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Abstract

A wide range of solvent contents (1–2.5 molar), pressures (150–4000 kPa), and temperatures (313.15–353.15 K) were used to explore the vapour-liquid equilibrium of the CO₂-loaded aqueous potassium salt of L-histidine in this study. The outcomes of the experiment demonstrate that L-histidine has a superb capacity to absorb carbon dioxide. When compared to conventional solvent (monoethanolamine) and amino acid salt (potassium *L*-lysinate) at similar process conditions, *L*-histidine has superior absorption capacity. Moreover, modified Kent–Eisenberg model was used to correlate the VLE of the studied system with excellent agreement between the model and experimental values. The model exhibited an AARE% of 7.87%, which shows that it can satisfactorily predict carbon dioxide solubilities in aqueous potassium salt of *L*-histidine at other process conditions. Being a biological component in origin, almost negligibly volatile, and highly resistant to oxidative degradation, *L*-histidine offers certain operational advantages over other solvents used and has a promising potential for carbon dioxide capture.

1. Introduction

The acceptance of environmental norms has led to an increase in research efforts aimed at lowering carbon dioxide emissions. The primary task in this endeavour is to remove carbon dioxide from process exhaust and fuel streams. There are various techniques which have been applied for this purpose [1]. Of these techniques, removal of carbon dioxide (CO₂) by chemical absorption technique is regarded a standout amongst the most industrial process, technologically and commercially. The process has been broadly received in power plant industry. This involves a chemical reaction between the CO₂ containing industrial gas streams and a solvent which then results to a greener and cleaner gas released to the

atmosphere. Aqueous alkanolamines such as monoethanolamine (MEA) are commonly used. However, this class of solvents has a few downsides like limiting the cyclic CO₂ loading capacity and causing an implication in regeneration economically. Aside from being corrosive, they also add to formation of toxic degradation products and solvent losses due to evaporation [2]. The fugitive losses in the environment have been shown to be directly associated with occurrences of cancer and other medical complexities, apart from their adverse contribution in destroying marine and atmospheric ecology [3].

In the current years, research on using amino acid saltbased solvents as another alternative has

been centred for carbon dioxide separation related technology. Interestingly, these amino acid salts have similar functional group to the conventional alkanolamines. Hence, it is expected that their reactivity toward carbon dioxide is as good as alkanolamines-based solvents. Apart from that, they possess high resistance to thermal and oxidative degradation as well as low in volatility for they are naturally ionic compounds, potentially are a greener solvent for capturing carbon dioxide [4, 5]. Their application shall result in a much cleaner and environmentally friendly process. Few studies on these systems are presently available in the literature. Majority of these already scant works are oriented toward the provision of precursor vapour-liquid equilibrium (VLE) data for studies, pertaining to kinetics and transport property-based investigations. The VLE data form the base for all design and simulation studies, which eventually leads to proper equipment sizing and better selection of operational parameters, resulting in optimal production.

One of the initial works was performed by Muñoz et al. [6] as part of their study on structure/function relationship in various solutions of amino acid salts, namely, proline, serine, taurine, ornithine, and arginine. They examined that the carbon dioxide capacity in these aforementioned solvents at concentration of 1 molar was comparable to the conventional MEA [6]. Recently, the carbon dioxide solubility in aqueous potassium lysinate solutions has been

studied at temperature (313.15–353.15 K), concentration (1–2.5 M), and pressure (150–4040 kPa). It was discovered that lysine offered good absorptive capacity for carbon dioxide, and model results developed based on the Kent–Eisenberg model are coherent with experimental findings [7]. A comprehensive literature review of the similar studies was conducted in the field. Table 1 provides exhaustive summary about the recent studies in the discussed field.

However, it was interesting to note that VLE data for carbon dioxide-loaded aqueous potassium histidinate (HisK) are absent. Although there was a reported literature on physical properties and kinetics of CO₂ absorption into this HisK solution from the work of Shen et al. [30], the VLE data for the said system are fictional. Hence, in this study, CO₂ solubility of aqueous potassium histidinate solution was measured at pressure ranging from 150 to 4000 kPa, temperature from 313.15 to 353.15 K, and solvent concentrations of 1 and 2.5 molar. A reliable high-pressure vapour-liquid equilibrium apparatus was used to perform this experimental study.

