

Iranian Journal of Oil & Gas Science and Technology, Vol. 10 (2021), No. 2, pp. 51–61
<http://ijogst.put.ac.ir>

Simulation of H₂S Solubility in Three Acetate-based Ionic liquids Using PC-SAFT EoS together with RETM

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Highlights

- Pure [emim][Ace], [bmim][Ace], and [hmim][Ace] were modeled;
- H₂S solubility in three carboxylates ionic liquids was correlated using PC-SAFT EoSs;
- RETM was applied to calculate the liquid-phase concentrations;
- RETM–PCSAFT presents AADs% equal to 2.29%, 3.09%, and 7.65% for H₂S–[emim][Ace], H₂S–[bmim][Ace], and H₂S–[hmim][Ace] systems respectively;
- The results of RETM–PCSAFT were compared with those of RETM–CPA.

Received: April 09, 2021; revised: April 20, 2021; accepted: May 12, 2021

Abstract

In current work, perturbed chain-statistical associating fluid theory (PC-SAFT) equation of state (EoS) together with the reaction equilibrium thermodynamic model (RETM) was employed to correlate H₂S solubility in three carboxylate ionic liquids including [emim][Ace], [bmim][Ace], and [hmim][Ace]. The RETM proposes a chemical reaction approach between ionic liquid (IL) (B) and H₂S (A) in the liquid phase. Moreover, PC-SAFT EoS contributes to VLE calculations. All the H₂S and the investigated ILs, as self-associating components, are assumed to follow the 2B association scheme. Five adjustable variables of PC-SAFT EoS for pure components were calculated using experimental data of liquid density and vapor pressure. Afterward, the binary systems were investigated by applying RETM. Indeed, two nested loops calculate the liquid phase, total pressure, and vapor phase concentrations, respectively. For these systems, an AAD% of 2.29%, 3.09%, and 7.65% was obtained for H₂S–[emim][Ace], H₂S–[bmim][Ace], and H₂S–[hmim][Ace] systems, respectively.

Keywords: Acetate anion, Acid gas solubility, Ionic liquid, PC-SAFT EoS, RETM

How to cite this article

Afsharpour A, Simulation of H₂S Solubility in Three Acetate-based Ionic liquids Using PC-SAFT EoS together with RETM, Iran J. Oil Gas Sci. Technol., Vol. 10, No. 2, pp. 51–61, 2021.

DOI: <http://dx.doi.org/10.22050/IJOGST.2021.276176.1586>, This is an Open Access article under Creative Commons Attribution 4.0 International License (creativecommons.org/licenses/by/4.0)



1. Introduction

Because of several technical, environmental, and economic concerns, the removal of acid gases, especially H₂S, from gas streams is essential (Afsharpour and Haghtalab, 2017a). In this way, the most common approach is using aqueous alkanolamine solutions because of their numerous advantages such

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as rapid absorption kinetics, high absorption capacity, low price, and relevant accessibility. However, some disadvantages of these solvents make their applications restricted and costly (Afsharpour and Haghtalab, 2017b). Recently, a novel category of solvents entitled “room temperature ionic liquids (RTILs or ILs)” has been proposed as valuable components in many applications. The ILs (a liquid constructed from cations and anion) are liquid salts at ambient temperature (e.g., below 100 °C) constructed of an organic cation (e.g., alkyl-imidazolium and alkyl-pyridinium) and an inorganic/organic anion (e.g., acetate and formate). According to particular demand, combinations of different kinds of cations and anions will lead to different properties (Haghtalab and Afsharpour, 2015). ILs present excellent properties such as insignificant vapor pressure, chemical and thermal stability (even up to 400 °C or more), non-flammability, and tunable nature, making them a good candidate for different applications (Haghtalab and Afsharpour, 2015).

Although several practical studies on the solubility of H₂S in various ILs have been done, the expensive, time- and energy-consuming nature of such experimental works proposed the necessity of a reliable modeling knowledge as an excellent alternative to investigate the solubility of acidic gases in ILs (Macías-Salinas et al., 2013). From a technical point of view, the solubility of acid gases into ILs is very similar to alkanolamines. Some differences may return to lower kinetics (more time demand), lower gas loadings, and different absorption mechanisms (physical versus chemical). More details could be found in our previous works (Afsharpour and Haghtalab, 2017b; Haghtalab and Afsharpour, 2015). Accordingly, up to now, some modeling studies have been performed in the literature; few of them are mentioned here.

