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Modeling and Optimization of Carbon Dioxide Absorption in Deep Eutectic Solvent

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ABSTRACT

Reducing carbon dioxide (CO2) emissions into the atmosphere is the most crucial objective since this results in higher temperatures, pollution, health problems and acid rain. This research focuses on the modeling and optimization of CO2 capture from flue gas by deep eutectic solvent (DES) synthesized from choline chloride/monoethanolamine (ChCl/MEA) using statistical design of experiments (DoE). The synthesized DES and the raw materials were characterized for the presence of functional groups using Fourier transform infrared (FTIR) spectrometry. The impact of three process parameters, operating temperature (25–45°C), molar ratio of ChCl to MEA (0.1–0.5) and inlet CO2 concentration (5–20%) on the CO2 absorption loading performance were investigated. A model to correlate the impact of process parameters on CO2 absorption loading was constructed using the response surface methodology (RSM) in conjunction with central composite design (CCD). The analysis of variance (ANOVA) validated the quadratic model's high significance at a 95% confidence interval to identify the optimal process parameters for the absorption performance. Furthermore, CO2 absorption loading was computed according to the experimental data; the optimal process parameters to achieve the maximum CO2 absorption loading at 8.647 mole CO2/kg solvent at a molar ratio of ChCl to MEA 0.1, an inlet CO2 concentration of 20% and an operating temperature of 32°C.

1. Introduction

Global warming is a major concern for humans and is believed to be primarily caused by CO_2 emissions, mostly produced by burning fossil fuels for transportation and electricity generation [1, 2]. CO_2 is one of the most common waste gases that factories, businesses, and cars emit frequently [3]. Based on scientific estimations, CO_2 concentrations have significantly increased from the pre-industrial ideal of less than 300 ppm to about 420 ppm at present [4]. Many researchers are interested in sequestering and storing CO_2 from fossil fuel-powered power plants to reduce greenhouse gas emissions. However, several technological, economic, and environmental issues, as well as safety problems, remain to be solved, such as (i) enhancing the effectiveness of CO_2 capture, (ii) cutting process expenses, and (iii) CO_2 storage aims to keep CO_2 out of the atmosphere [5, 6]. Various separation methods (e.g., adsorption, membrane separation, cryogenic distillation) can successfully capture CO_2 from the gas streams. The gas and petroleum industries use absorption technology to capture CO_2 from sour natural gas and refinery gas [7, 8].

Chemical absorption is the most feasible technique for removing CO_2 from power plants by 2030[9, 10]. Alkanolamines are the most widely used solvents for the chemical

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absorption technique of CO_2 due to their great ability to absorb acid gases [11, 12]. Despite their advantages, many researchers are looking for a replacement for alkanolamines because of their drawbacks, which include metal corrosion [13], high volatility [14], high recuperative energy [15, 16] and conversion into amine salts [11]. However, several DESs show promise than conventional aqueous amines due to their high CO_2 solubilities [17], low vapor pressures, and high thermal stabilities [18 ,19]. They also have other benefits, such as being less expensive, easier to prepare, non-toxic [17, 20-22], and biodegradable [23]. DESs are a unique class of ionic liquids (ILs) with properties similar to conventional ILs. They are eutectic salt or complexing agent mixes with a preset stoichiometric ratio. A different of salts and complexing agents, including metal salts, metal oxides, and hydrogen bond donors (HBDs), i.e., amides, amines, alcohols, and carboxylic acids, can be used to create DESs [1]. Li and members proposed the use of DES in the CO_2 absorption process as early as 2008, five years after it was discovered using the same HBD and HBA [24]. More research and studies have since been carried out to test additional HBDs and HBAs, such as glycerol, ethylene glycol, ammonium-based, phosphonium-based, and amine-based, to increase CO_2 solubility [25]. It seems that the CO_2 solubility of DES is influenced by the molar ratio of HBA to HBD. Temperature harms CO_2 solubilities in DES, whereas absorption pressure has a beneficial effect. Three distinct DES were synthesized by M.B. Haider et al. using the same hydrogen bond acceptor (methyltriphenylphosphonium bromide) and three distinct hydrogen bond donors (ethylene glycol, glycerol, and diethylene glycol). Since hydrogen bond donors were used, these synthesized DESs can be classified as Type III DESs because they include alcohols, carboxylic acids, or amides. Experimental research is being done on CO_2 absorption from flue gas. The experiment was run up to 15 bars and at different temperatures (303, 313, and 323 K). FTIR analysis was used to characterize the DES before and during the CO_2 collection procedure. According to the findings, DESs based on diethylene glycol exhibited the maximum CO_2 solubility at 303 K and 12 bar [26].