VLE data on this said system are likely the most essential ancestor data for the development of mathematical models particularly at predicting the CO₂ loading values. For this reason, a mathematical model based on the modified Kent and Eisenberg approach is extended to correlate the equilibrium solubility data of the aforementioned system, with satisfactory results.

Although there are several models available for the prediction of CO₂ equilibrium data, the thermodynamic modeling efforts for the aqueous amino acid salt solutions have been limited to modified Kent–Eisenberg model [31, 32]. Being computationally simple, this model has been preferably and broadly used by previous researchers with good correlation of their experimental data [7, 25, 29]. Usually, all the nonidealities of the process system are combined in a single/dual correction parameter(s) of the model, that is a function of amine concentration, carbon dioxide loadings, and/or pressure [33], yielding a good relationship between the model's results and the experimental data. Hence, a study on the modeling of CO₂ solubility using the Kent and Eisenberg approach appears desirable.

2. Materials and Methods

The chemicals used throughout the experimentation are tabulated in Table 2. All chemicals were of sufficient purity and used without further purification. Samples were weighed using a mass balance Sartorius BSA224S-CW ($u = 0.1$ mg). Separate aqueous solutions of 1.0 and 2.5 molar of potassium hydroxide and *L*-histidine were prepared in 250 ml volumetric flasks ($u = 0.1$ ml) using deionized water and micropipettes (Duran). Both solutions were then mixed in equal volumes to create 1.0 molar and 2.5 molar aqueous potassium salt of *L*-histidine. The results of the study were reiterated

thrice to ensure the repeatability of the results, using freshly prepared sample of aqueous potassium salt of *L*-histidine, each time.

Pressurized reactor system (PRS) was used to measure the carbon dioxide solubility in the solvent and is shown in Figure 1. The apparatus has two vessels primarily made up of stainless steel and designed as 600 ml and 200 ml for feed cell and solubility cell, respectively. Each vessel is jacketed with electrically operated heaters. The apparatus has been used previously at various instances to reaffirm the carbon dioxide solubility in various alkanolamines with good reliability [7, 34, 35]. The feed vessel and reactor cell are equipped with a temperature (type: Autonics TK-4S) and pressure (type: Keyence GP-100M) gauge each. The digital temperature and pressure gauges extract data from the system and transfer it to computer data acquisition system. The computer uses a USB data link with LAB View software for data storage and utilization.

In a usual run, the solubility cell was filled with 40 ml of freshly prepared solvent. The system was purged with lowpressure nitrogen (0.1 kPa) for two minutes to ensure the removal of air/oxygen present in the solubility cell. While purging, the feed cell was filled initially with a known quantity of carbon dioxide, n_{IQ} . After completion of nitrogen flush, carbon dioxide gas was then transported to the solubility cell and n_{FQ} is introduced as CO₂ number of moles in the feed tank after transferring to the solubility cell. Thus,

the number of moles of CO₂ being fed to the solubility cell is calculated as follows:

$$n_{FD} = n_{IQ} - n_{FQ} \quad (1)$$

In the solubility cell, the pressure of CO₂ gas dropped by times as the gas chemically reacts and dissolves in the solvent which then brought to an equilibrium state. The residual number of moles of CO₂ or undissolved gas were calculated by the tmPR-LCVM-UNIFAC equation of state/excess Gibbs energy model [36], using partial pressure of carbon dioxide, P_{RS} at equilibrium, using

$$P_{RS} = P_{PT} - P_{NT} - P_{WT} - P_{AA} \quad (2)$$

where P_{PT} is denoted as the total pressure in solubility cell at equilibrium whilst P_{NT} , P_{WT} , and P_{AA} are the equilibrium partial pressures of nitrogen, water, and amino acid in the solubility cell, respectively. The value of P_{RS} was then further