A simple association-type equation of state (EoS), known as Peng–Robinson two-state (PR-TS) EoS, was applied to simulate the pressure-volume-temperature behavior of H₂S solubility in 12 imidazolium-based ILs by Shojaeian (2017). The best achieved overall absolute average deviation percentage (AAD %) in this work is 3.40.

In the work of Hamzehie et al. (2015), the solubility of acidic gases (H₂S and CO₂) in 32 commonly single and mixed amine and ionic liquid solutions were predicted over broad ranges of operating conditions using an artificial neural network (ANN) model. The outputs of the model illustrate that the implemented model can accurately compute the solubility of acid gases in various solutions with a mean relative error (MRE) value of 3.104.

Modeling the solubility of H₂S and CO₂ single gases in the fourteen ionic liquids ([C₂mim][eFAP], [C₂mim][EtSO₄], [C₂mim][OTf], [C₂mim][Tf₂N], [C₄mim][BF₄], [C₄mim][PF₆], [C₆mim][PF₆], [C₆mim][Tf₂N], [C₈mim][PF₆], [C₈mim][Tf₂N], [HOC₂mim][BF₄], [HOC₂mim][OTf], [HOC₂mim][PF₆], and [HOC₂mim][Tf₂N]) using the CPA EoS was performed by Soltani Panah (2017) through a novel approach. He obtained good compatibility between experimental data and the calculated results, so an overall AAD% below 10% was observed.

The work of Haghtalab and Kheiri (2015) studied the solubility of mixtures of CO₂ and H₂S in [C₂mim][Ace] experimentally and theoretically using the CPA equation of state. Moreover, the reaction equilibrium thermodynamic model (RETM) proposed by Huang et al. (2013) was employed to obtain the liquid-phase concentrations. The computed results show the acceptable accuracy of the model.

Afsharpour (2021b) followed an approach based on the RETM to correlate the solubility of CO₂ and H₂S in four protic ionic liquids, including [MDEAH][Ace], [MDEAH][For], [MDEAH][Ace], and [MDEAH][For] using the CPA EoS. The effect of the RETM was studied by comparing the model's

results with and without using the RETM. The RETM played an important role in reducing the overall deviation according to the achieved outputs. In this way, the total AAD% below 1% was calculated.

The present study thermodynamically models the solubility of H₂S in ionic liquids [emim][Ace], [bmim][Ace], and [hmim][Ace] using the perturbed chain-statistical associating fluid theory (PC-SAFT) EoS together with the RETM.

2. Thermodynamic modeling

2.1. Reaction equilibrium thermodynamic model

The RETM was proposed by Huang et al. (2013) and considers two chemical reactions in the liquid phase as below:



where A , B , AB , and AB_2 stand for H₂S, ionic liquid, and two possible complex concentrations, respectively.

Three fundamental relations, including Henry's law, reaction equilibria, and mass balance, should be satisfied in these systems. These equations have been described in detail by Huang et al. (2013). Merging Equations (2)–(6) leads to Equation (7):

$$P = Hm_A \quad (2)$$

$$K_1 = \frac{m_{AB}}{P.m_B} \quad (3)$$

$$K_2 = \frac{m_{AB_2}}{P.m_B^2} \quad (4)$$

$$m_{B_0} = m_B + m_{AB} + 2m_{AB_2} \quad (5)$$

$$m_{A_0} = m_A + m_{AB} + m_{AB_2} \quad (6)$$

$$m_{A_0} = \frac{4K_2 P m_{B_0} + (1 - K_1^2 P^2) \left[1 - \sqrt{\frac{8K_2 P m_{B_0}}{(1 + K_1 P)^2} + 1} \right]}{8K_2 P} + \frac{P}{H} \quad (7)$$

where m_{A_0} and m_{B_0} are the initial H₂S and ILs molalities, respectively.

The main parameters, K_1 (first reaction equilibrium constants), K_2 (second reaction equilibrium constant), and H (constant of Henry's law), could be computed through fitting the experimental solubilities. The first reaction (K_1) constant was amazingly computed equal to zero for all the studied systems, and the K_2 and H parameters were obtained from the literature (Huang et al., 2013). These parameters can be correlated as temperature functions as follows:

H₂S+ [emim][Ace] binary:

$$H \text{ (KPa)} = 0.0018 \times T^3 - 1.5876 \times T^2 + 482.96 \times T - 49142 \quad (8)$$

$$K_2 = -10^{-5} \times T^3 + 0.0147 \times T^2 - 4.8181 \times T + 529.5 \quad (9)$$