However, the modeling and optimization of the process variables for CO_2 absorption loading using synthesized DES has been documented in relatively few studies. The one-factor-at-a-time (OFAT) method, implemented by changing only one process variable at a time to fix all the others, has been the subject of numerous studies. The time-consuming nature of this method and the difficulty in determining how the process variables interact are its drawbacks [27, 28]. Temperature, molar ratio of ChCl to MEA, and the inlet CO_2 concentration are among the most significant variables that affect the CO_2 absorption loading performance that is being studied [29]. In this work, a statistical technique called Design of Experimentation (DoE) is applied to find the optimum process parameters for the absorption of CO_2 using synthesized DES, assess the interaction between the variables, and develop an equation that is used to predict the CO_2 absorption loading.

2. Methodology

2.1 Chemicals

Choline Choline chloride (ChCl, 98%) was obtained from Macklin China. Whereas, monoethanolamine (MEA, 99%) was gained from Loba India, the N2 gas (99.99%) and the CO_2 gas (99.99%) cylinders used for the synthesis of flue gas were obtained from the Biladi plant for gases in Iraq.

2.2 Synthesis of DES.

In this work, ChCl was used as hydrogen bonding acceptor (HBA), while MEA was used as hydrogen bonding donor (HBD) in the synthesis of DES. The DES solvent was prepared by drying ChCl for 48 hours at 65 °C to get rid of any possible moisture, then heating first (MEA) up to 80 °C on a hotplate with magnetic stirring at 500 rpm. After that, gradually add 1 mole of HBA to HBD with a different molar ratio, then leave the mixture stirred for 4 hours. The translucent and homogenous liquids were then produced. The moisture from DES was removed by drying at 80 °C overnight. At this stage, the prepared DES is ready for absorption experiments [20]. Figure 1 shows the schematic of the procedure for the formation of DES.

2.3 Absorption process

Experiments of CO_2 absorption were achieved in a continuous mode for the gas and liquid phases. The experimental set-up for the absorption process is shown in Figure 2. 40 ml of the prepared DES at various mole ratios of 0.1–0.5 is placed in a flask and then in a water bath that Memmert purchased from Germany, and then let the gas mixture (15 volume percent CO_2 and 85 volume percentN_2) come into contact with the solvent to absorb CO_2. Mass flow controllers that were purchased from Beijing Ifan Peng Instrument Co., Ltd. in China were used to regulate the gas flow rates. The absorption process was operated between 25 and 45°Cat atmospheric pressure and 100 ml/min of gas mixture flow rate, or between 5 and 20 ml/min for CO_2 and 80 to 95 ml/min for N_2. Every five minutes, an analysis of the CO_2 in the absorption cell's outlet gas (AtmoCheck Double from the USA) was done to determine the saturation of the solvent, where the solvent stopped absorbing CO_2.

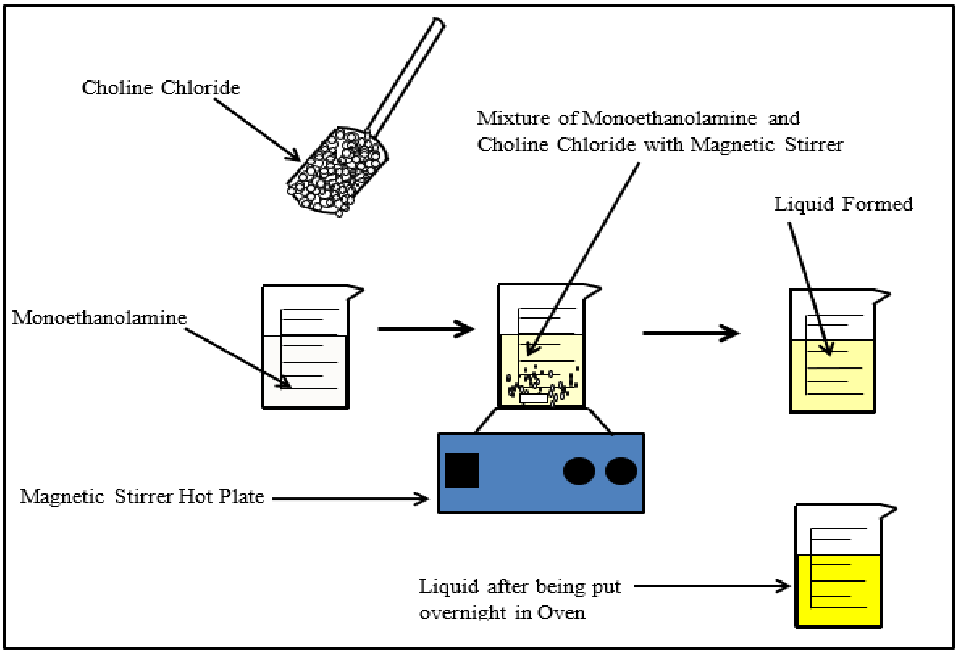

Figure 1. The schematic of the formation of DES.

