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Prediction the Experimental Data of CO_2 and H_2S Solubility in Ionic Liquids Using PR-EoS with Three Different Mixing Rules

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ABSTRACT

In this study, Peng-Robinson equations of state associated with three different mixing rules used to predict the experimental solubility data of two acid gases, carbon dioxide and hydrogen sulfide in seven ionic liquids. The solubility data were obtained from different literature in pressure range (0.119 – 65.2) bar and verity range of temperatures (298.2 – 353) K. Mixing rules, used the modified Van der Waal (MR1), the Quadratic (MR2) and the Wong Sandler (MR3). The ionic liquids critical properties were correlated by modified Lydersen-Joback-Reid technique. The Average Absolute Relative Deviation (%AARD) was applied to compare the experimental data and that obtained from the model. The evaluated critical properties give a very close result with the literature. The mathematical model in almost systems using the three mixing rule gives good agreement with experimental data only in H2S - ILs systems gives very high deviation from the experimental data when use MR3. Quadratic mixing rule (MR2) was the best comparing with MR1 and MR3, give the lowest range %AARD 0.9 to 21.

1. Introduction

Carbon dioxide (CO_2) and hydrogen sulfide (H_2S) are hazardous to human health and the environment[1][2] and regarded as the primary cause of climate change and global warming [3]. To eliminate acidic gases from natural gas, various procedures are adopted [4]. Ionic liquids (ILs) can be utilized in absorbing environmentally harmful acidic gases[5]. Machine learning can be used to check ILs for gas absorption because they are cost effective and non-toxic in nature. In many oil and gas fields, methane and other light hydrocarbons are produced along with the acid gases including carbon dioxide and hydrogen sulfide. The solubility is important when assessing ILs for future application in commercial natural gas treating procedures [6]. Common uses for ILs include liquid-liquid separation, extraction, lubricants, fuel cells, and the creation of basic materials like gels and membranes [7].

The length of the alkyl chain showed a linear correlation with the solubility of CO_2 in the ionic liquids. Solubility increases with the increase in alkyl chain and the decrease in error, which develops a relationship directly affecting the prediction of data across equations of state [8]. The solubility of acidic gases in ILs is largely temperature-dependent, increasing with a decrease in temperature, which depends on the kinetic energy of gases in liquid. When temperature increases, the motion of gas particles increases, which makes gas particles

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escape the solution and reduces the solubility of the gas in a liquid. In imidazolium based ILs the cation has a moderate impact on solubility, and H_2S solubility increases by lengthening the alkyl chain on the cation The anion fluorination process can enhance H_2S solubility by increasing the number of trifluoromethyl (CF3) groups on the anion surface [9].

Sakhaeinia et al. 2010, [10] study the solubility of hydrogen sulfide gas in 1-ethyl-3-methylimidazolium bis(trifluoromethyl) sulfonylimide ([emim][TF2N]) at temperature ranges (303.15 -353.15) K and pressures up to about 2.0 MPa. A volumetric-based static apparatus was used for the purpose, where it was concluded that H_2S is more soluble in [emim][TF2N] than [emim][PF6] [9]. In 2012 Jalili et al. calculated the critical properties and measured solubility of carbon dioxide and hydrogen sulfide gases in 1-octyl-3-imidazoliumbis-(trifluoromethyl)sulfonylimide. Both the gases were observed to be dissolved physically in ILs, where H_2S was found to be more soluble in [C8mim] [TF2N] than CO_2. It has been demonstrated that increasing the number of carbons in the alkyl substituent of the methylimidazolium cation ring increased the solubility of both CO_2 and H_2S gases in [Cnmim][TF2N] IL [11].

Furthermore, thermodynamic modeling is necessary for process simulation, design, and optimization because it provides knowledge of the fundamental variables that influence gas solubility and selectivity. Several thermodynamic models have reportedly been used to represent the phase behavior of mixtures containing ILs in recent years [12]. In 2009 Sylvia et al. measured and modelled the CO_2 solubility, volume expansion, and mixture critical points in the synthesis of a model imidazolium ionic liquid 1-hexyl-3-methylimidazolium bromide ([HMIm][Br]) from 1-bromohexane and 1-methylimidazole. The solubility and volume expansion of CO_2 was determined at 313.15 K and 333.15 K for pressures ranging from 10 to 160 bar in 1-methylimidazole, 1-bromohexane, a 1:1 mixture of 1-methylimidazole and 1-bromohexane and [HMIm][Br]. A mathematical model using Peng-Robinson equation coupled with quadratic mixing (Two adjustable parameters) has been established. The model with estimated critical properties gives good results close to the experimental data [13].

Mohammad and Farhad in 2010 examined CO_2 solubility in 1-alkyl-3 methylimidazolium bis (trifluoromethylsulfonyl) imide ([Cn-mim] [TF2N]; n=2, 4, 6, and 8). They predicted a mathematical model using Peng-Robinson (PR) with the Van Laar model for excess Gibbs free energy determination. According to Mohammad and Farhad the model gives a very good agreement with experimental data even at high pressure compared with other mixing rules like Van der Waal [14].

John studied the experimental solubility data of CO_2 in pure ILs over a wide range of temperatures and pressures. Peng-Robinson (PR) with Van der Waals two-parameter mixing rules were used, and the model results showed very good agreement with the experimental data [15].

The difficulty of measuring the solubility of acid gases in ionic liquids is often time-consuming and expensive. Therefore, the main objective of the investigation is to construct a thermodynamic model by applying PR-EoS coupled with three different mixing rules to correlate the experimental data obtained from the literature at various pressure and temperature, conditions.

2. Thermodynamic model

For modeling and correlating the solubility of acidic gases in ionic liquid, the Peng Robinson equation of state (1979) was chosen [16]. As expressed,

$$P = \frac{RT}{(v-b_m)} - \frac{a_m(T)}{v(v+b_m)+b_m(v-b_m)} \quad (1)$$

where a_m and b_m are the mixtures attractive and v is molar volume and T is temperature and P pressure, At the critical point

$$a(T_c) = 0.45724\frac{R^2T_c^2}{P_c} \quad (2)$$

$$b(T_c) = 0.0778\frac{RT_c}{P_c} \quad (3)$$

where R is ideal gas constant and T_c, P_c, critical properties

At the other temperatures, the parameter a (T) temperature is corrected to

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

Correlation terms of the vapor pressure curve up the critical point gives

$$\alpha^{0.5} = 1 + (1 - T_r^{0.5})(0.37464 + 1.5422\,\omega - 0.26992\,\omega^2) \qquad (5)$$

where the acentric factor (ω) and the reduced temperature (Tr) are represented. By utilizing a suitable mixing rule, as shown in Table (1), PR EoS can be used for mixtures.

