional groups of the solvent (particularly the O-H and C=O sites), promoting enhanced physical dissolution. This relationship has been reported by several researchers, who demonstrated that the solubility of CO<sub>2</sub> in PEG-based and carbonate solvents increases almost linearly with pressure, particularly at lower temperatures. These findings collectively confirm that CO<sub>2</sub> absorption in the DMC-PEG400 system is primarily governed by physical dissolution rather than chemical reaction, consistent with the weakly interacting nature of the solvent components.

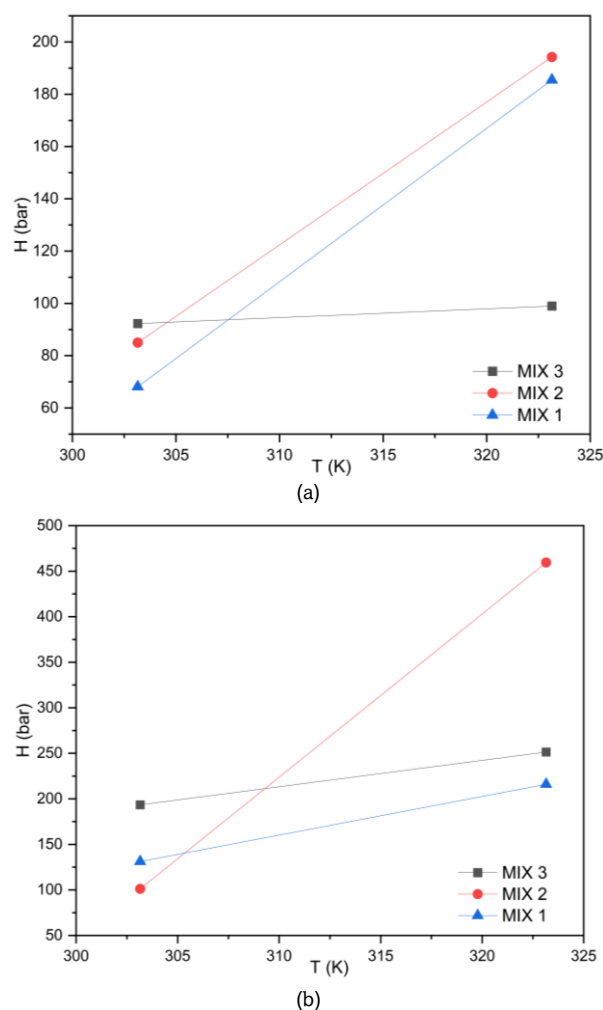
### 3.4 Henry's constants of CO<sub>2</sub> solubilities

The solubility of CO<sub>2</sub> increases with increasing pressure in accordance with Henry's law, which states that at a constant temperature, the amount of gas absorbed by a liquid is proportional to the partial pressure of that gas (Y. Li *et al.*, 2018). The following equation mathematically expresses this relationship:

$$H_x = \frac{P}{x} \quad (8)$$

The term  $H_x$  refers to Henry's constant expressed on a mole-fraction basis, where  $x$  represents the mole fraction of CO<sub>2</sub> dissolved in the liquid phase, which is usually calculated as the number of moles of CO<sub>2</sub> gas absorbed per mole of solvent, and  $P$  is the partial pressure of the gas (J. Li *et al.*, 2012; Y. Li *et al.*, 2018). Since the gas used consists only of CO<sub>2</sub>, the partial pressure can be considered equal to the absorption pressure as the equilibrium system pressure.

Therefore, an increase in pressure causes an increase in the solubility of CO<sub>2</sub> in the solvent, as shown in the experimental results in Figure 6 (Gui *et al.*, 2010; Haider *et al.*, 2018). Henry's constant characterizes the proportional relationship between gas concentration and pressure at infinite dilution. Therefore, its



**Fig 6.** Henry's constant of CO<sub>2</sub> in solvents: (a) at 3 bar and (b) at 7 bar

value can be determined from the slope of the linear correlation between pressure and solute concentration.

In this work, that governed by physical absorption, the solvent's capacity is primarily controlled by the gas partial pressure, meaning that the process typically follows Henry's law. According to this relationship, Henry's law constant corresponds to the slope of the pressure-mole fraction ( $P-x$ ) plot. As shown in Figure 6, Henry's law constant increases with rising temperature, consistent with the observed decrease in CO<sub>2</sub> solubility in DMC as temperature increases under the examined pressure range. It indicates a reduced affinity between CO<sub>2</sub> molecules and the solvent structure, resulting in a diminished ability of the DMC-PEG400 mixture to stabilize dissolved gas (J. Li *et al.*, 2012). This behavior is consistent with the thermal disruption of hydrogen-bonding interactions observed in the FTIR analysis, where weakening intermolecular forces lead to fewer favorable sites for CO<sub>2</sub> accommodation.

### 3.5 Effect of molar ratio on CO<sub>2</sub> solubility

The molar ratio of DMC:PEG400 also affects CO<sub>2</sub> absorption capacity. In most cases, increasing the molar ratio of PEG enhances CO<sub>2</sub> uptake because a higher proportion of glycol groups provides more active sites for interaction with CO<sub>2</sub> (Isaifan & Amhamed, 2018; J. Li *et al.*, 2012; Song *et al.*, 2023). This general trend has been widely observed in various mixed green solvents and binary molecular systems, where the solvent composition modifies polarity, hydrogen-bond networks, and

local free volume, ultimately affecting the solvation environment for CO<sub>2</sub>. Interestingly, for DMC:PEG400, the CO<sub>2</sub> solubility decreases when the molar ratio shifts from 1:3 to 1:4. Based on the results, the highest absorption capacity order according to the molar ratio is 1:3; 1:2; 1:4. This indicates that the 1:3 composition is the optimal condition at room temperature, likely due to the balance between molecular interaction ability and viscosity that is still low enough to facilitate CO<sub>2</sub> gas diffusion into the solution.