H₂S+ [bmim][Ace] binary:

$$H(KPa) = \exp\left(-0.8599 - \frac{369.9}{T} + 0.02168T\right) \quad (10)$$

$$K_2 = \exp\left(16.38 + \frac{7.911}{T} - 0.0493T\right) \quad (11)$$

H₂S+ [hmim][Ace] binary:

$$H(KPa) = 0.0429 \times T^2 - 24.321 \times T + 3518 \quad (12)$$

$$K_2 = 0.0006 \times T^2 - 0.5756 \times T + 127.4 \quad (13)$$

By determining K_2 and H parameters, other concentrations will be achieved through Equations (2), (5), and (6) (Huang et al., 2013):

With the liquid phase values, VLE calculations can be accomplished through the PC-SAFT EoS.

2.2. PC-SAFT equation of state

Gross and Sadowski introduced the PC-SAFT as a SAFT variant EoS (Gross and Sadowski, 2001). The main difference between this model and other variants of SAFT EoS returns to the implemented dispersion term, and this term tries to take the dispersion attraction between whole chains into account. A conceptual molecular model of PC-SAFT EoS is presented in Figure 1.

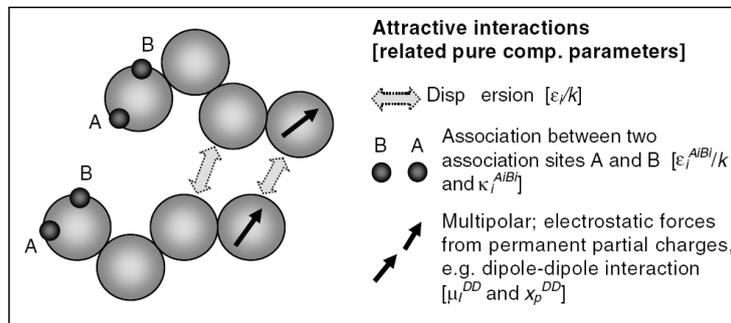


Figure 1

The conceptual molecular model of PC-SAFT EoS.

The PC-SAFT can be presented based on reduced residual Helmholtz energy as follows:

$$\tilde{a}^{res} = \tilde{a}^{hc} + \tilde{a}^{disp} + \tilde{a}^{assoc}. \quad (14)$$

where \tilde{a}^{hc} , \tilde{a}^{disp} , and \tilde{a}^{assoc} denote reduced Helmholtz energy of the rigid chain, dispersion, and association terms, respectively. According to the PC-SAFT variation, the mentioned terms could be defined as given below.

a. Hard chain term

The reduced Helmholtz energy of the hard chain term is defined as:

$$\mathcal{V}^{hc} = m\mathcal{V}^{hs} - \sum_i x_i (m_i - 1) \ln g_{ii}^{hs}(\sigma_{ii}) \quad (15)$$

where m , \tilde{a}^{hs} , and $g_{ii}^{hs}(\sigma_{ii})$ stand for the segment number, hard-sphere reduced Helmholtz energy, radial distribution function, respectively. The mentioned parameters are defined as:

$$m = \sum_i x_i m_i \quad (16)$$

$$\tilde{a}^{hs} = \frac{1}{\xi_0} \left[\frac{3\xi_1\xi_2}{(1-\xi_3)} + \frac{\xi_2^3}{\xi_3(1-\xi_3)^2} - \left(\xi_0 - \frac{\xi_2^3}{\xi_3^2} \right) \right] \ln(1-\xi_3) \quad (17)$$

$$g_{ij}^{hs} = \frac{1}{1-\xi_3} + \left(\frac{d_i d_j}{d_i + d_j} \right) \frac{3\xi_2}{(1-\xi_3)^2} + \left(\frac{d_i d_j}{d_i + d_j} \right)^2 \frac{2\xi_2^2}{(1-\xi_3)^3} \quad (18)$$

where

$$\xi_k = \left(\frac{\pi}{6} \rho \right) \sum x_i m_i d_i^k \quad n \in \{0, 1, 2, 3\} \quad (19)$$

$$d_i = \sigma_i \left[1 - 0.12 \exp\left(-3 \frac{\epsilon_i}{kT}\right) \right] \quad (20)$$

$$\tilde{a}_1 = (-2\pi\rho I_1 \overline{m^2 \epsilon \sigma^3}) + (-\pi\rho m C_1 I_2 \overline{m^2 \epsilon^2 \sigma^3}) \quad (21)$$