The critical values and acentric factor of the ionic liquids were determined using the modified Lydersen-Joback-Reid technique, as shown in Table (2),

Table 1: Mixing Rules (MR)

Name	Mixing rules	Adjustable parameters
Modified Van der Waal mixing rules (MR1)	$a_m = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j a_{ij}$ $b_m = \sum_{i=1}^{n} x_i b_i$ $a_{ij} = \sqrt{a_i a_j}\,(1 - k_{ij})$	k_{ij} =value
Quadratic mixing rules (MR2)	$a_m = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j a_{ij}$ $b_m = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j b_{ij}$ $a_{ij} = \sqrt{a_i a_j}\,(1 - k_{ij})$ $b_{ij} = \frac{b_i + b_j}{2}(1 - l_{ij})$	k_{ij} =value l_{ij}= value
Wong Sandler mixing rules (MR3)*	$a_m = b_m \left[\sum_{i}^{n} \frac{x_i a_i}{b_i} + \frac{A_\infty^E}{\Omega}\right]$ $\frac{A_\infty^E(x)}{RT} = \frac{(A_{12}/RT)x_1 x_2}{x_1(A_{12}/A_{21}) + x_1}$ $b_m = \frac{\sum_i^n \sum_i^n x_i x_j \left(b - \frac{a}{RT}\right)_{ij}}{1 - \sum_i^n \frac{x_i a_i}{b_i RT} - \frac{A_\infty^E(x)}{\Omega RT}}$ $(b - a/RT)_{ij} = \frac{1}{2}(b_i + b_j) - \frac{\sqrt{a_i a_j}}{RT} + (1 - k_{ij})$	k_{ij} =value

*Van laar model was used to determine excess gibbs free energy (AE) in the Wong Sandler mixing rules (MR3).

Table 2: Critical properties of the modified Lydersen-Joback-Reid method

	Model Equations	**Constants**
Boiling point temperature	$T_b(K) = 198.2 + \sum n\Delta T_{bm}$	A=0.5703 B=1.0121
Critical temperature	$T_c(K) = {T_b}/{([A + B\sum T_{cm} - (\sum n\Delta T_{cm})^2])}$	C=0.2573
Critical pressure	$P_c(bar) = M/([C + \sum n\Delta P_{cm}]^2)$	
Acentric factor	$\omega = \frac{(T_b - 43)(T_c - 43)}{(T_c - T_b)(0.7T_c - 43)} log\left[\frac{P_c}{P_b}\right] - \frac{(T_b - 43)(T_c - 43)}{(T_c - T_b)} log\left[\frac{P_c}{P_b}\right] - 1$	

3. Results and discussion

Predicting the experimental solubility data obtained from the literature for a few binary systems of CO_2 and H_2S with various types of ionic liquid is a key objective of the current effort. CO_2 and H_2S solubility in ionic liquid are obtained from different researcher works [10][11][17-20]. PR-EoS implementing by the critical properties, which are calculated by the modified Lydersen-Joback-Reid method. Table 3 shows the critical properties of ionic liquid and acidic gases.

Three different mixing rules were employed with PR-EoS, MR1, MR2, and MR3. The predicted binary interaction parameter k_{12} by fitting the experimental data in (MR1, MR2, MR3) it was fixed at each temperature in three mixing rules for all the systems. Trial and error are used to calculate the L_{12} in MR2. Also, A_{12} and A_{21} are calculated by iteration in MR3. The three mixing adjustable parameter values for CO_2 and H_2S -ILs are appear in Table (4,5) respectively, which give the lowest percentage of average absolute relative deviation (%AARD).

$$\text{AARD} = \sum \left|\frac{X_{exp}-X_{cal}}{X_{exp}}\right|/N \times 100 \qquad (6)$$

where N refers to the total number of data points.

Tables (6,7) shows %AARD values for all mixing rules utilizing PR-EoS for CO_2 & H_2S in IL systems at various temperatures.

Tables (4,5) show that k_{12} are increased in almost the systems, the second binary interaction for MR2 (L_{12}) are arbitrary change with temperature seems to be depending on the solvent naturality.

The calculated mole fraction of CO_2 and H_2S in Ionic Liquids are presented graphically in Figures (1-4) of CO_2 (1)-ILs (2) and (5-8) H_2S (1)-ILs (2). The results showed in almost the systems MR2 gave smaller %AARD and good agreement with experimental data than MR1 and MR3.

Applying MR3 with PR in all H_2S -ILs systems give very bad agreement with experimental data and give high values of %AARD.It is challenging to evaluate the correlation and support our conclusion concerning MR3 because the modeling data on H2S solubility in ionic liquids comes from a limited number of sources. According [14] H_2S solubility in Ionic liquids it was about three times more than CO_2 in the particular ionic liquid . studied for the third mixing rule working better in CO_2. From all the studied systems results, concluded that MR3 cannot be work for high solubility.

The estimated mole fraction of CO_2 in [Amim][HCOO] is presented in Figure 1 shows very high deviation from the experimental in all temperature range data with %AARD range (15-37). The experimental data of this system obtained from [21]. They conclude that ideal mixing rule cannot be used to estimate the properties of the aqueous [Amim][HCOO], this means the critical properties estimated were not correct. The results of all other systems were very close for that our conclusion is the experimental were not correct.

MR3 gives the lowest %AARD than the other mixing rules of system CO_2-[C8mim]

[TF2N] system form temperatures (313.15 - 353.15) K as shown in Figure 2. Also, in Figure 3 for CO_2-[emim] [DEP] and Figure 4 for CO_2 - [HOPMim] [TF2N], MR2 give minimum %AARD.

The calculated mole fraction of H_2S was determined from figures (5-8), which MR2 was give the lowest value of % AARD. For all temperatures in each system.

