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Mathematical Modeling of the Solubility of Carbon Dioxide in Deep Eutectic Solvents

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ABSTRACT

The increase in energy consumption, along with an increase in human population and industrial activities after the industrial revolution, has caused to increase in the consumption of fossil fuels. Carbon dioxide from fossil fuels has the most significant effect on the production of greenhouse gases and global warming. The absorption of CO2 emitted into the atmosphere is the most crucial method to reduce carbon dioxide in the air. Recently, a new solvent has been developed to absorb greenhouse gases under the name of deep eutectic solvents (DES). These solvents are biodegradable, non-toxic, or low-toxic compounds that are easily obtained. A mathematical model based on the Peng–Robinson (PR) equation of state (EOS) with three different mixing rules Modified van der Waal's (M1), Quadratic (M2) and Wong Sandler (M3) was developed to correlate the CO2 solubility in six types of DESs. The model was validated and compare with the obtained experimental data reported in the literature at temperatures (293.15 – 333.15) K and pressure (0.405 – 30.408) bar. The experimental and calculated data of PR EOS with three mixing rules were generally in a good agreement by obtaining % AARD a round (0.08 – 8.08), (0.05 – 7.58) and (0.09 – 6.56) for M1, M2 and M3 respectively, and the best results with less %AARD was obtained from Wong-Sandler mixing rule in the most of cases.

1. Introduction

One of the most pressing problems confronting humanity is global warming.[1] The human greenhouse effect is at the forefront of the present conversation concerning climate change and global warming.[2] Given that it is present in the environment in quite high concentrations, CO_2 has a major effect on global warming.[2, 3] There is a swift coming to the consensus that CO_2 emissions must be decreased to mitigate the impacts of climate change and global warming.[4]

The most developed method over the recent years has been thought to be CO_2 capture from the natural gas sweetening unit.[5] There are many different CO_2 capture systems for separating and capturing CO_2 from gas sources [6, 7] depending on various physical and chemical processes, such as absorption, adsorption, membranes, and cryogenics.[8]

Aqueous amine absorbents are the most well-known and industrially accepted CO_2 collection technique. These solvents do, however, have significant flaws such as the loss of amine chemicals and the injection of water into the gaseous state throughout the desorption process, chemical decomposition that produces caustic compounds. For industry applications, they are diluting with water since they are viscous in their pure state, and owing to the necessity to heat the extra water, high energy

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use during regeneration, and low carbon dioxide collection capability, resulting in a large parasitic energy loss.[9]

Ionic liquids (IL) have so garnered a lot of interest as a substitute for conventional organic solvents.[10] These solvents initially sparked attention because to their low vapor pressure, which is crucial for industrial uses, good thermal stability, broad liquidus variety, significant non-flammability, performance factor, and renewability. They can also be readily tailored for a particular purpose and then can take a variety of substances, including CO2. [11, 12] Large-scale applications of ILs also are difficult to implement, and among the challenges is their massive cost.[13] Deep Eutectic Solvents (DESs) have begun to grow in prominence among scientists for a variety of uses, particularly in CO_2 absorption.[14]

Binary mixes of two components that accept and donate hydrogen bonds in a predetermined molar ratio are known as DESs.[15] These substances, which are divided into many broad kinds based on their components, are mixes of two compounds having eutectic melting points that are considerably lower than the melting points of the pure elements.[16] At temperatures between 298.15 K and 343.15 K, the majority of DESs are liquid.[2]

Thus, many DESs have several advantageous qualities that make them appropriate choices with high potential for various uses, including a wide liquidus range, biodegradability, simplicity of production, relatively inexpensive, nonreactivity with water, such little byproduct creation, environmental friendliness, etc. [17, 18, 19]

The experimental assessment of CO_2 solubility in DESs has been the primary concern of the majority of DES-based CO_2 absorption research. Nevertheless, even taking into account the vast number of HBA-HBD configurations at various ratios, have still included a minor part of DES possibilities. It is particularly essential in this situation to have a trustworthy mathematical model for forecasting the CO_2 absorption capability of DESs.[20]

The time and economic constraints, hazards, and dangers posed by experimental circumstances must also be taken into account, in addition to all the complexity and difficulty that may be encountered when undertaking laboratory operations.[21] As a result, it is very desired to have accurate prediction models for estimating experimental findings under various conditions.[22]

Whereas the interaction parameters for the binary mixes were necessary, modeling these systems is a good way to simplify the experimental observations. Adequate equilibrium data across a broad temperature range are needed for the estimation of the binary interaction parameters.[23] The cubic equations of state, including Peng-Robinson (PR) is without a doubt the most popular models.[24]

In 2015 Mirza et al. examined experimentally the solubility of CO_2 in three different DESs, namely, reline, ethaline, and malinine in a wide range of temperatures and pressures. They modified PR EOS to correlate the experimental data. Their results showed excellent agreement with the complete set of experimental data, whereas a maximum average absolute relative deviation of 1.6%. [25] In addition, Ali et al. in 2016 developed a mathematical model based on the PR-EOS to calculate the VLE conditions in the desorption unit and estimate the CO_2 solubility. The research employed eight distinct DESs. According to their findings, the model gives very close results to the experimental data. [26]