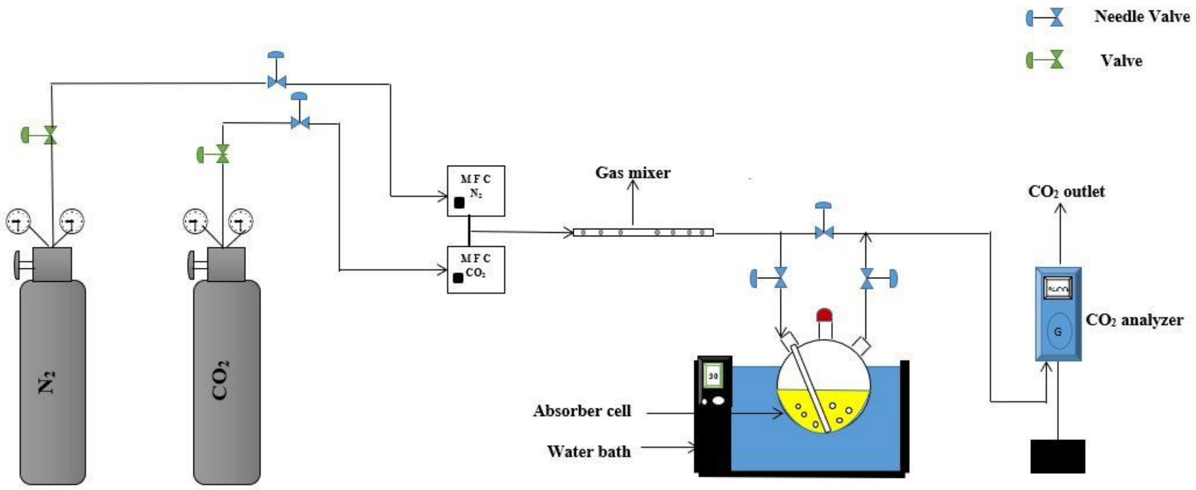

Figure 2. The schematic of the absorption experimental.

2.4 CO_2 analysis

The calibrated CO_2 analyzer can utilized to measure the vol % vol. % of CO_2 gas from the input and output of the absorption cells, through which the saturation of the solvent (when the vol. % of CO_2 in the outlet stream equals the vol. % of CO_2 in the outlet stream) can measured as a guide to the end of the CO_2 absorption experiment. The rate absorption of CO_2 by DES is the differential in the carbon dioxide gas rate between the inlet and output of the absorber from the gas phase. On the other hand, the absorption loading of CO_2 of the absorbents was acquired by determining the integral value of the rate absorption of CO_2 to time absorption [30], as in the subsequent equations:

$$r = \frac{Q_{in} - Q_{out}}{m \times 22.4 \times 1000} \qquad (1)$$

Where: r is the absorption rate of solvent (mole per kg. min); Q_{in} and Q_{out} are the input and output gas flow rate (ml per min); m is the weight of solvents (kilogram).

$$C_T = \int_0^t r\,dt \qquad (2)$$

Where: C_T is the absorption loading of solvents (mole per kg), t is the absorption time (min).

2.5 FTIR Spectroscopy

The chemical structure of the resulting DESs is ascertained using Fourier transform infrared spectroscopy (FTIR), which examines modifications in covalent chemical bonding in molecules The Shimadzu spectroscope was utilized to acquire the FTIR spectra of the specimens (Shimadzu Corporation FT/IR Affinity-1 spectrometer, SN: A21375003264 CZ/PIN 206-73500-38, Japan) at the College of Science/Department of Chemistry/University of Diyala, Iraq. The potassium bromide (KBr) pellet technique was used to record the infrared spectra within the wavenumber range of 4000-400 cm^{-1}. The sample and KBr were dried at 105 °C for two hours before analysis, and the resulting transparent pellet was then ground at a mass ratio of 1:20 (KBr: sample). By applying pressure of up to 75 MPa using uniaxial presses, the fine powder mixture was compressed into a thin, one-millimeter-long pellet. Once inside a sample holder, the pellet was subsequently placed under the FT-IR unit's infrared radiation and exposed vertically.

2.6 Design of experiment (DoE)

The experiments were designed with the purpose of modeling and optimizing CO_2 absorption loading using DoE software with version 6.0.6. Three independent variables were examined for their effects on CO_2 absorption loading: operating temperature (25 - 45°C), inlet CO_2 concentration (5-20 vol.%), and molar ratio of ChCl to MEA (0.1-0.5). Studies have shown that the CO_2 absorption loading in synthesized DESs increases with increasing temperature to 45°C and then begins to decrease between 45°C and 65°C. However, inlet CO_2 concentration has a positive effect on CO_2 absorption loading, the CO_2 absorption loading became more soluble with an increase in the molar ratio of amine in the synthesized DESs [6, ٣١-33]. For this statistical model, 20 experimental runs were advised by the RSM and the CCD, both of which are included in the DoE software. Finding the functional correlations between independent variables with the fewest tests is made possible by the Design-Expert program. By using multiple regression analysis on the experimental data, it also creates an empirical model for the desired response as a function of the chosen factors [27]. To minimize bias resulting from systematic trends in the variables, the experimental runs were carried out randomly. One response taken into consideration to investigate the impact of process factors was CO_2 absorption loading. This is the empirical model displayed:

$$\begin{aligned} Y = \beta_o + \beta_1 A + \beta_2 B + \beta_3 C + \beta_{12} AB \\ + \beta_{13} AC + \beta_{23} BC + \beta_{11} A^2 \\ + \beta_{22} B^2 + \beta_{22} B^2 \\ + \beta_{33} C^2 \qquad (3) \end{aligned}$$