Table 3: Critical properties calculated by the modified Lydersen-Joback-Reid method

Component	Tc (K)	Pc (bar)	ω
CO_2	304.25	73.8	0.225
[Amim][HCOO]	909.3	33.19	0.799
[C8mim] [TF2N]	975.5793	13.3042	0.9594
[emim][DEP]	864.783	21.1764	0.6638
[HOPMim][TF2N]	1309.5	30.35	0.5617
H_2S	304.2	89.4	0.081
[C6mim][TF2N]	1355.858	22.5793	0.4594
[C8mim][PF6]	810.8483	14.0501	0.9384
[C8mim][TF2N]	975.5793	13.3042	0.9594
[emim][TF2N]	1244.9	32.9	0.1818

Table 4: Values of adjustable parameters obtained from fitting with PR-EoS for CO_2

System	T (K)	MR	MR2	MR3		
		K_{12}	L_{12}	K_{12}	A_{12}	A_{21}
CO_2+ [Amim][HCOO]	298.2	-0.0559	0.2010	-0.0559	-0.1	-0.2
	313.2	-0.0700	0.2430	-0.0700	0.1	-0.2
	333.2	0.0918	0.2870	0.0918	-0.1	-0.2
CO_2 + [C8mim] [TF2N]	303.15	-0.0814	0.4890	-0.0814	-0.1	-0.2
	313.15	-0.1013	0.5910	-0.1013	-0.1	-0.2
	323.15	-0.1150	0.5910	-0.1150	-0.436	-0.453
	333.15	-0.1298	0.5560	-0.1298	-0.476	-0.651
	343.15	-0.1460	0.5360	-0.1460	-0.52	-0.86
	353.15	-0.1648	0.4640	-0.1648	-0.556	-1.36
CO_2 + [emim] [DEP]	313.15	0.0971	0.0670	0.0971	0.817	3.4872
	333.15	0.0979	0.0210	0.0979	0.5394	10
	353.15	0.1241	-0.0010	0.1241	0.6134	10
CO_2 + [HOPMim][TF2N]	303.15	-0.0551	0.0830	-0.0551	-0.1	-0.2
	323.15	-0.0649	0.0370	-0.0649	-0.55	-0.389

Table 5: Values of Adjustable Parameters Obtained from Fitting with PR-EoS for H_2S

System	T (K)	MR	MR2	MR3		
		K_{12}	L_{12}	K_{12}	A_{12}	A_{21}
H_2S + [C6mim] [TF2N]	303.15	-0.0147	0.4450	-0.0147	-0.1	-0.2
	313.15	-0.0515	-0.5310	-0.0515	-0.1	-0.2
	323.15	-0.0556	-0.4450	-0.0556	-0.1	-0.2
	333.15	-0.0658	0.4110	-0.0658	-0.1	-0.2
	343.15	-0.0612	0.3950	-0.0612	-0.1	-0.2
	353.15	-0.0652	0.3680	-0.0652	-0.1	-0.2
H_2S + [C8mim] [PF6]	303.15	-0.0733	-0.3380	-0.0733	-0.1	-0.2
	313.15	-0.0766	-0.3870	-0.0766	-0.1	-0.2
	323.15	-0.0804	-0.4810	-0.0804	-0.1	-0.2
	333.15	-0.0844	-0.5990	-0.0844	-0.1	-0.2
	343.15	-0.0885	-0.3110	-0.0885	-0.1	-0.2
	353.15	-0.0888	-0.4770	-0.088	-1.041	-6.26

H_2S + [C8mim] [TF2N]	303.15	-0.0836	-0.2110	-0.0836	-0.1	-0.2
	313.15	-0.0937	-0.2630	-0.0937	-0.1	-0.2
	323.15	-0.1023	-0.2820	-0.1023	-0.1	-0.2
	333.15	-0.1117	0.3110	-0.1117	-0.1	-0.2
	343.15	-0.1245	-0.2130	-0.1245	-0.1	-0.2
	353.15	-0.1356	-0.1480	-0.1356	-0.1	-0.2
H_2S + [emim] [TF2N]	303.15	-0.0204	-0.3470	-0.0204	-0.1	-0.2
	313.15	-0.0290	-0.6210	-0.0290	-0.1	-0.2
	323.15	-0.0352	-0.6610	-0.0352	-0.1	-0.2

Table 6: %AARD between the experimental and predicted mole fraction solubility of CO_2 in IL with three different mixing rules

Acidic gas +IL	**T (K)**	**1st MR**	**2nd MR**	**3rd MR**
CO_2+ [Amim][HCOO]	298.2	23	21	32
	313.2	21	19	35
	333.2	17	15	37
CO_2+[C8mim] [TF2N]	303.15	7	5	9
	313.15	6	3	13
	323.15	5	3	0.7
	333.15	5	3	0.6
	343.15	4	2	0.5
	353.15	3	2	0.5
CO_2+ [emim] [DEP]	313.15	5	5	7
	333.15	7	7	8
	353.15	4	4	4
CO_2 + [HOPMim][TF2N]	303.15	7	7	29
	323.15	7	7	10
	343.15	8	8	8

Table 7: %AARD between the experimental and predicted mole fraction solubility of H_2S in IL with three different mixing rules

Acidic gas +IL	T (K)	1st MR	2nd MR	3rd MR
H_2S + [C6mim] [TF2N]	303.15	8	3	67
	313.15	8	4	65
	323.15	6	2	65
	333.15	6	3	65
	343.15	5	2	64
	353.15	4	2	64
H_2S + [C8mim] [PF6]	303.15	8	5	45
	313.15	9	6	50
	323.15	8	5	51
	333.15	8	5	50
	343.15	8	6	51
	353.15	6	5	49
H_2S + [C8mim] [TF2N]	303.15	6	5	59
	313.15	9	7	59
	323.15	7	5	59
	333.15	6	5	59
	343.15	6	5	61
	353.15	5	5	62
H_2S + [emim] [TF2N]	303.15	8	4	63
	313.15	7	4	63
	323.15	4	2	64
	333.15	4	2	63
	343.15	2	1	64
	353.15	2	0.9	2