where

$$\overline{m^2 \epsilon \sigma^3} = \sum_i \sum_j x_i x_j m_i m_j \left(\frac{\epsilon_{ij}}{kT} \right) \sigma_{ij}^3 \quad (22)$$

$$\overline{m^2 \epsilon^2 \sigma^3} = \sum_i \sum_j x_i x_j m_i m_j \left(\frac{\epsilon_{ij}}{kT} \right)^2 \sigma_{ij}^3 \quad (23)$$

$$C_1 = \left(1 + m \frac{8\eta - 2\eta^2}{(1-\eta)^4} + (1-m) \frac{20\eta - 27\eta^2 + 12\eta^3 - 2\eta^4}{[(1-\eta)(2-\eta)]^2} \right)^{-1}; \eta = \xi_3 \quad (24)$$

$$I_1(\eta, m) = \sum_{i=0}^6 a_i(m) \eta^i \quad (25)$$

$$I_2(\eta, m) = \sum_{i=0}^6 b_i(m) \eta^i \quad (26)$$

where

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j) \quad (27)$$

$$\epsilon_{ij} = \sqrt{\epsilon_{ii}\epsilon_{jj}}(1 - k_{ij}) \quad (28)$$

$$a_i(m) = a_{0i} + \frac{m-1}{m} a_{1i} + \frac{m-1}{m} \frac{m-2}{m} a_{2i} \quad (29)$$

$$b_i(m) = b_{0i} + \frac{m-1}{m} b_{1i} + \frac{m-1}{m} \frac{m-2}{m} b_{2i} \quad (30)$$

Constant a_{ki} and b_{ki} are reported in the literature (Senol, 2011). Moreover, k_{ij} s is the binary interaction coefficients between species i and j and can be optimized utilizing experimental data.

b. Association term

The association is given by the Wertheim's association term as follows:

$$a^{\text{assoc.}} = \sum_i X_i \sum_{A_i} \left[\ln X_{A_i} - \frac{1}{2} X_{A_i} + \frac{1}{2} \right] \quad (31)$$

where X_{A_i} is the critical parameter of the association term. It stands for the site fractions of type A at molecule i that do not establish hydrogen bonding with the other active sites. It is calculated by:

$$X^{A_i} = \frac{1}{1 + \rho \sum_j X_j \sum_{B_j} X^{B_j} \Delta^{A_i B_j}} \quad (32)$$

where $\Delta^{A_i B_j}$ denotes the association strength computed by:

$$\Delta^{A_i B_j} = d_{ij}^3 g_{ij}^{hs} (d_{ij}) \kappa^{A_i B_j} \left[\exp\left(\frac{\varepsilon^{AB}}{kT}\right) - 1 \right] \quad (33)$$

where ε^{AB} and $\kappa^{A_i B_j}$ are the association energy and volume, respectively.

3. Results and discussion

3.1. The pure component parameters

As can be seen in Equations (14), (18), and (31), there exist five pure parameters (m , σ , $\frac{\varepsilon}{k}$, κ^{AB} , and $\frac{\varepsilon^{AB}}{k}$) for self-associating components (Gross and Sadowski, 2001). H₂S pure component parameters were obtained from the work of Rahmati-Rostami et al. (2011).

A usual method to find the model parameters is to utilize vapor pressure and liquid density data through the following objective function (OF). Because ILs are almost involatile components, their vapor pressure data do not exist in the literature; therefore, the parameters of the EoS can be found utilizing experimental liquid density data according to the following objective function:

$$OF = \frac{100}{N} \left[\sum_i^N \frac{|\rho_i^{\text{exp}} - \rho_i^{\text{calc}}|}{\rho_i^{\text{exp}}} + \sum_i^N \frac{|P_i^{\text{exp}} - P_i^{\text{calc}}|}{P_i^{\text{exp}}} \right] \quad (34)$$

$$OF = \frac{100}{N} \sum_i^N \frac{|\rho_i^{\text{exp}} - \rho_i^{\text{calc}}|}{\rho_i^{\text{exp}}} \quad (35)$$

where N denotes the number of data points.

The experimental density data for all the considered ionic liquids were taken from the literature (Ma et al., 2013). For H₂S and the ILs, the pure parameters in addition to AADs% of the liquid density data are presented in Table 1.

Table 1
The PC-SAFT parameters of the pure components.