Where: Y is the predicted response. A, B, and C are the actual forms of inlet CO_2%, operating temperature, and molar ratio of ChCl to MEA, respectively. The term β_0 is the offset, β_1, β_2 and β_3 are the linear expressions. While, β_{11}, $\beta 22$

and β_{33} are the quadratic expressions, and β_{12}, β_{13} and β_{23} are the interaction expressions. The analysis of variance (ANOVA) was used to establish the statistical significance of the empirical model. The numerical optimization method built into the Design Expert program was then used to improve the replies.

3. Results and discussion

3.1 (FT-IR) analysis

FTIR spectra of pure ChCl, pure MEA, and synthesized DES before absorption of CO_2 are displayed in Figure 3. The pure ChCl material exhibits IR vibrational bands that have been assigned at 948 cm^{-1} referred to as C-C symmetric [3٤]. Whereas the vibrational bands at 1134 cm^{-1} refer to $C-N^+$ symmetry stretching [3٥]. In the meantime, the vibrational bands at 1470 cm^{-1} indicate the presence of CH_2 bending and an alkyl group. However, the band C-H stretches around 3000-2850 cm^{-1} due to absorbed water [36], and the broad O-H stretch around 3300 cm^{-1} [6].

On the other hand, in the FT-IR spectra of the pure MEA, it can be seen that the vibrational bands at 950 cm^{-1} refer to C-C symmetry [3٤]. The vibrational bands at 1134 cm^{-1} indicated C-N [3٦]. However, the vibrational bands at 1050 cm^{-1} indicated C-O stretching [37]. The vibrational bands at 1470 cm^{-1} refer to–CH_2 [36], the vibrational bands at 1597 cm^{-1} indicated NH bending of primary amine bend [37]. However, the peaks at 3300-3100 cm^{-1} refer to N-H stretches [36], and the broad band around 3300 cm^{-1} refer to O-H cm^{-1} [6].

FT-IR spectra of the created DES before absorption of CO_2, results have been verified for the creation of DES, as from the reported spectra, all of the functional groups of both compounds have been identified, and the bands that are more noticeable at 950 cm^{-1} represent C-C [34]. However, it can be observed, the band is less obvious at 1224 cm^{-1} refer to the C-N stretch [36]. It is evidence of ChCl-MEA interactions because the presence of aliphatic amines. The FT-IR spectra of synthesized DES after absorption of CO_2. The IR bands of synthesized DES after the absorption of CO_2 show that the structure of DES changed due to the reaction of CO_2 with DES. It can be observed in small bands at 950 cm^{-1} that are less obvious or weakened. While the bands at 1224 cm^{-1}, 1470 cm^{-1} and 1650 cm^{-1} disappeared, this indicates this indicates the formation of carbamate [35]. The results of the FT-IR spectra demonstrated that even after CO_2 is absorbed, the amine group present in the DES is still present. This suggests that even when the solvent is completely saturated with CO_2, some amines have not yet reacted. This implies that, in addition to the process's chemical absorption, there may also be physical absorption. The development of a carbamate indicates that there has been chemical absorption between 2241 cm^{-1} and 2023 cm^{-1} [6].

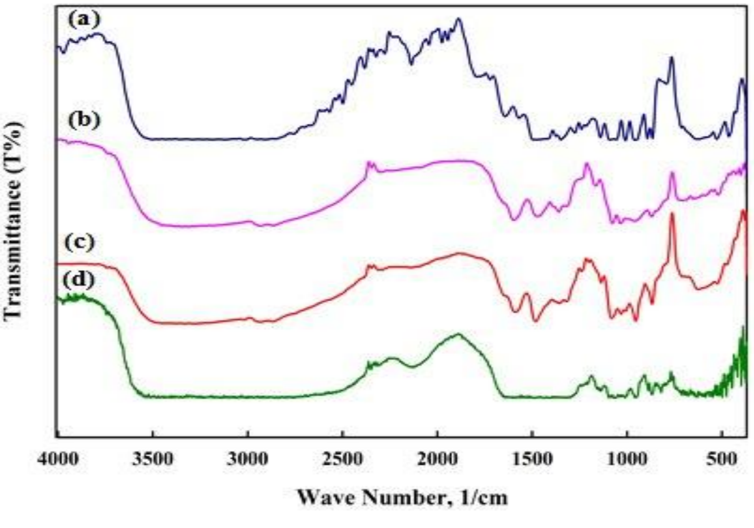

Figure 3. FTIR spectra of synthesized DES prior to CO_2 absorption; (a) pure ChCl; (b) pure MEA; (c) DES before adsorption; and (d) DES after absorption.