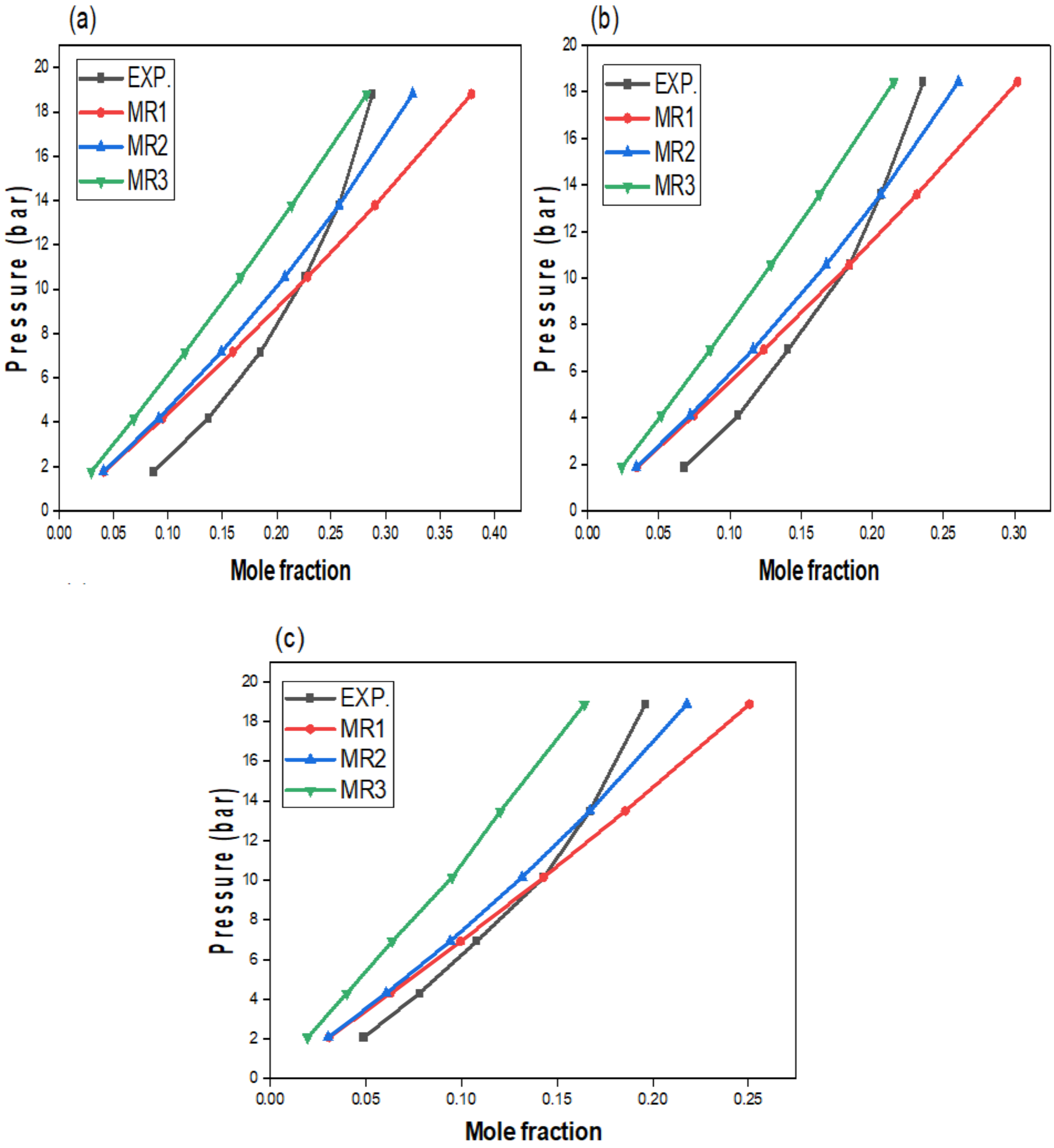

Figure 1. Phase composition diagram of CO_2- [Amim][HCOO] system at (a) 298.1K, (b) 313.2K, (c) 333.2K using PR with three different mixing rules.[21]

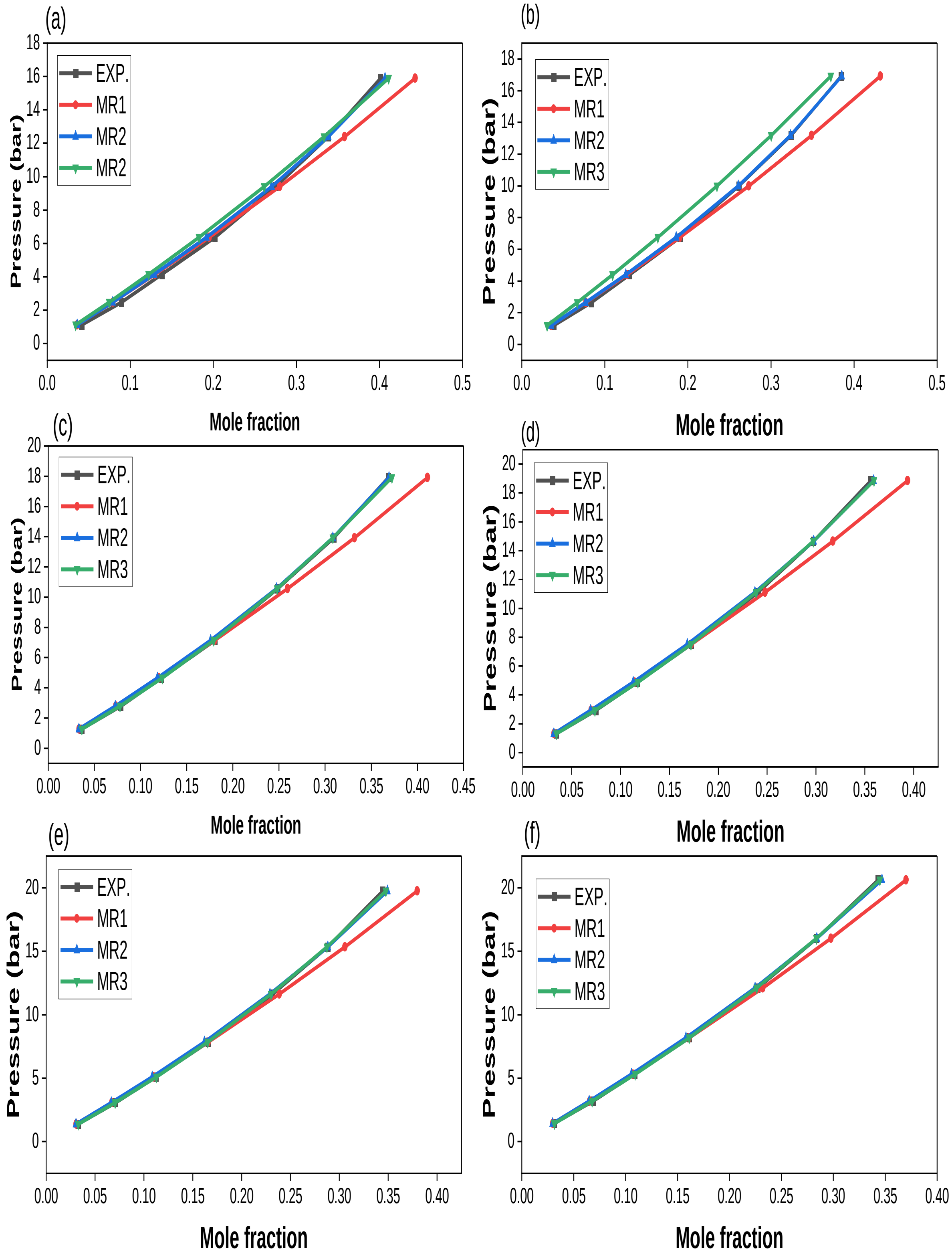

Figure 2. Phase composition diagram of CO_2- [C8mim][TF2N] system at (a) 303.15K , (b) 313.15K, (c) 323.15K , (d) 333.15K, (e) 343.15K, (f) 353.15K, using PR with three different mixing rules.[11]