used to determine the value of n_{RS} . This n_{RS} is important for determination of CO₂ number of moles absorbed in the solvent, as demonstrated in the following equation:

$$n_{AB} = n_{FD} - n_{RS} \quad (3)$$

The number of moles in each case (n_{IQ} , n_{FQ} , and n_{RS}) were determined by translated modified Peng–Robinson equation of state [37] and Span and Wagner EoS [38] for pressures lower and higher than 3000 kPa, respectively. Hence, the carbon dioxide loading was determined as follows:

$$n_{AB} \alpha n_{AA} \quad (4)$$

where n_{AA} is the number of moles of unloaded amino acid initially fed to the solubility cell.

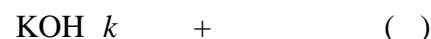
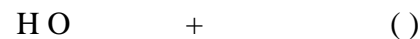
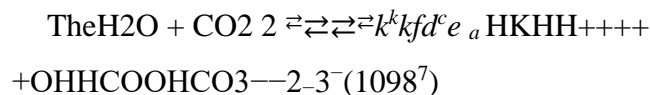
3. Thermodynamic Framework

3.1. *Modified Kent–Eisenberg Model for Absorption of Carbon Dioxide in Aqueous Potassium Histidinate Solution (HisK)*. The chemical reaction between carbon dioxide and amino acid salt like histidine is best explained by the zwitterion mechanism which broadly recognized for the development of model for CO₂ absorption in the aqueous solutions of alkanolamines and amino acid salts [39]. The equations describing the equilibrium of CO₂ with HisK are as follows [30]:

k_a



k_b



are equilibrium constants, k_a – k_b , for reactions (5)–(10)

given as k_a $\frac{[RRHCOO^-][NH_3]}{[RRHCOO^-][NH_3]} = 3$

$$H^+ + K^+ [OH_2[RR] + NCOOHCO] + [2RRCO-NH^-] \quad (19)$$

$[[HH^{++}], 3^- , (1211) kb$

$$\frac{RR [HCO^-]}{[RR^-NCOO^-]} [] ()$$

$$k_e [] () k f d c$$

$$OHOHCOHCOKOH-3-CO_2$$

$$-HK32^{++}+[H^{+}, ,] (141315)$$

$$k_e [] ()$$

The potassium hydroxide value of equilibrium constant is assumed to be very high as compared to other equilibrium constants, k_a to k_e , and the strength of molar for potassium ion, $[K^+]$, is presumed to be equal to the strength of molar for potassium hydroxide $[KOH]$ rearrangement]. Therefore, value of equations of $[K^+]$ is known. The solution and

Moreover, as follows: balances for [reactions []] given in (5)-(10)(16 are)

(11)-(17) and (19) yield the equation of polynomial given below:

$${}^5 B^4 C^3 D^2 E F (20) A H^+ + H^+ + H^+ + H^+ +$$

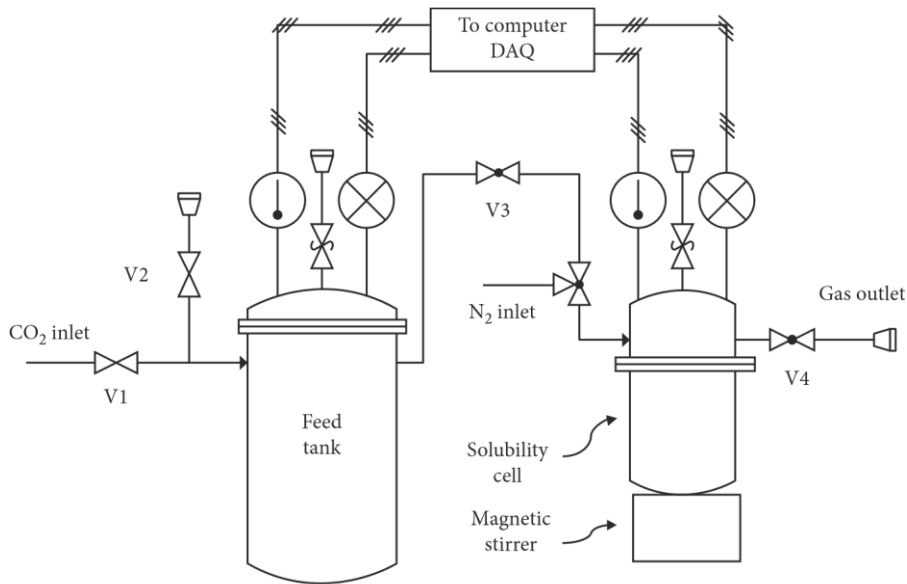


FIGURE 1: Pressurized reactor system.

Amino acid $[RR-NH_2] + [RR-NCOO^-] (17)$ CO balance:
 $\alpha AMT_2 CO_2 + HCO^- -3^- + CO_3^- -32^- + [RR_32^- NCOO^- 18]$
 ()

$H^+ + 0,$
 where
 $A = k_{bx},$
 $B = K^+ + k_a k_b x,$

Electroneutrality balance:

$$k_{bx}k_e k_{ax}k_{bx} \text{AMT}, D \text{---} \text{CO} \quad \text{K}^+ \quad \square \text{CO}_2 \text{H}_{\text{---}}\text{co}_2. \quad (24)$$

The value of hydrogen ion concentration, $[\text{H}^+]$, was equation (20). The carbon dioxide loading in the aqueous determined within the range of 10^{-5} to 10^{-12} , according to HisK solution thereby can be calculated based on the folthe relevancy of pH value of HisK solutions and solved by lowing equation:

$$\frac{\square \text{CO}_2 \square + k_c \square \text{CO}_2 \square [\text{H}^+] \square + k_c k_d \square \text{CO}_2 \square [\text{H}^+]^2 \square + [\text{RR}^-\text{NCOO}^-] \square}{\square \text{AMT} \square} \quad \alpha \quad (22)$$

where the value of $[\text{RR}^-\text{NCOO}^-]$ is governed by the equation as follows:

$$\text{RR}^-\text{NCOO}^- \frac{\square k_c [\text{K}^+] \square \text{CO}_2 \square [\text{H}^+]^2 + k_c \square \text{CO}_2 \square [\text{H}^+]^3 + \dots}{\dots} \square \text{CO}_2 \square [\text{H}^+] - 2k^2 c k d \square \text{CO}_2 \square^2 \square. \quad (23) \quad k_{bx}[\text{H}$$

$$2 \quad \text{CO} \quad (21)$$

c

$$-k k_k \text{---} a_x b_x a_x k k k a_x k k a_x a_x c b_x k k k 2 c k 2 c K b_x$$

$$-k k + d k c^2 k c 2 k a_x + d 2 k k - b_x a_x k k k - a_x e c - k k C$$

$$\text{O} c^{a_x} k k e k_{b_x} 2^c k - c k k d b_x^2 k c_{\text{ACOMT}}, 2$$

$$a_x b_x 2 \quad \text{CO}_2 E \text{CO} \quad \text{CO}_2$$

$$2 \quad \text{CO}_2,$$

$$F 2 \quad \text{CO}_2^2.$$

3.2. Modified Kent–Eisenberg Model Parameters for Absorption of Carbon Dioxide in Aqueous Potassium Histidinate Solution(HisK). Henry’s law equation given below is used in the model of modified Kent and Eisenberg for determination of carbon dioxide value in the liquid phase:

$$P_{\text{CO}_2}$$

On the other hand, the values of equilibrium constants in equations (7)–(10) are obtained from published literatures and calculated based on

$$k_i \exp \square \dots \square. \quad (25)$$

$$T + b_i \ln T + c_i$$

From the equation above, the value of factors from a_i to c_i is tabulated in Table 3. The values of apparent equilibrium constants for amino acid, k_{ax} and k_{bx} , are regressed to the experimental data.