Component	H ₂ S	[emim][Ac]	[bmim][Ac]	[hmim][Ac]
Association scheme	2B	2B	2B	2B
Range of T	190–340	298.15–338.15	293.15–343.15	298.15–338.15
AAD% in P^{sat}	0.688	---	---	---
AAD% in ρ_{liq}	2.418	0.0063	0.3000	0.0156
Parameter				
m	1.649	2.172	2.245	2.216
σ	3.055	4.832	5.572	4.904
$\frac{\epsilon}{k}$	229.840	504.691	315.594	455.785
κ^{AB}	0.001	0.001	0.132	0.0001
$\frac{\epsilon^{AB}}{k}$	536.600	4221.231	2690.783	4965.509
Reference	(Rahmati-Rostami et al., 2011)	This work	This work	This work

3.2. Binary systems

For H₂S–IL systems, the binary interaction coefficients, k_{ijS} , can be adjusted via minimizing the following objective function:

$$OF = \frac{100}{N} \sum_i^N \left| \frac{P_i^{cal} - P_i^{exp}}{P_i^{exp}} \right| \quad (36)$$

Experimental data on H₂S solubility were obtained from the literature (Huang et al., 2013). The interaction coefficients and the AADs% of all the investigated IL–H₂S systems are reported in Table 2.

Table 2

The binary interaction parameters and AAD% of the solubility of H₂S in the pure ionic liquids using PC-SAFT EoS.

	H ₂ S–[emim][Ace]	H ₂ S–[bmim][Ace]	H ₂ S–[hmim][Ace]
	$K_{ij} = 1.173 \times 10^{-5}T^2 - 0.0073T + 1.099$	$K_{ij} = 4.3084 \times 10^{-4}T - 0.2356$	$K_{ij} = -2 \times 10^{-5}T^2 + 0.0124T - 1.9869$
T (K)		AAD%	
293.15	1.85	3.80	7.95
303.15	2.85	2.65	7.80
313.15	2.32	3.10	6.80
323.15	2.76	3.05	5.98

333.15	1.62	2.66	9.60
Overall AAD%	2.29	3.09	7.65

Figures 2–4 delineate the experimental versus calculated results for the H₂S–[emim][Ace], H₂S–[bmim][Ace], and H₂S–[hmim][Ace] binaries at various temperatures.

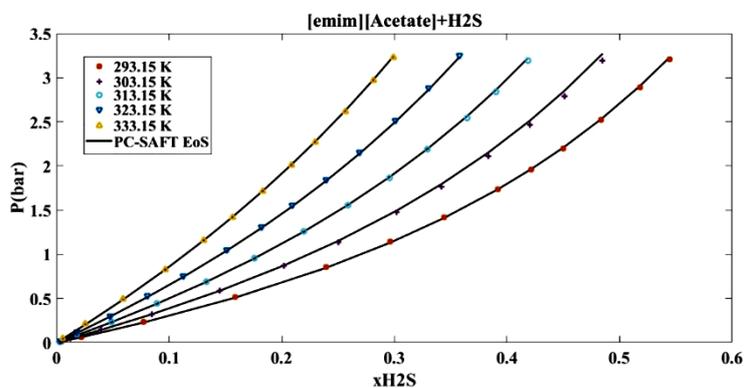


Figure 2

The experimental and calculated pressure versus H₂S liquid molality in ionic liquid [emim][Ace] at different temperatures.

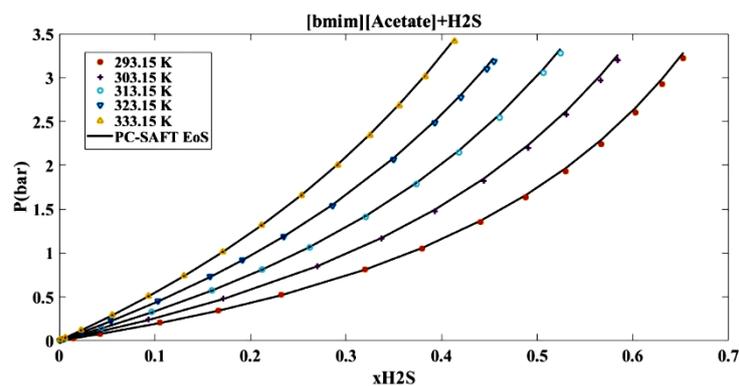


Figure 3

The experimental and calculated pressure versus H₂S liquid molality in ionic liquid [bmim][Ace] at different temperatures.