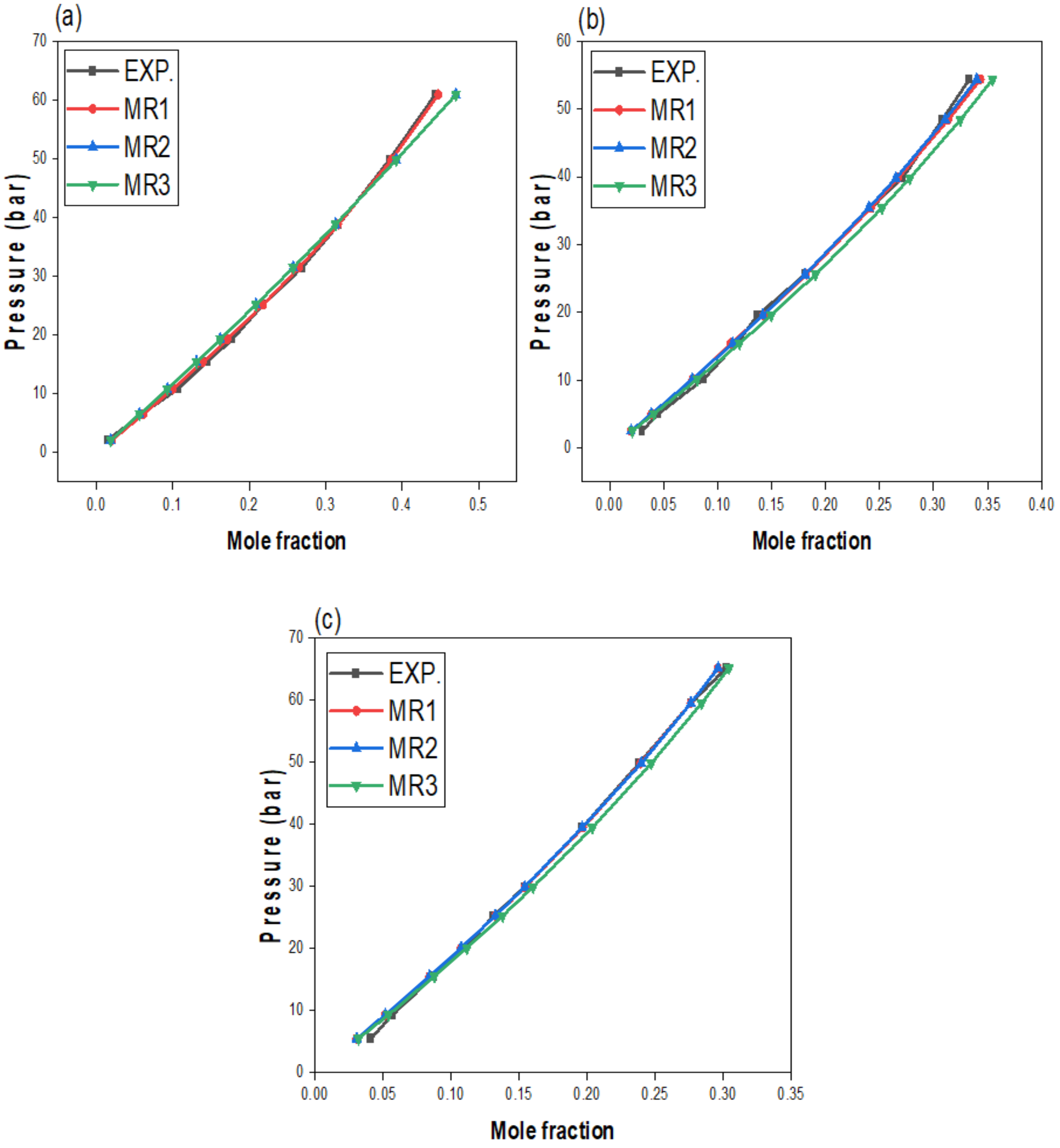

Figure 3. Phase composition diagram of CO_2- [emim][DEP] system at (a) 313.15K, (b) 333.15K, (c) 353.15K using PR with three different mixing rules.[18]