3.2. Response surface modelling of CO_2 absorption loading

DoE was utilized to evaluate and model the CO_2 absorption experimental data using DES synthesized from ChCl/MEA according to surface response methodology (RSM). DoE can provide an empirical model for CO_2 absorption loading as a function of specific process conditions. Table 1 gives the experimental design matrix of the 20 full factorials with CCD for the CO_2 absorption loading. A total of 20 experimental runs are needed for a three-factor full factorial design, which consists of 8 factorial points, 6 axial points, and 6 replicates at center points. The reproducibility of the experimental data was examined using the replicate at center point (experimental runs of 15-20). Randomization was employed in the experimental runs to reduce bias resulting from systematic trends in the variables. The CO_2 absorption loading ranges from 1.988 to 7.484 mole CO_2/kg solvent.

Table 1: Experiment matrix and respective responses for the CCD for CO_2 loading absorption using DES

Std	Run	Point Type	Temperature, °C	Inlet CO_2 concentration, vol. %	Mole Ratio of ChCl to MEA	absorption loading, mol CO_2/kg solvent
1	15	Fact	29	8	0.18	3.150
2	17	Fact	41	8	0.18	3.630
3	16	Fact	29	17	0.18	6.107
4	4	Fact	41	17	0.18	7.484
5	11	Fact	29	8	0.42	1.988
6	19	Fact	41	8	0.42	2.412
7	14	Fact	29	17	0.42	2.040
8	12	Fact	41	17	0.42	3.433
9	20	Axial	25	13	0.30	2.682
10	2	Axial	45	13	0.30	3.479
11	7	Axial	35	5	0.30	2.362
12	8	Axial	35	20	0.30	3.982
13	1	Axial	35	13	0.10	4.575
14	18	Axial	35	13	0.50	2.001
			Repeted runs for reproducibility test			
15	3	Center	35	13	0.30	3.813
16	9	Center	35	13	0.30	2.954
17	10	Center	35	13	0.30	3.411
18	6	Center	35	13	0.30	3.053
19	5	Center	35	13	0.30	3.253
20	13	Center	35	13	0.30	2.782

The statistical findings of the ANOVA analysis for CO_2 absorption loading using DES synthesized from ChCl/MEA are shown in Table 2. According to the ANOVA data, the quadratic model recommended by the RSM software provides the best representation of the CO_2 absorption loading. Eq. (4) shows the modified quadratic model in reality. In front of model terms, the positive sign (+) denotes a synergistic effect that increases CO_2 absorption loading, while the negative sign (-) denotes an antagonistic effect that decreases CO_2 absorption loading.

$$\mathrm{CO_2\ absorption\ loading} = +4.970 - 0.206 \times \mathrm{A} + 0.130 \times \mathrm{B} + 1.471 \times \mathrm{C} + +1.352 \times \mathrm{B} \times \mathrm{C} \quad (4)$$

Where: A is the operating temperature (°C), B is the inlet CO_2 concentration (vol.%) and C is mole ratio of ChCl to MEA.

Table 2: ANOVA results for CO_2 absorption loading using DES synthesized from ChCl/MEA.

Source	Sum of squares	DF*	Mean square	F-Value	Prob > F	
Model	31.26	9	3.47	9.06	0.0010	Significant
A	1.84	1	1.84	4.80	0.0532	
B	8.24	1	8.24	21.49	0.0009	
C	16.10	1	16.10	41.98	<0.0001	
A^2	0.094	1	0.094	0.25	0.6305	
B^2	0.18	1	0.18	0.48	0.5032	
C^2	0.34	1	0.34	0.89	0.3665	
AB	0.44	1	0.44	1.14	0.3117	
AC	$2*10^{-4}$	1	0.19	0.52	0.9822	
BC	4.12	1	4.12	10.73	0.0083	
Residual	3.83	10	0.38			
Lack of Fit	3.16	5	0.63	4.65	0.0586	Not Significant
Pure Error	0.68	5	0.14			
Cor Total	35.09	19				
Dev**	0.62					
R^2	0.8907					

DF*= Degree of Freedom and Dev**= Standard Deviation

The main variable effects and any potential interactions on the CO_2 absorption loading are estimated using an ANOVA. The associated probability value (Prob>F) and Fisher value (F-value) are the two most significant outputs from the ANOVA results. The probability equals the fraction of the F-distribution's area under the curve that is outside of the observed F-value, as indicated by the (Prob>F) value. In other words, a term is deemed to significantly affect the CO_2 absorption loading when the (Prob>F) value is small. Model terms that have a probability greater than 0.05 (Prob>F) suggest that the terms hold significance in the CO_2 absorption loading model. There is a 95% confidence level that indicates the developed model is significant, as indicated by the model F-value of 25.72 and the Prob>F value of less than 0.05. Terms B, C and AC are important for CO_2 absorption loading at 95% in the current study. The terms A^2, B^2, C^2, AB, and AC in Eq. (4) are not significant to the model because their values of probability (Prob>F) are greater than 0.05, so they were removed from Eq. (4) [38]. The ratio of pure error to residuals indicates a lack of fit. In light of the fact that the F-value of 4.65 indicates a lack of fit when compared to the pure error resulting from noise (Prob>F) of0.0586, the proposed model for CO_2 absorption loading in Eq. (4) is appropriate for the current investigation. Figure 4 presents a comparison between the predicted values by the RSM model and the experimental data of CO_2 absorption loading.