The PR, Soave-Redlich-Kwong (SRK) and Perturbed-Chain SAFT (PC-SAFT) equations of state were employed to predict the vapor liquid equilibria of several different CO_2 in DES systems over a range of temperature and pressure conditions by Animasahun et al. in 2017. The predictive capability of the three EOSs were compared based on the percentage average absolute relative deviation (AARD%) of the predicted values from the experimental data. Their results show that all three EOSs performed to a high degree of accuracy. Their results showed that both the PR and SRK EOSs were able to predict 81% of the system with an AARD less than 5%, while the Perturbed-Chain SAFT EOS predicts 72% of the systems with an AARD% less than 5%. [27]

The solubility of CO_2 in many DES was studied experimentally by a wide of researchers in wide range of temperature and pressures. In this study, PR-EOS coupled with three different mixing rules was employed to predicted the experimental solubility of CO_2 in multiple DESs. The experimental data were obtained from the literatures [17, 25, 28, 29, 30, and 31] for various temperature and pressure range. Average absolute relative deviation (AARD%) was utilizing to compare between a predicted and experimental data.

2. Thermodynamic model

Acid gases can dissolve chemically and physically in different solutions. Mathematical models can be used to explain and examine this process.[32] It was investigated in several of the publications from our study to forecast gas solubility in DESs.[18] Several thermodynamic models were employed to characterize the solubility characteristic of CO_2 in the electrolyte and nonelectrolyte mixture.[33]

The solubility of CO_2 in DESs was calculated using PR EOS described as follows: [34]

$$P = \frac{RT}{(v-b)} - \frac{a(T)}{v(v+b)+b(v-b)} \qquad (1)$$

In this equation, P is the pressure (bar), v is the molar volume (m^3/mol), T is the e absolute temperature (K), R is the universal gas constant (8.314 J/mol·K), b is the mixture size parameter and a is the mixture attractive (energy) parameter of the chemical species and are the functions of critical properties as follows:[31]

$$a = 0.4572\frac{R^2T_c^2}{p_c} \qquad (2)$$

$$b = 0.0778\frac{RT_c}{p_c} \qquad (3)$$

When T_c is critical temperature and p_c is critical pressure.

$$a(T) = a\,\alpha(T_r;\omega) \qquad (4)$$

while α is a temperature-dependent parameter and is calculating by using:

$$\alpha(T_r;\omega) = [1 + (0\cdot 37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{1/2})]^2 \qquad (5)$$

And ω is the acentric factor, T_r is the reduced temperature (ratio of temperature to critical temperature).[25]

The compressibility factor, Z, must be included in solubility studies when using the cubic EOS.

$$Z = \frac{Pv}{RT} \qquad (6)$$

$$Z^3 - (1-B)Z^2 + (A - 2B - 3B^2)Z - (AB - B^2 - B^3) = 0 \qquad (7)$$

A and B for a binary system, are defined as follows:

$$A = \frac{a\alpha P}{R^2T^2} \qquad (8)$$

$$B = \frac{bP}{RT} \qquad (9)$$

The component fugacity coefficient in each phase may then be calculated using the compressibility factor.[34].

Table 1: Mixing rules equations utilizing in this work

No.	Mixing rule	Equation	Adjustable parameters
1	Modified van der Waal's [35]	$a_m = \sum\sum x_i x_j a_{ij}$ $b_m = \Sigma\Sigma x_i x_j b_{ij}$ $a_{ij} = \sqrt{a_i a_j}(1 - k_{ij})$ $b_{ij} = \frac{b_i + bj}{2}$	k_{12}
2	Quadratic [36]	$a_m = \sum\sum x_i x_j a_{ij}$ $b_m = \Sigma\Sigma x_i x_j b_{ij}$ $a_{ij} = \sqrt{a_i a_j}(1 - k_{ij})$ $b_{ij} = \frac{b_i + bj}{2}(1 - l_{ij})$	k_{12} , l_{12}

3	Wong Sandler [37]	$a_m = D\frac{Q}{1-D}$ $b_m = \frac{Q}{1-D}$ $Q = \sum_i \sum_j x_1 x_j \left(b - \frac{a}{RT}\right)_{ij}$ $D = \Sigma_i x_i \frac{a_i}{b_i} + \frac{G^E}{CRT}$ $\left(b - \frac{a}{RT}\right)_{ij} = \frac{b_i + b_j}{2} - \sqrt{a_i a_J} \cdot (1 - k_{ij})$ $\frac{G^E}{RT} = \frac{A_{12} x_1 x_2}{x_1 (A_{12} / A_{21}) + x_2}$	k_{12} , A_{12}, A_{21}

3. Critical properties

It is important to understand acentric factors (ω) and critical characteristics (T_C, V_C, P_C) in order to carry out solubility modeling for CO_2 in different DES systems.[25] The critical properties of the DES should be determined because it is a mixture of several chemical substances.[34] The "modified Lydersen-Joback-Reid" (LJR) technique was initially employed to assess each of the DESs precursor's important individual qualities.