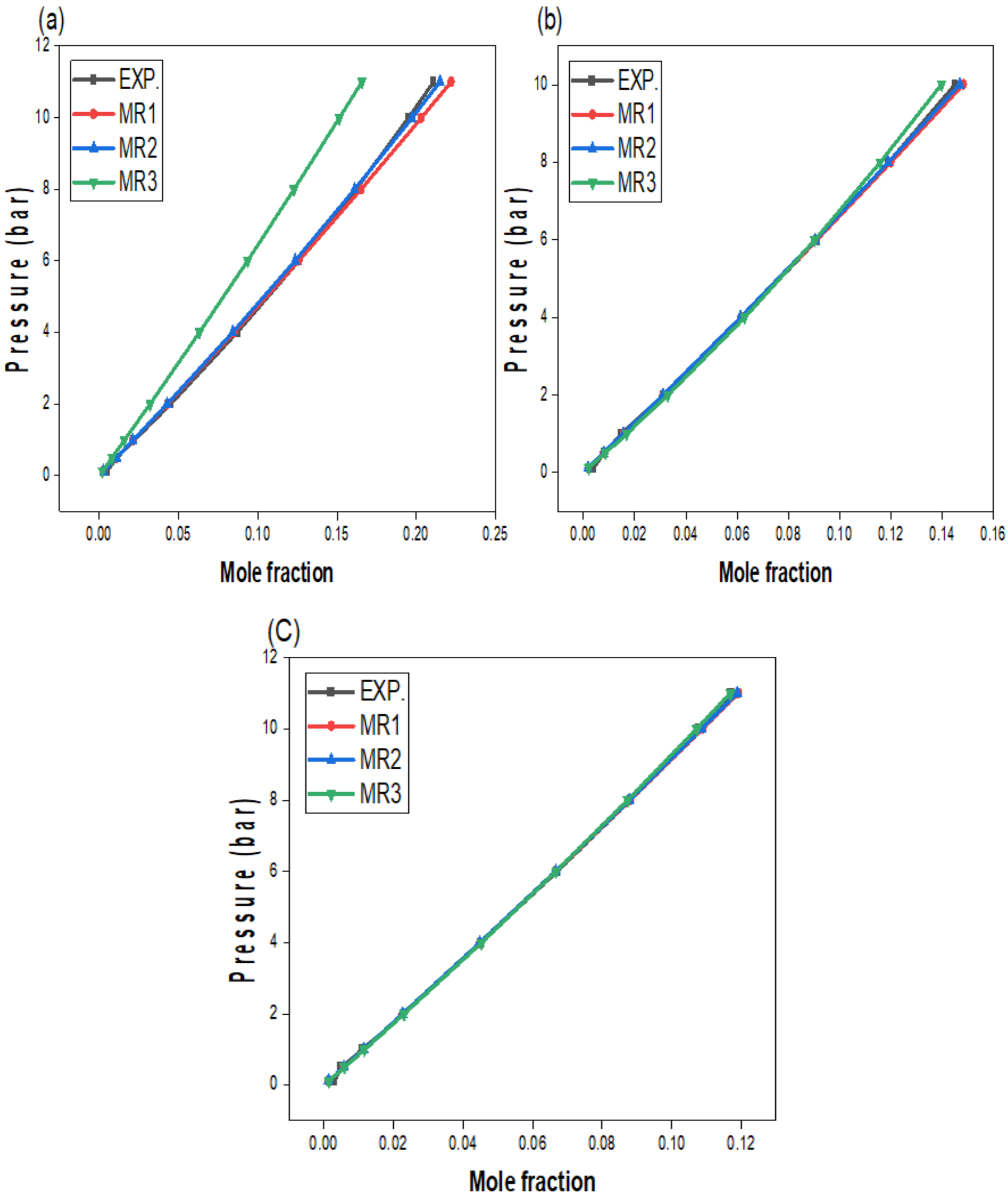

Figure 4. Phase composition diagram of CO_2- [HOPMim][TF2N] system at (a) 303.15K, (b) 323.15K, (c) 343.15K using PR with three different mixing rules.[19]

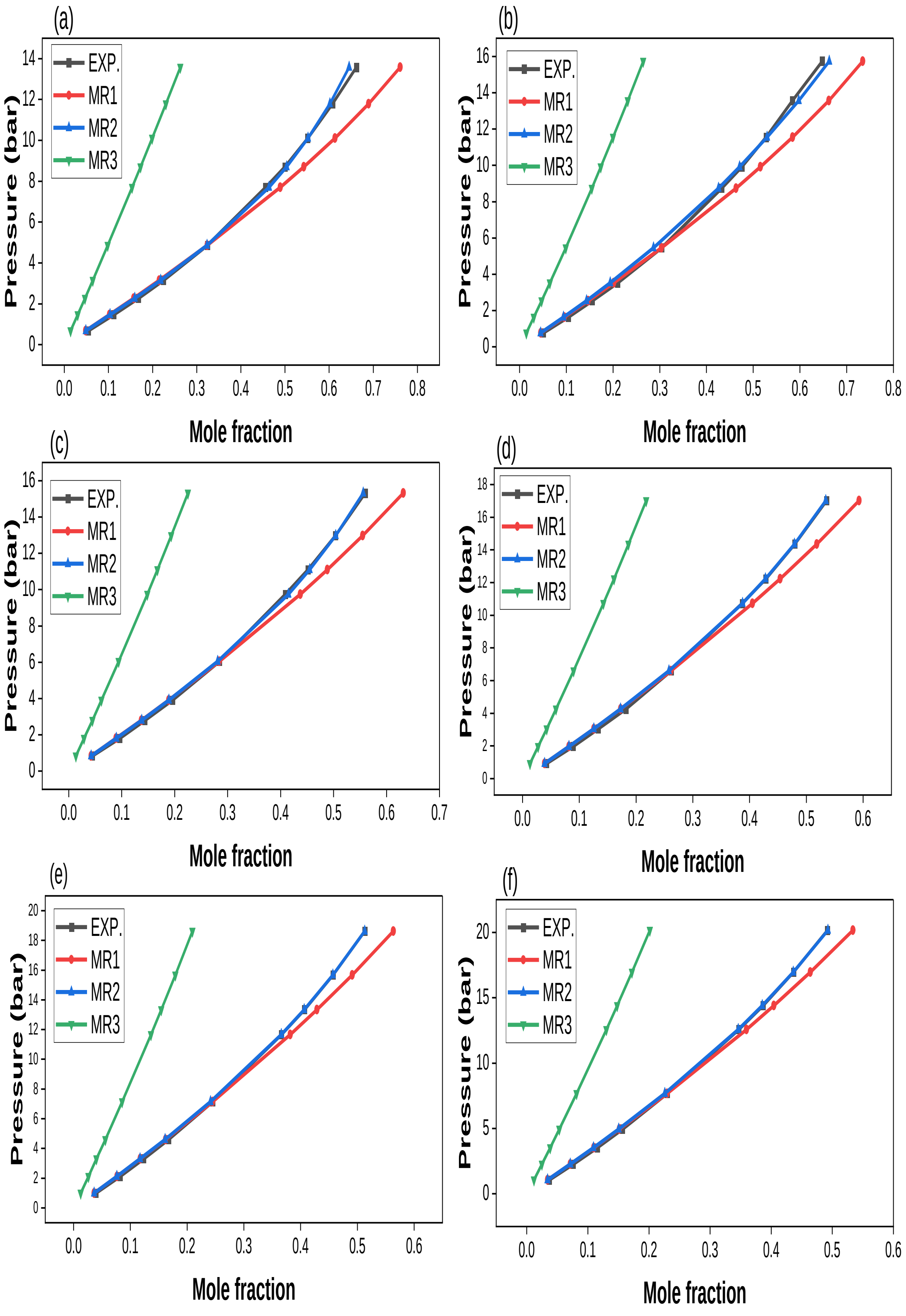

Figure 5. Phase composition diagram of H_2S- [C6mim][TF2N] system at (a) 303.15K , (b) 313.15K, (c) 323.15K , (d) 333.15K, (e) 343.15K, (f) 353.15K, using PR with three different mixing rules.[11]