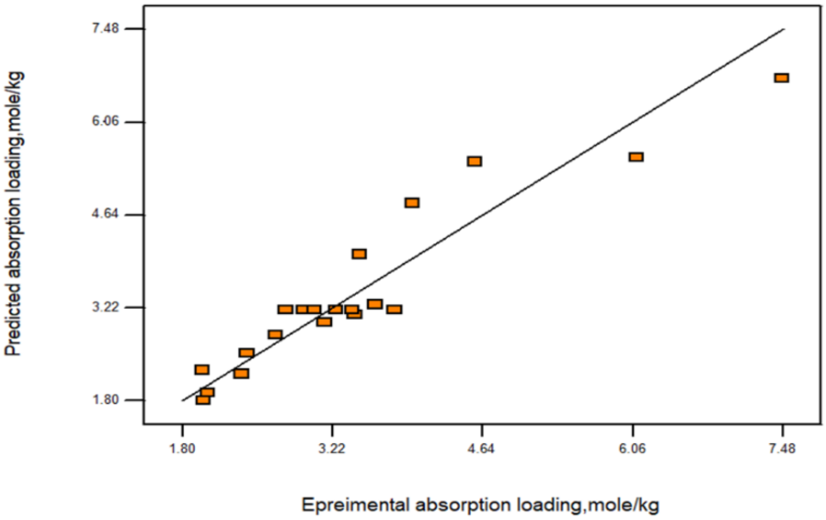

Figure 4. Experimental vs. RSM predicted results of CO_2 absorption loading

The interaction between temperature and inlet CO_2 concentration on the CO_2 absorption loading at the center point of the molar ratio of ChCl to MEA (0.3) is illustrated in Figure 5. It can be noted that CO_2 absorption loading increases with an increase in inlet CO_2 concentration from 5 to 20 for a temperature range of 25 to 45 °C. This result agrees with those reported previously [31-33]. The synthesized DES continued to show good CO_2 absorption loading at high operating temperatures, while the CO_2 uptake was expected to reduce when the operating temperature was raised from 45 to 65 °C as reported previously [31]. However, higher inlet CO_2 concentration led to an increase in the CO_2 absorption loading for the DES [33]. The increase in CO_2 absorption loading is not very noticeable and fall between 3.789 and 6.325 mole/kg solvent. This conduct is consistent with earlier reports [31-33].

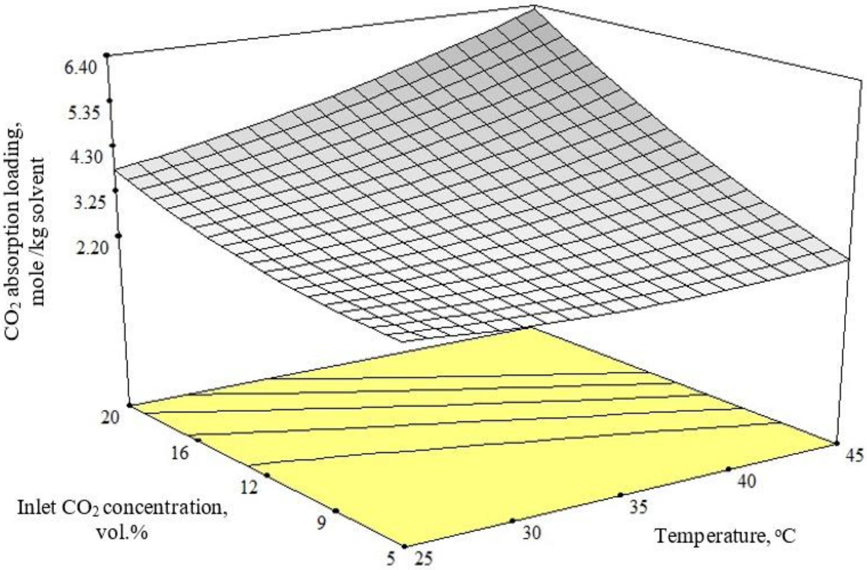

Figure 5. Effect of inlet CO_2 concentration and operating temperature on the CO_2 absorption loading at a mole ratio (ChCl/MEA) of 0.3

Figure 6 illustrates the effect of inlet CO_2 concentration and mole ratio of ChCl to MEA on the CO_2 absorption loading at the center level of operating temperature (35 °C). It is observed that for the molar ratio of ChCl to MEA, which ranges from 0.1 to 0.5, the CO_2 absorption loading increases with an increase in the inlet CO_2 percentage from 5 to 20. This outcome is consistent with previously reported results: An increase in CO_2 absorption loading for DES was caused by higher CO_2 concentrations in the inlet gas stream [6, 33]. Although the physical absorption is believed to be caused by ChCl's ability to form hydrogen bonds with amines, Meanwhile CO_2 became more soluble with an increase in the molar ratio of amine in the DES. This is understandable since the concentration of amines increases the probability of a hydrogen bond network forming with ChCl, resulting in DESs [6]. Additionally, it shows that the CO_2 absorption loading increases but not significantly, the inlet CO_2 concentration rises with increasing mole ratio of ChCl to MEA, and the results range from 3.207 to 3.328 mole/kg. This behavior is in line with previous reports [6, 33].