The regressed values of k_a and k_b in this work are represented by a set of apparent equilibrium constants given in [41]:

$$k_{ax} k_{af_a}, \quad (26) \quad k_{bx} k_{bf_b}, \quad (27)$$

where the values of k_a and k_b are determined similarly as equilibrium constants given in Table 3, on the basis of equation (25). The regressed parameters for both k_a and k_b are tabulated in Table 4.

Moreover, the values of correction factors, f_a and f_b , are determined by $f_a \exp[s_1 A_{MT} + s_2 P_{CO_2} + s_3 A_{MT}^2]$, (28) $f_b \exp[s_4 A_{MT} + s_5 P_{CO_2} + s_6 A_{MT}^2]$. (29)

The values of correction parameters for f_a and f_b are given in Table 5.

4. Results and Discussion

The experimental equilibrium CO₂ loadings in 1 M and 2.5 M aqueous HisK solutions are presented in Table 6.

With increase in pressure, the solubility of carbon dioxide increases, whereas increase in temperature leads to decrease in loading values. An overall increase in carbon dioxide solubility is seen with increase of the HisK solvent concentration. However, the individual values of gas loading are reduced with increase in solvent concentration, since the HisK concentration appears in the denominator of loading equation as defined in equation (4). Moreover, the trend of the carbon dioxide loadings with respect to pressure, temperature, and concentration was congruent with the common understanding [7, 10, 29, 34, 42, 43]. Additionally, the exothermic reaction of CO₂ with HisK creates a further increase in

temperature, leading to a lower loading of CO₂ [44]. From the table below, it can also be seen that carbon dioxide loadings in HisK solutions were significant with maximum values reaching 2.399 moles of CO₂ per mole of HisK solvent at equilibrium partial pressure of CO₂ (3901 kPa).

Additionally, the behaviour of experimental equilibrium CO₂ loading data and literature data of monoethanolamine (MEA) are studied and observed. Figure 2 shows the behaviour of carbon dioxide loadings in 1 molar MEA and 1 molar HisK solutions. Similarly, Figure 3 presents the behaviour of carbon dioxide loadings in 2.5 molar MEA and 2.5 molar HisK solutions. Graphical analysis based on Figures 2 and 3 shows that the CO₂ loading of HisK is superior to that of MEA. As seen in Figure 2, HisK exhibits very high absorptive capacity than that of MEA at lower temperature (313.15 K). Contrarily, the carbon dioxide loadings at 353.15 K are similar to MEA. This means that HisK solutions can absorb more carbon dioxide per mole of solvent. Hence, more carbon dioxide is taken up the absorber section of the carbon dioxide separation system and can be stripped easily in the stripper section with same equilibrium loading. Additionally, based on Figure 3, HisK shows better CO₂ absorption at high temperature (353.15 K) than MEA, which further strengthens its potential for carbon dioxide absorption and stripping in respective sections. This provides a larger window of absorptive potential (the amount of carbon dioxide transferred

from absorption section to a stripping section of a carbon dioxide capture plant), where the HisK solutions are capable of carrying more carbon dioxide gas per cycle of carbon dioxide removal system than MEA, provided that the kinetics of both systems are deemed equal.

For example, the carbon dioxide loading for 1 molar aqueous potassium salt of *L*-histidine at 313.15 K and a pressure of 1000kPa is 1.503 mol/mol, whereas the carbon dioxide loading in 1 molar MEA at similar process conditions is 1.143 mol/mol. This means that HisK solutions can pick 0.36 more moles of carbon dioxide than MEA at absorber conditions. Similarly, the carbon dioxide loading for 1 molar aqueous potassium salt of *L*-histidine at 353.15K and a pressure of 360 kPa is 0.632 mol/mol, whereas the carbon dioxide loading in 1 molar MEA at almost similar process conditions (316 kPa than 360 kPa) is 0.772 mol/mol. This means that, at stripping conditions (assuming that stripper operates at 353.15 K), HisK solutions will be less loaded at equilibrium than the MEA (quantitatively by a difference of 0.14mol/mol). Eventually, HisK solutions can separate 0.871 moles of carbon dioxide per mole of solvent per cycle, whereas MEA can only transfer 0.371 moles at similar process conditions.