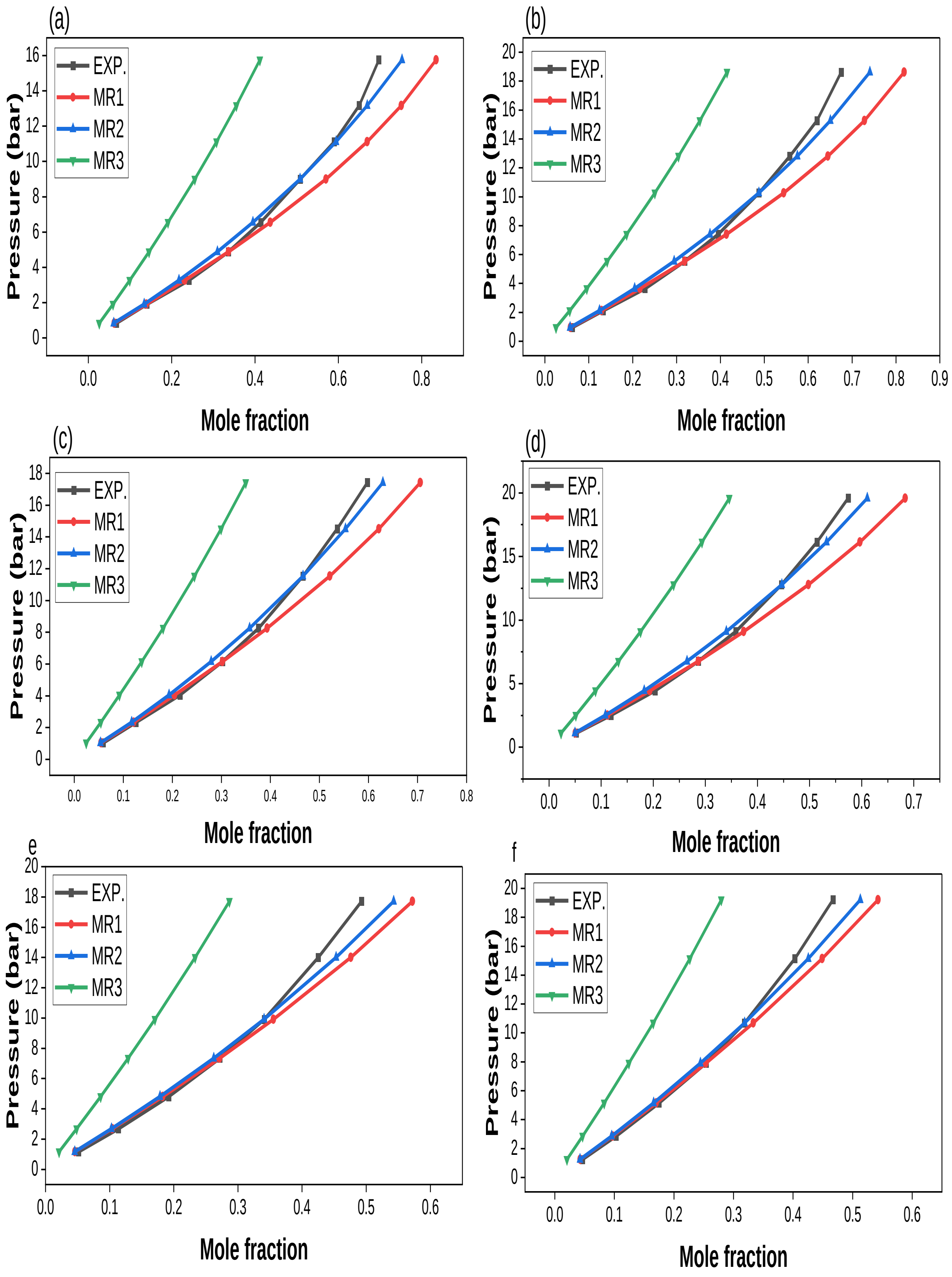

Figure 6. Phase composition diagram of H_2S- [C8mim][PF6] system at (a) 303.15K , (b) 313.15K, (c) 323.15K , (d) 333.15K, (e) 343.15K, (f) 353.15K, using PR with three different mixing rules.[20]

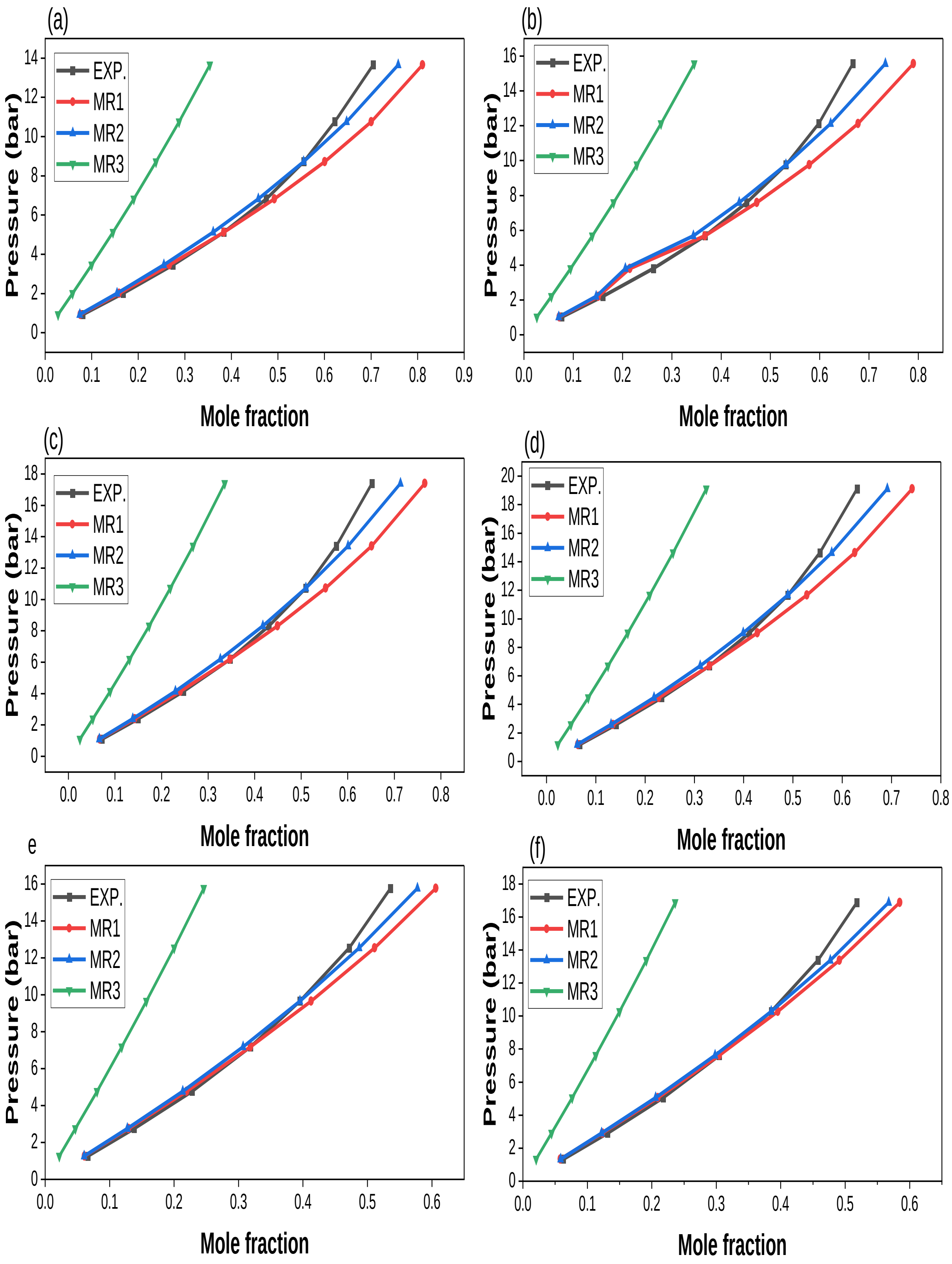

Figure 7. Phase composition diagram of H_2S- [C8mim][TF2N] system at (a) 303.15K , (b) 313.15K, (c) 323.15K , (d) 333.15K, (e) 343.15K, (f) 353.15K, using PR with three different mixing rules.[11]