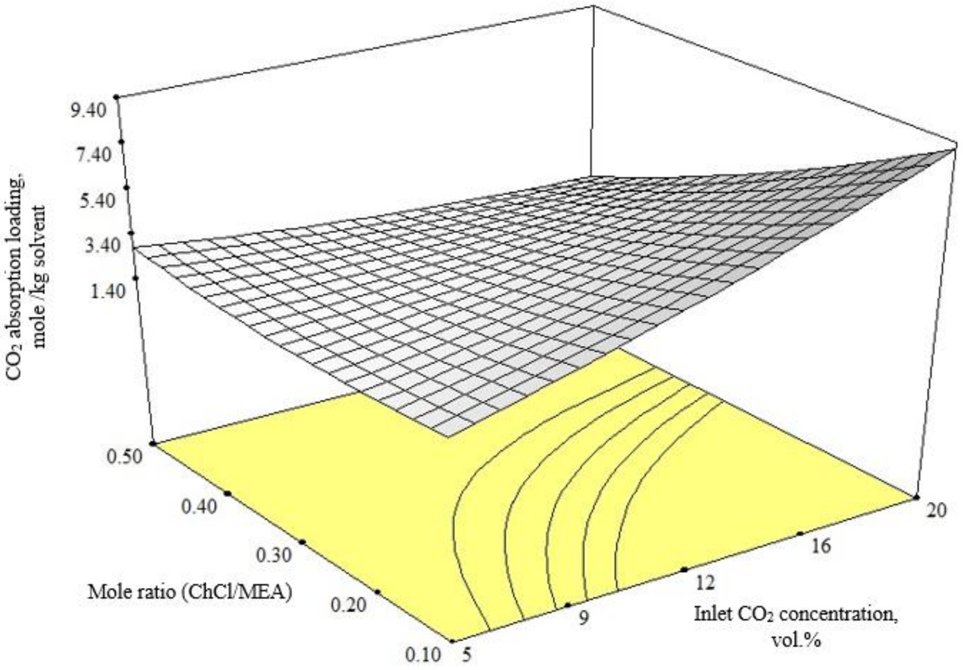

Figure 6. Effect of inlet CO_2 concentration and mole ratio of ChCl/MEA on the CO_2 absorption loading at an operating temperature of 35°C

The interaction temperature and molar ratio of ChCl to MEA on the CO_2 absorption loading at the center level of the inlet CO_2 concentration (13%) are shown in the Figure 7. It can be noted that the CO_2 absorption loading increases with an increase in temperature from 25 to 45 for mole ratios of amine in DES ranging from 0.1 to 0.5. This result agrees with those reported previously. Good CO_2 absorption loading was still demonstrated by the synthesized DES at high operating temperatures, although, as previously reported [6, 31-33], CO_2 uptake was predicted to decrease at higher operating temperatures of 45 to 65 °C.

CO_2 can be absorbed in DES both chemically and physically. For chemical absorption, the equilibrium reaction mechanisms determine the reaction steps of the solubility of CO_2 in amines. The reaction mechanisms for primary amines proceed in two steps and do not require the addition of water to produce carbamate. The first step for the primary amines is bimolecular, second order, and rate-determining, while the second step is immediate. On the other hand, the physical absorption is caused by the ability of ChCl to create hydrogen bonds (O–H and N–H) with the amines. The solubility of CO_2 increased with increasing molar ratio of amine in the DES. This is made obvious as there is a greater chance of a hydrogen bond network forming with the ChCl when more amine is available in DES [6]. Moreover, the increase in temperature resulted in a slight increase in CO_2 absorption loading (1.428 to 3.871 moles/kg), this was owing to the exothermic CO_2 absorption thermodynamic mechanism, which caused undesirable reactions at high temperature. This behaviour matches previous reports [6, 33].