$$T_b = 198.2 + \sum n_i \Delta T_{bMi} \tag{10}$$

$$T_c = \frac{T_b}{0.5703 + 1.0121 \sum n_i \Delta T_{Mi} - (\sum n_i \Delta T_{Mi})^2} \tag{11}$$

$$P_c = \frac{M}{(0.2573 + \sum n_i \Delta P_{Mi})^2} \tag{12}$$

$$V_c = 6.75 + \sum n_i \Delta V_{Mi} \tag{13}$$

In such formulas, n_i is the frequency of occurrence of the ith group of atoms in the molecule, ΔT_{bMi} is the contribution of these atoms to the normal boiling temperature (K), ΔT_M is the contribution of these atoms to the critical temperature (K), ΔP_M is the contribution of these atoms to the critical pressure (bar), ΔV_M is the contribution of these atoms to the critical molar volume ($cm^3 \cdot mol^{-1}$), and M is the molar mass of the molecule ($g \cdot mol^{-1}$). [38]

Additionally, the critical properties of DESs were estimated using the Lee-Kesler mixing rule.[39]

The following are the theoretical procedures to determine the critical properties:[34]

$$T_{Cm} = \frac{1}{V_{Cm}^{1/4}} \sum_i \sum_j x_i x_j V_{C_{ij}}^{1/4} T_{C_{ij}} \tag{14}$$

$$P_{Cm} = \frac{(0.2905 - 0.085\omega_m) R T_{Cm}}{V_{Cm}} \tag{15}$$

$$V_{Cm} = \sum_i \sum_j x_i x_j V_{C_{ij}} \tag{16}$$

$$\omega_m = \sum_i x_i \omega_i \tag{17}$$

With:

$$T_{C_{ij}} = \left(T_{C_i} T_{C_j}\right)^{1/2} k_{ij} \tag{18}$$

$$V_{C_{ij}} = \frac{1}{8}\left(V_{C_i}^{1/3} V_{C_j}^{1/3}\right)^3 \tag{19}$$

Where T_{Cm} is critical temperature of mixture (K), P_{Cm} is critical pressure of mixture (bar), V_{Cm} is critical volume of mixture (m^3), ω_m is acentric factor of mixture, T_{C_i} is critical temperature of component *i* (K), V_{C_i} is critical volume of component *i* (m^3), and ω_i is acentric factor of component *i*.

4. Result and discussion

The Peng Robinson EOS was used to predict the solubility of CO_2 in sixteen different DESs systems by identifying the critical properties and acentric factors of the pure components. Table 2 shows the calculated critical properties. It is also needed to introduce an interaction parameter of the carbon dioxide and the DES systems with the data observed from the literature.

Table 2: Critical properties of DESs

		T_C	P_C	ω
DES1	Choline Chloride + 3 triethyline glycol	712.693	27.376	1.020
DES2	Choline-Chloride +1,2propanediol (1:3)	620.93	38.44	0.9290
DES3	Choline Chloride + diethylene glycol (1:3)	657.341	33.226	0.968
DES4	Choline Chloride + diethylene glycol (1:4)	660.161	33.797	0.982
DES5	Choline Chloride + Levulinic acid (1:3)	712.147	36.706	0.726
DES6	Choline Chloride + Levulinic acid (1:4)	718.668	37.543	0.724
DES7	Choline Chloride + Levulinic acid (1:5)	723.060	38.115	0.722
DES8	Choline Chloride + Phenol (1:2)	646.250	44.165	0.540
DES9	Choline Chloride + Phenol (1:3)	651.470	47.590	0.512
DES10	Choline Chloride + Phenol (1:4)	654.910	49.846	0.496
DES11	Choline Chloride + Triethylene glycol (1:3)	712.693	27.376	1.020
DES12	Choline Chloride + Triethylene glycol (1:4)	718.888	27.413	1.037
DES13	Lactic acid and tetramethylammonium chloride (1:2)	636.43	40.2	0.86
DES14	Lactic acid and tetraethylammonium chloride (1:2)	658.39	33.0	0.92
DES15	Lactic acid and tetrabutylammonium chloride (1:2)	695.02	24.7	1.03
DES16	Choline Chloride + Urea (1:2)	644.4	49.3	0.651

For correlating experimental data of solubility of each system, PR-EOS is often utilized, with the mixing rules provided by the equations M1, M2, and M3 with one or more interaction parameters.

The interaction parameter k_{12} that used with this mixing rule is examined by fitting the experimental data, otherwise l_{12} was found by trial and error, and A_{12} and A_{21} are also obtained to get Gibbs free energy in M3 to get the minimum %AARD as accepted value.

$$\text{AARD} = \sum \left| \frac{X_{exp} - X_{cal}}{X_{exp}} \right| / N \times 100 \quad (20)$$

When X_{exp} is experimental mole fraction, X_{cal} is calculated mole fraction and N is the number of data points.

Table 3 shows the adjustable parameter k_{12}, l_{12}, and A_{12} and A_{21} that used and determined in this work in some selected temperatures, and complete data with all temperatures obtained in this work are presented in the supplementary material part.