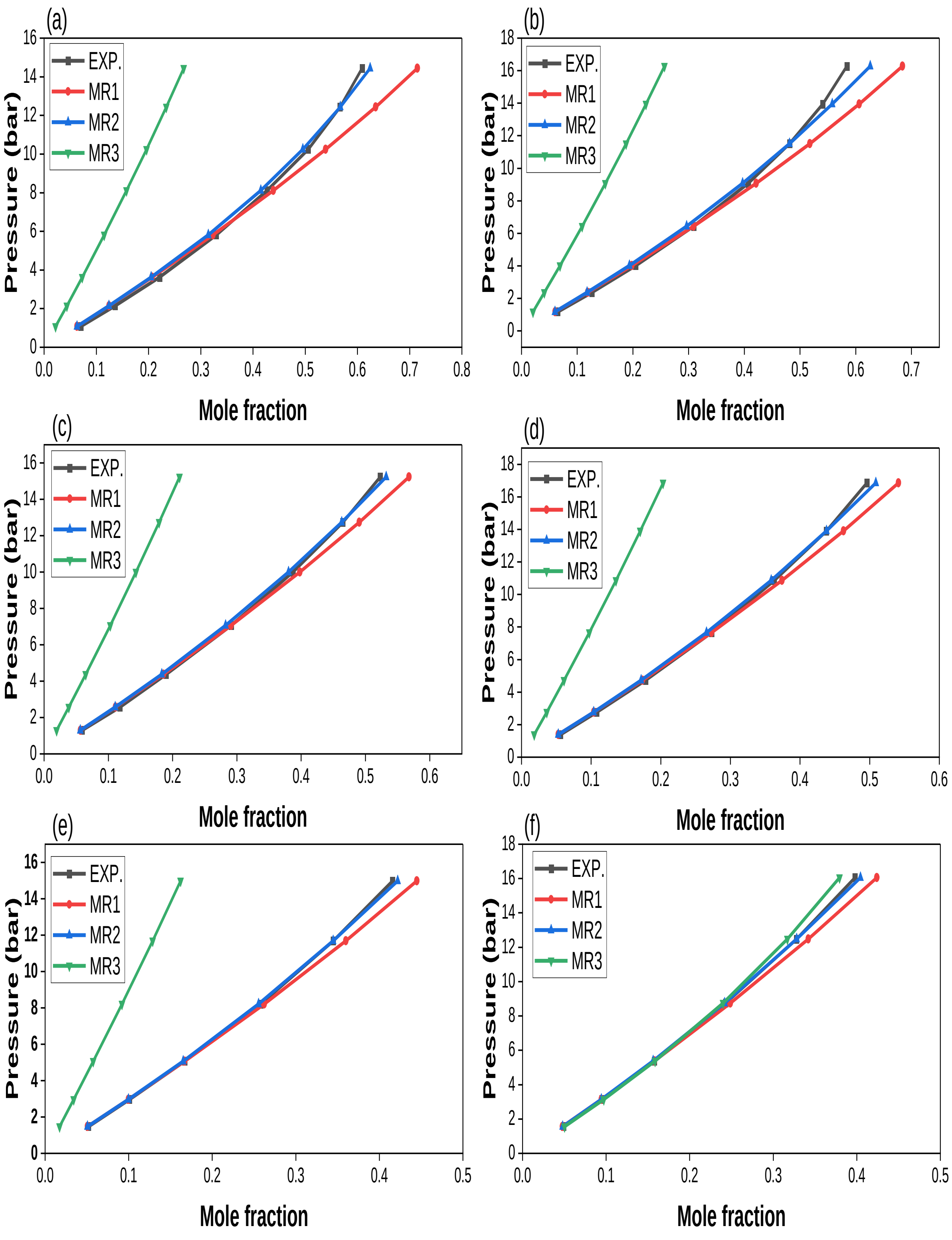

Figure 8. Phase composition diagram of H_2S- [Emim][TF2N] system at (a) 303.15K , (b) 313.15K, (c) 323.15K , (d) 333.15K, (e) 343.15K, (f) 353.15K, using PR with three different mixing rules.[10]

4. Conclusions

In the presented study, PR-EoS was successfully employed with three different mixing rules in order to predict carbon dioxide and hydrogen sulfide solubility in various ionic liquids at temperatures and pressures range (298.2–353.15) K, (0.119–65.2) bar, respectively. The research was conducted on various experimental data gathered from literature sources. The mixing rule MR2, which has two adjustable parameters (k_{12} and L_{12}) provides the best agreement with experimental data in comparison to other mixing rules. Finding L_{12} also is a little bit difficult, therefore, for easy calculation and save time, MR1 was utilized for PR, which provides acceptable results compared to the experimental data. %AARD values obtained by using MR2 and MR1 in all system studied in this work have a range (0.9-8) and (2-8) excluding CO_2+ [Amim][HCOO] system due to our conclusion the e experimental data was not correct. Concerning MR3 with PR-Eos, in CO_2 -ILs systems gives arbitrary % AARD range (0.5 - 29), but in some systems it was observed best, while in H_2S-ILs system it shows very bad agreement with experimental data with high range of %AARD (2-67), depending to the structure and solubility of the system.

List of Symbols

Symbol	Total Name of Symbols
a, b	parameters in the equation of state
A, B	dimensionless parameters
f	fugacity, bar
$k_{ij}, l_{ij}, A_{12}, A_{21}$	adjustable parameters
n	number of components
n_i	number of moles of component i, mole
N	number of data points
P	pressure, bar
R	universal gas constant, 0.08314 lit. bar/ mole K
T	temperature, K
x,y	liquid and gas mole fractions, respectively
Z	compressibility factor
$\underline{V}$	total system volume, lit
v	total system molar volume, lit./mole
A^E_∞	excess Gibbs free energy
AARD	average absolute relative deviation
PR–EoS	Peng Robinson Equation of State
MR	Mixing Rules
Greek litters	
$\hat{\phi}_i$	fugacity coefficient in mixture
ω	a centric factor
Ω	Omega, dimension less constant in PR-EoS, -0.62323
Subscripts & Superscripts	
c	critical condition
Exp	experimental value
calc	calculated value
g	gas phase
l	liquid phase
i, j	Component
m	mixture
r	reduced property
ILs	Ionic liquids

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