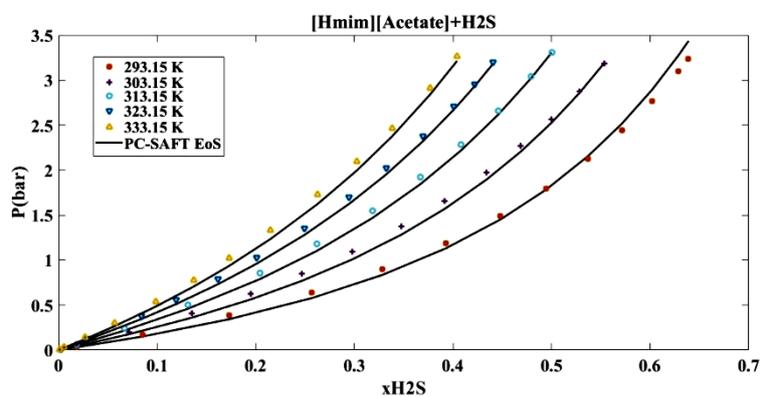


Figure 4

The experimental and calculated pressure versus H₂S liquid molality in ionic liquid [hmim][Ace] at different temperatures.

According to the obtained results, all the figures demonstrate that the solubility of H₂S (mole fraction of H₂S in the ionic liquids) increases with the operational pressure. Moreover, lower solubility is observed at higher temperatures in all cases. In fact, absorption is promoted at higher pressures and lower temperatures. In addition, from the curvature trends of the figures, it could be deduced that a chemical absorption mechanism is predominant. Indeed, Equations (3) and (4) play significant roles, so a curve trend is seen instead of a linear one.

According to the figures and on the basis of the results in Table 2, the AADs% of H₂S–[emim][Ace], H₂S–[bmim][Ace], and H₂S–[hmim][Ace] systems is 2.29%, 3.09%, and 7.65%, respectively. Significant compatibility between the experimental data and the modeling outputs is observed.

A comparison was made between the present results and those of other models to show the capability of the used models. In this way, for the investigated systems, the results of PC-SAFT–RETM were compared with those of CPA–RETM (Afsharpour, 2019, 2021a) in Table 3. PC-SAFT EoS presents a much higher degree of accuracy, so more than 50% improvement in overall AAD% is noticed.

Table 3
Comparison between results of the PC-SAFT and the CPA EoSs.

Binaries	Applied models	
	PC-SAFT–RETM	CPA–RETM
H ₂ S–[emim][Ace]	2.29	4.75
H ₂ S–[bmim][Ace]	3.09	13.42
H ₂ S–[hmim][Ace]	7.65	12.44
Reference	This Work	(Afsharpour, 2019, 2021a)

4. Conclusions

H₂S solubility in ionic liquids [emim][Ace], [bmim][Ace], and [hmim][Ace] was correlated implementing PC-SAFT EoS. The RETM was employed to calculate the liquid-phase concentrations. This model proposed an AB₂ type chemical complex reaction between acidic gas and the ionic liquids. In other words, at the inner loop, the RETM calculates the liquid-phase concentrations, and at the outer loop, VLE calculations are performed through PC-SAFT EoS. The 2B association scheme was supposed for both H₂S and the ILs. Pure components parameters were adjusted using the PC-SAFT with very a high degree of accuracy. In addition, binary systems, including H₂S–[emim][Ace], H₂S–[bmim][Ace], and H₂S–[hmim][Ace], were correlated by implementing PC-SAFT together with RETM. An AAD% of 2.29%, 3.09%, and 7.65% was obtained for H₂S–[emim][Ace], H₂S–[bmim][Ace], and H₂S–[hmim][Ace] systems, respectively. Combining RETM with PC-SAFT EoS results in excellent accuracy in correlating such systems. A comparison was made with the CPA EoS to trust the applied model. In this way, for all the studied systems, a total AAD% of 4.34% and 10.20% was obtained by PC-SAFT and CPA EoSs, respectively. Based on these results, PC-SAFT presents a much lower AAD%. Because of the no particular restriction in the applicability of the model (including RETM and PC-SAFT), it is expected that all the results are reproducible. In addition, some suggestions for future works can be using other EoSs, applying the nonideal RETM, studying new types of ionic liquid, and investigating CO₂ removal.

Nomenclature

AAD	Average deviation percentage
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ANN	Artificial neural network
EoS	Equation of state
IL	Ionic liquid
MRE	Mean relative error
OF	Objective function
PC-SAFT	Perturbed chain-statistical associating fluid theory
PR-TS	Peng–Robinson two-state
RETM	Reaction equilibrium thermodynamic model
RTIL	Room temperature ionic liquids

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