The results indicated that binary interaction parameter k_{12} depends on temperature and increase directly with temperature rising. In general, l_{12} is independent of temperature fluctuations. The quantities of l_{12} are different for a system regardless of temperature for the majority of the systems tested utilizing PR EOS.

Table 3: Binary interaction parameters

	T	k_{12}	l_{12}	A_{12}	A_{21}
DES1	303.15	0.1743	-0.0705	1.336135	2.32213
DES2	303.15	0.233	0.0710	1.98027107	0.5861753118
DES3	303.15	0.2227	0.0920	1.729685	1.35468257
DES4	303.15	0.2186	0.1955	1.80593109	0.61915975

DES5	303.15	0.1474	-0.0071	1.125929	10.000
DES6	303.15	0.1367	-0.0663	1.1040613	1.130391339
DES7	303.15	0.1227	0.0191	1.0013159	1.35814996
DES8	303.15	0.2121	0.1307	1.63386489	10.0000
DES9	303.15	0.2016	0.0248	1.777160099	0.5420753795
DES10	303.15	0.1961	0.1392	1.759482236	0.6438152389
DES11	303.15	0.1948	0.3118	1.585999	0.47350926
DES12	303.15	0.1839	-0.1352	1.402657831	0.73804749
DES13	308	0.19934	-0.0003	1.66310225	1.832139678
	318	0.21154	-0.02860	1.582322696	4.03894607
DES14	308	0.1987	0.01310	1.50198513	2.45136322
	318	0.210693	0.05780	1.4235682	10.0
DES15	308	0.1464	-0.00330	1.030070518	2.844034049
	318	0.15222	0.01120	0.96082261	10.0
DES16	309	0.21584	0.02020	1.828787882	10.0
	319	0.22946	-0.6404	1.809963396	10.0
	329	0.24069	-0.2708	1.814543828	-2.03146349

% AARD between the predicted and the data of literature of CO_2 solubility in various deep eutectic solvents system for three different mixing rules used at some selected temperatures are presented in Table 4, and complete data with all temperatures obtained in this work are presented in the supplementary material part. It is obvious M3 provides a lower AARD percent than the other two mixing rules.

Table 4: Comparison %AARD between the three different mixing rules

N	**T(K)**	**%AARD**		
		M1	**M2**	**M3**
DES1	303.15	5.10	4.41	3.90
DES2	303.15	3.59	3.47	2.66
DES3	303.15	1.75	1.64	1.02
DES4	303.15	4.43	4.34	0.54
DES5	303.15	0.72	0.71	0.69
DES6	303.15	1.34	1.34	0.39
DES7	303.15	0.96	0.90	1.01
DES8	303.15	2.42	2.31	2.16
DES9	303.15	4.71	4.66	0.59
DES10	303.15	4.15	3.95	0.53
DES11	303.15	6.37	6.37	1.38
DES12	303.15	2.64	2.53	1.50
DES13	308	0.20	0.21	1.23
	318	0.19	0.43	0.62

DES14	308	0.25	0.12	0.92
	318	0.55	0.09	0.65
DES15	308	0.07	0.11	0.58
	318	0.16	0.05	0.05
DES16	309	0.08	0.07	0.09
	319	2.72	2.68	2.21

For the sake of results are very close a few obtained data were presented graphically in this article. Figures (1-6) presented the pressure-equilibrium phase composition diagram of CO_2 in six selected DESs.