Interestingly, the DMC:PEG400 system does not follow a strictly monotonic trend. Although increasing the PEG400 content generally enhances the availability of interaction sites, the CO<sub>2</sub> solubility decreases when the molar ratio increases from 1:3 to 1:4. This behavior suggests that factors beyond simple functional group availability play an important role. At higher PEG400 content, the solvent structure becomes more dominated by PEG–PEG intermolecular interactions, which may reduce the effective free volume available for CO<sub>2</sub> accommodation. As a result, the ability of the solvent to physically dissolve CO<sub>2</sub> at equilibrium may decrease. In addition, while increased viscosity at higher PEG400 content can hinder mass transfer, it is not the sole factor controlling equilibrium solubility. Therefore, the reduced CO<sub>2</sub> uptake at the 1:4 ratio is more likely associated with a combination of reduced free volume and altered thermodynamic interactions within the binary liquid mixture.

The deviation at the 1:4 ratio can be attributed to excessive viscosity introduced by the higher PEG400 content. PEG400 is inherently a highly viscous compound, and increasing its molar fraction elevates the overall viscosity of the solution, which is estimated to follow the order 1:4 > 1:3 > 1:2. Elevated viscosity reduces molecular mobility, restricts free volume, and slows down CO<sub>2</sub> diffusion, ultimately lowering the equilibrium absorption capacity (Meng *et al.*, 2016; Z. Zhao *et al.*, 2022). This aligns with previous reports that overly viscous green solvents, regardless of high functional group density, tend to show diminished gas solubility due to kinetic limitations on mass transfer.

Thus, increasing the PEG400 ratio as a cosolvent does not always correlate directly with increased CO<sub>2</sub> absorption capacity (Haider *et al.*, 2018). Solvent effectiveness depends on the combination of intermolecular interactions, viscosity, free volume, and temperature effects on solvent structure. Similar non-linear behavior has been observed in other environmentally benign binary systems such as choline chloride/levulinic acid and choline chloride/furfuryl alcohol mixtures, where optimal solubility occurs at intermediate molar ratios rather (Aboshatta & Magueijo, 2021; Martins *et al.*, 2019). These findings reinforce the importance of identifying a balanced molar ratio that simultaneously maximizes favorable CO<sub>2</sub> solvent interactions while preserving adequate transport properties for efficient absorption.

#### 4. Conclusion

This study demonstrates that the DMC–PEG400 binary mixture functions as an effective and environmentally benign solvent for physical CO<sub>2</sub> absorption under isothermal conditions. FTIR analysis verified that CO<sub>2</sub> is absorbed physically, as indicated by the appearance of characteristic peaks at 2330–2350 cm<sup>-1</sup> without any alteration in the fingerprint region, confirming the absence of chemical reactions or formation of carbonate-based species. This is consistent with typical behavior of physical solvents, where absorption is governed by weak intermolecular interactions. The solubility results indicate that CO<sub>2</sub> absorption decreases with increasing temperature but increases significantly with operating pressure, in accordance with

Henry's law. The highest CO<sub>2</sub> solubility obtained was 0.0606 mole CO<sub>2</sub>/mole solution at 303.15 K and 7 bar. Temperature elevation weakens hydrogen-bond networks and increases molecular motion, reducing CO<sub>2</sub> retention, while higher pressure enhances the dissolution driving force.

The solvent composition strongly influences absorption performance. Among the tested mixtures, the DMC:PEG400 ratio of 1:3 exhibited the greatest CO<sub>2</sub> solubility. This composition provides an optimal balance between available interaction sites from PEG400 and a viscosity low enough to maintain effective CO<sub>2</sub> diffusion. Increasing PEG400 content beyond this ratio (e.g., 1:4) raises viscosity and limits free volume, reducing mass-transfer efficiency despite higher ether oxygen availability. Overall, the findings highlight the potential of the DMC–PEG400 system—particularly at a 1:3 ratio—as a promising green solvent for physical CO<sub>2</sub> capture. Its tunable properties, low toxicity, chemical stability, and favorable absorption behavior support its application in sustainable Carbon Capture and Storage (CCS) technologies and contribute to the development of low-energy, environmentally friendly decarbonization strategies.

#### Acknowledgments

The authors would like to express their sincere appreciation to the Department of Chemical Engineering, Institut Teknologi Sepuluh Nopember (ITS), for providing laboratory facilities, technical support, and an enabling research environment throughout the completion of this work.

**Author Contributions:** F.I.Q. – writing, editing, designing the study and experimental setup, and organization. I.H.S. – writing, visualization, methodology, and data collection. Y.R.D.R.N – data collection, data analysis, and designing the experimental setup. R.T. – supervision, validation, review, and data discussion. G.W. – supervision, validation, review, and project administration. W – supervision, validation, and review. R.P.A. – supervision and validation.

**Funding:** This work was financially supported by the Program Penelitian Pendidikan Magister menuju Doktor untuk Sarjana Unggul (PMDSU), Ministry of Higher Education, Science, and Technology of Indonesia, through the Directorate of Research and Community Service, Institut Teknologi Sepuluh Nopember, under contract number 1153/PKS/ITS/2025.

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

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