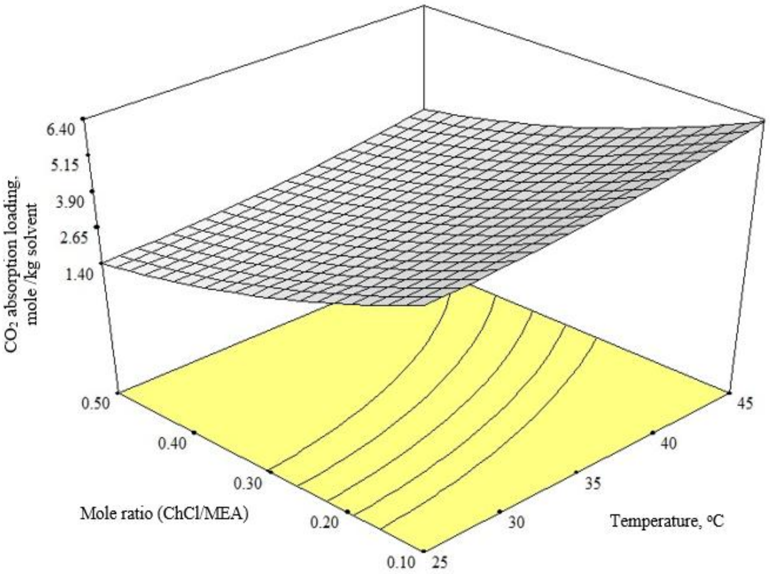

Figure 7. Effect of operating temperature and mole ratio of ChCl/MEA on the CO_2 absorption loading at an inlet CO_2 concentration of 13%

3.3 Process optimization using RSM

Table 3 displays the optimization criteria that were applied in order to ascertain the optimum value for the CO2 absorption loading of the synthesized DES.

Table 4 presents the total desirability optimum solutions found by Design Expert software. The optimum solutions are by default ranked from highest to lowest in terms of desirability. For additional process research, the optimum circumstances in Solution 1 with the highest total desirability of 1.000 are selected. The generated optimum conditions for the CO_2 absorption loading are obtained as follows: temperature 32 °C, inlet CO_2 concentration 20 vol.% and mole ratio of ChCl to MEA 0.1. According to the developed model, it is possible to achieve an optimal CO_2 absorption loading of 8.647 moleCO_2/kg,solvent.

Three more experimental runs are carried out at the ideal condition (Solution 1) to verify the accuracy of the DoE prediction. Table 5 displays the CO_2 absorption loading of the repeated experimental runs for DES synthesized from ChCl/MEA. The DoE software compares the experimental values of the CO_2 absorption loading under ideal conditions with the predicted values. The average % error for loading CO_2 absorption is 4.68. There is good agreement between the experimental and predicted values, as evidenced by the response's mean % error of less than 5%. It is possible to draw the conclusion that the model created by DoE software using RSM in the current study exhibits adequate reliability models for predicting reasonable predictability for the performance of the synthesized DES for the CO_2 absorption loading.

Table 3: Constraint used for optimization of CO_2 absorption loading using DES synthesized from ChCl/MEA.

Factors	**Goal**	**Lower limit**	**Upper limit**
Temperature, °C	Is in range	25	45
Inlet CO_2 concentration, vol.%	Is in range	5	20
Mole ratio of ChCl to MEA	Is in range	0.1	0.5
CO_2 absorption loading, mole CO_2/kg solvent	Maximize	1.989	7.484

Table 4: Optimum conditions of CO_2 absorption loading using DES synthesized from ChCl/MEA.

Solution	Temperature (℃)	Inlet CO_2 concentration, vol.%	Mole ratio of ChCl to MEA	CO_2 absorption loading, mole CO_2/kg solvent	Desirability	
1	32	20	0.10	8.647	1.000	Selected
2	45	20	0.20	8.328	1.000	
3	37	18	0.10	8.386	1.000	
4	30	20	0.11	8.208	1.000	
5	37	19	0.11	8.591	1.000	
6	44	17	0.11	8.608	1.000	
7	28	20	0.11	8.079	1.000	
8	32	19	0.11	8.148	1.000	
9	42	17	0.10	8.185	1.000	
10	42	19	0.18	7.842	1.000	

Table 5: Verification experiments at optimum conditions simulated by DoE for the CO_2 absorption loading using DES synthesized from ChCl/MEA.

Run	CO_2 absorption loading, mole CO_2/kg solvent		% Error
	Experimental	DoE	
1	9.165	8.647	5.99
2	8.431	8.647	4.38
3	8.965	8.647	3.68
Mean Error			4.68

4. Conclusions

Binary DES was successfully synthesized from ChCl/MEA with different molar ratios for enhancement of the absorption of CO_2. Process modeling and optimization of the CO_2 absorption loading using DES synthesized from ChCl/MEA by RSM coupled with CCD available in the statistical method of DoE. The effects of independent variables, such as temperature, inlet CO_2 concentration and the mole ratio of ChCl to MEA, on CO_2 absorption loading were investigated. The analysis revealed that when the temperature rises from 25 to 45 °C and the inlet CO_2 concentration rises from 5 to 20%, the CO_2 absorption loading increases. Conversely, a decrease in CO_2 absorption loading was brought about by raising the mole ratio of ChCl to MEA from 0.1 to 0.5. The optimum operating parameters were 32 °C temperature, 20% inlet CO_2 concentration and a

0.1 mole ratio of ChCl to MEA for maximum CO_2 absorption loading at 8.647 mole CO_2/kg solvent. The DoE-developed models showed sufficient reliability and good predictability for modeling and predicting the CO_2 absorption loading by DES, with correction coefficient (R^2) values greater than 0.8907.

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