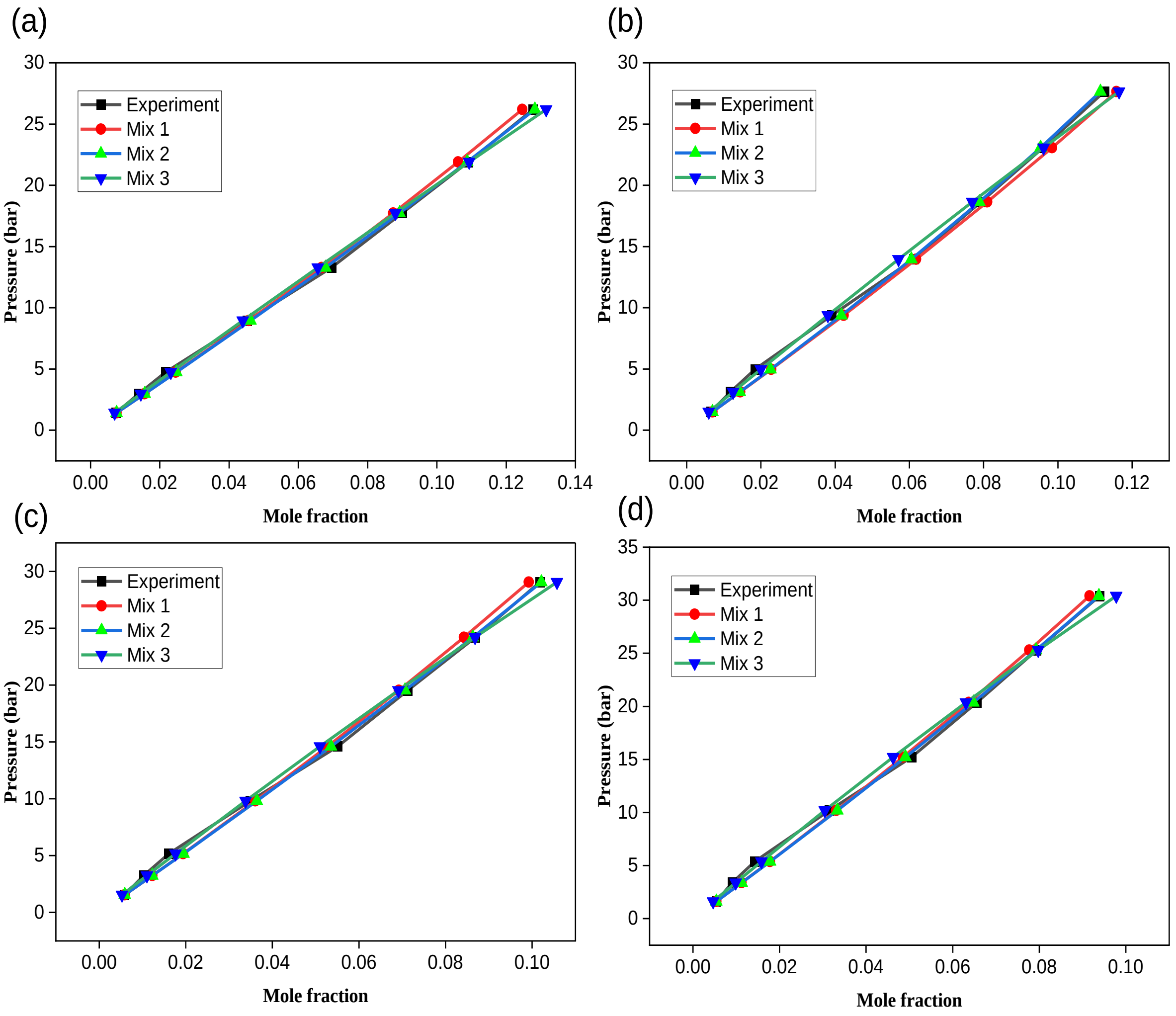

Figure 1. Pressure-equilibrium phase composition diagram of CO2 - DES1 system at 303.15K, 313.15K, 323.15K, 333.15K from (a) – (d) respectively

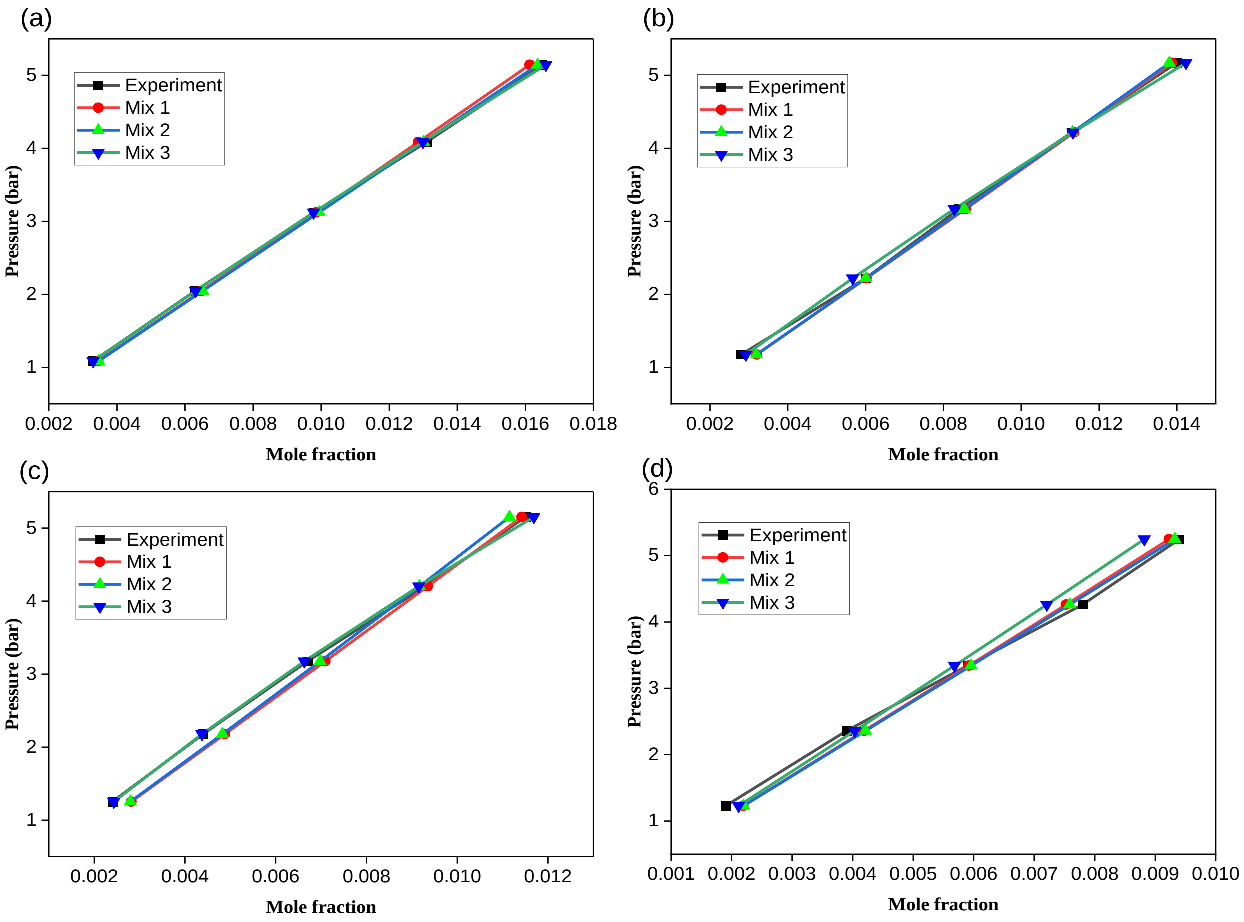

Figure 2. Pressure-equilibrium phase composition diagram of CO2 - DES2 system at 293.15K, 303.15K, 313.15K, 323.15K from (a) – (d) respectively.

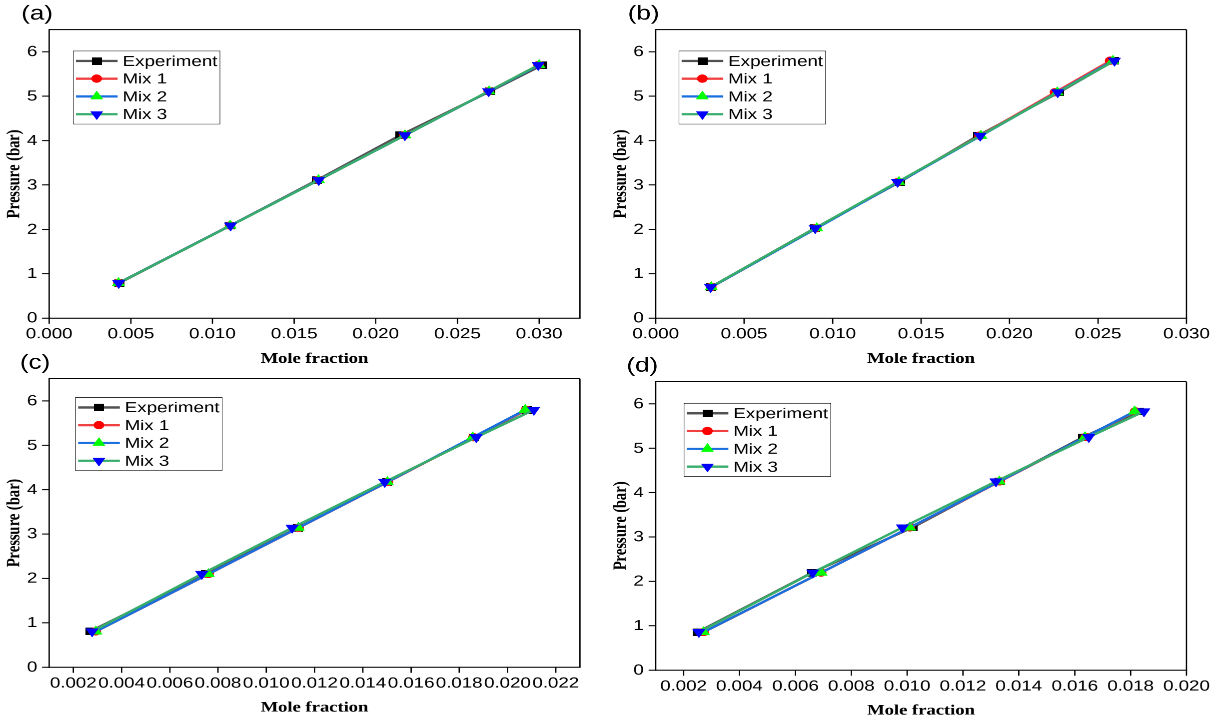

Figure 3. Pressure-equilibrium phase composition diagram of CO2 – DES3 system at 303.15K, 313.15K, 323.15K, 333.15K from (a) – (d) respectively.

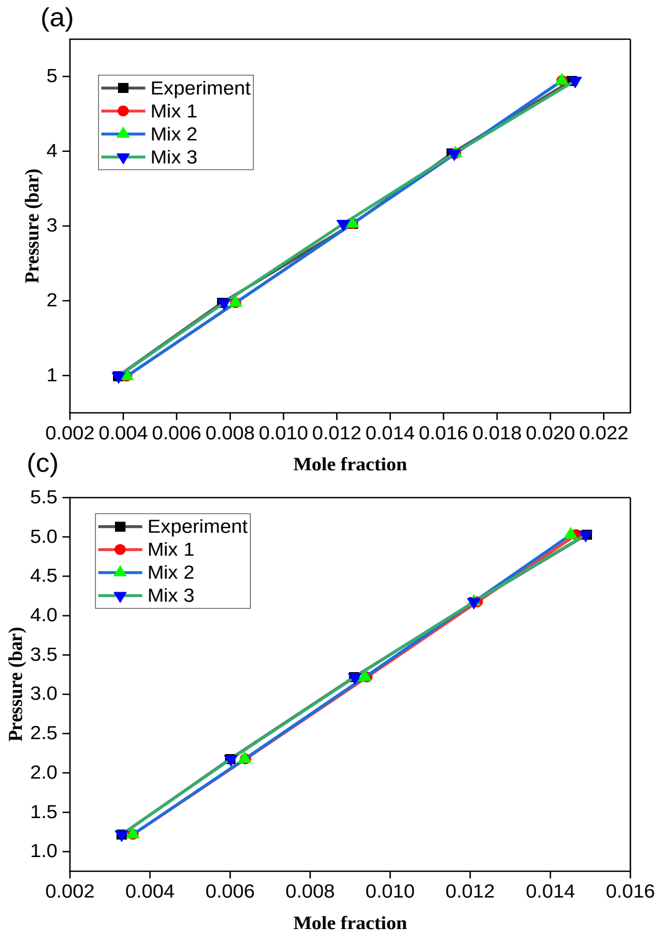

Figure 4. Pressure-equilibrium phase composition diagram of CO2 – DES4 system at 293.15K, 303.15K, 313.15K, 323.15K from (a) – (d) respectively

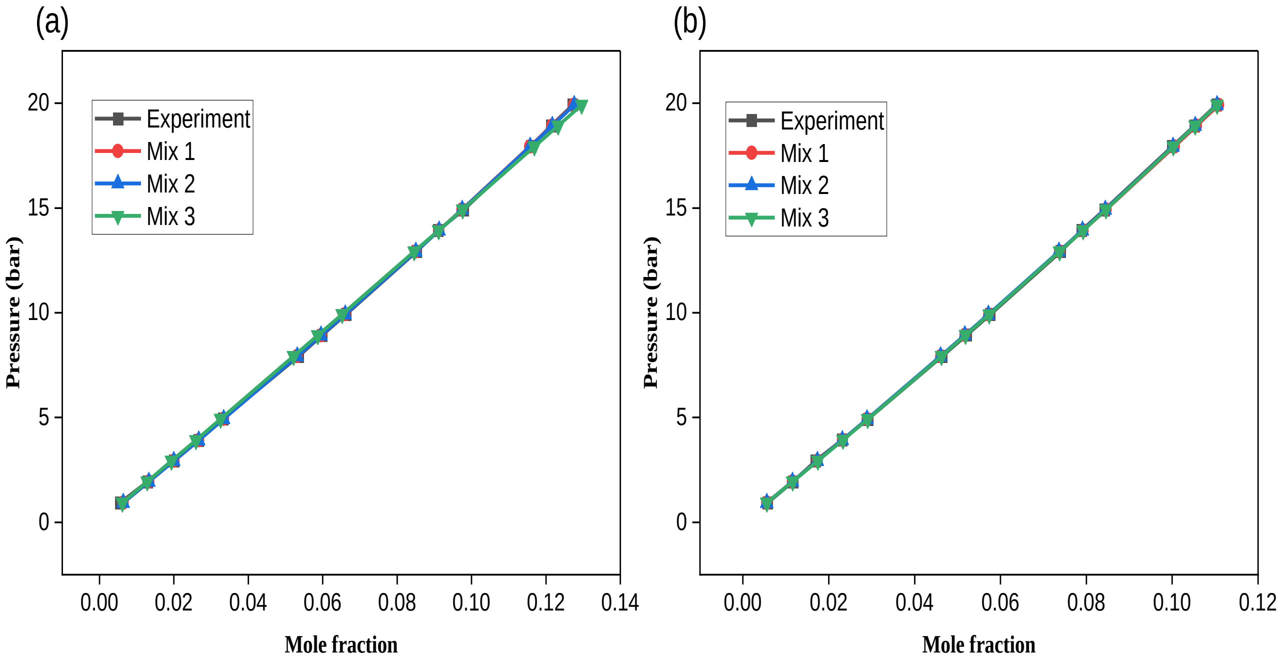

Figure 5. Pressure-equilibrium phase composition diagram of CO2 – DES5 system at 308K and 318K from (a) – (b) respectively

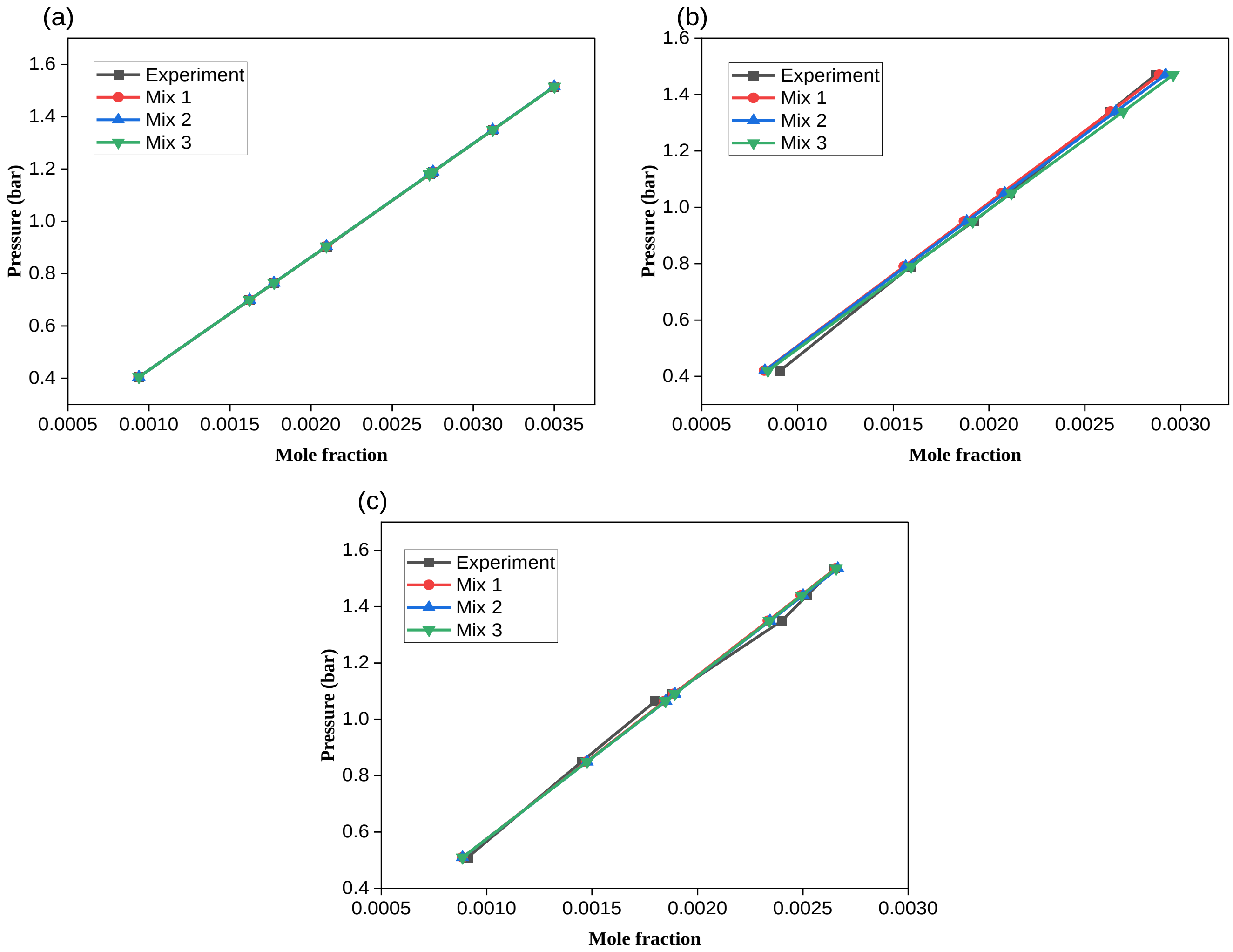

Figure 6. Pressure-equilibrium phase composition diagram of CO2 – DES6 system at 309K, 319K and 329K from (a) – (c) respectively

As it is shown the predicted data was very close to experimental one. In this way, according to the results obtained from the average, maximum and minimum errors and also by observing the mole fraction graphs (experimental and calculation) drawn according to the temperature of each system, it indicates that the model provided all three mixing rules for predicting the solubility of CO_2 in the mentioned DESs has a high accuracy.

For Peng-Robinson's equation of state, Wang-Sandler's mixing rule works better than two other mixing rules. Wong Sandler mixing rule, which take into account the additional Gibbs free energy, reduce the error to a suitable extent. As it is presented when the pressure increase, the solubility of CO_2 in DESs is increase, which leads to an increase in the additional Gibbs energy. And at the end the difference between Wong Sandler mixing rule and the other two mixing rules is more defined.

The hydrogen bond acceptors and hydrogen bond donors of DESs are also have affected on the accuracy of the modelling results, as presented in Table 4 %AARD for DES6 is negligible in M1, M2 and M3 compared to other DESs due to its structure, which used different hydrogen bond acceptors instead of using different hydrogen bond donors like the others.

5. Conclusion

The performance of six deep eutectic solvents for CO_2 capture was successfully modelled by using Peng-Robinson EOS correlating with three different mixing rules over a wide variety range of temperature and pressure.

The experimental mole fraction of CO_2 solubility in variety ranges of pressure in different temperatures are used from pervious works to calculate their equations fitting parameters.

The obtained results from calculation represent %AARD between (0.05284 - 8.69506) which gives acceptable results compared with experimental data that taken from the literature. Wong Sandler mixing rule provided the best result with experimental data in most of the systems. But according to some difficulties to obtain an excess Gibbs free energy model the two other mixing rules are presented acceptable results to use.

Taking into account that obtaining l_{12} for quadratic mixing rule also is a bit difficult modified Van der waals is able to utilizing with PR EOS which provides acceptable results compared to empirically ones. %AARD obtained from M1 in all the systems in our work have a range between (0.07256 - 8.69506) which is in good agreement with experimental data.

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