Furthermore, better absorptive potential also allows the stripping section to be operated at lower temperature (353.15 K) as compared to MEA (>373.15 K), resulting in lower energy penalty,

reducing thermal degradation of solvent, and reducing the fugitive emission of the solvent.

On the other hand, Figure 4 illustrates the behaviour of carbon dioxide loadings in 1 molar potassium salt of lysine (LysK) with 1 molar HisK solutions, whereas Figure 5 presents the behaviour of carbon dioxide loadings in 2.5 molar LysK and 2.5 molar HisK solutions. It can be seen

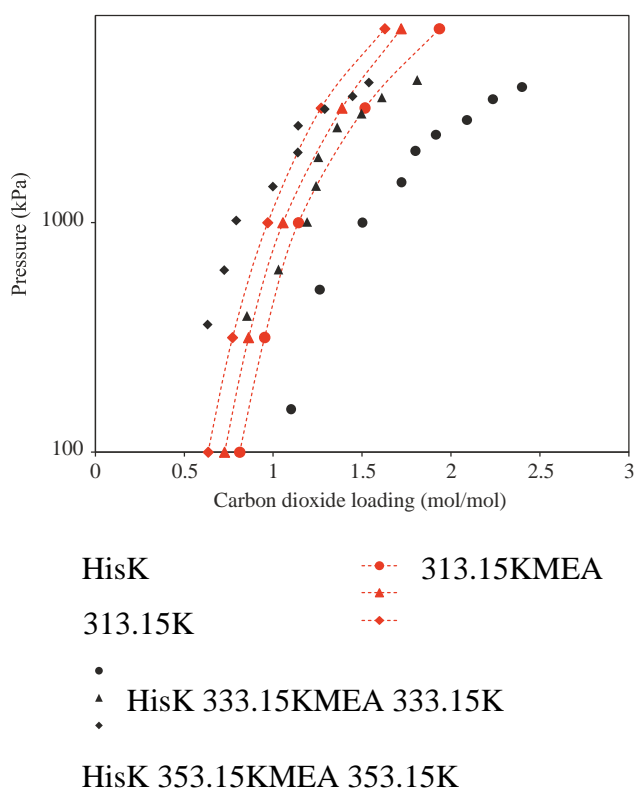


Figure 2: Experimental solubility behaviour of carbon dioxide in 1 M aqueous potassium salt of *L*-histidine and data of 1 M monoethanolamine [45].

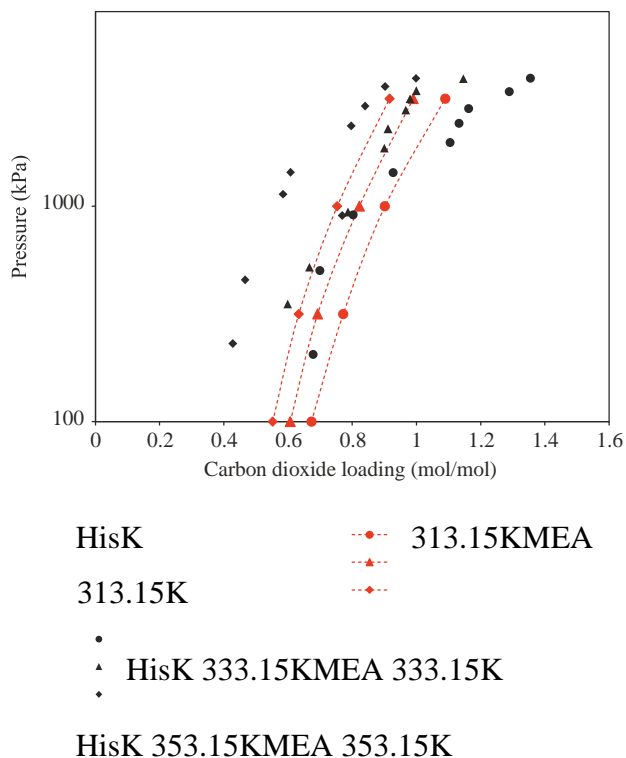
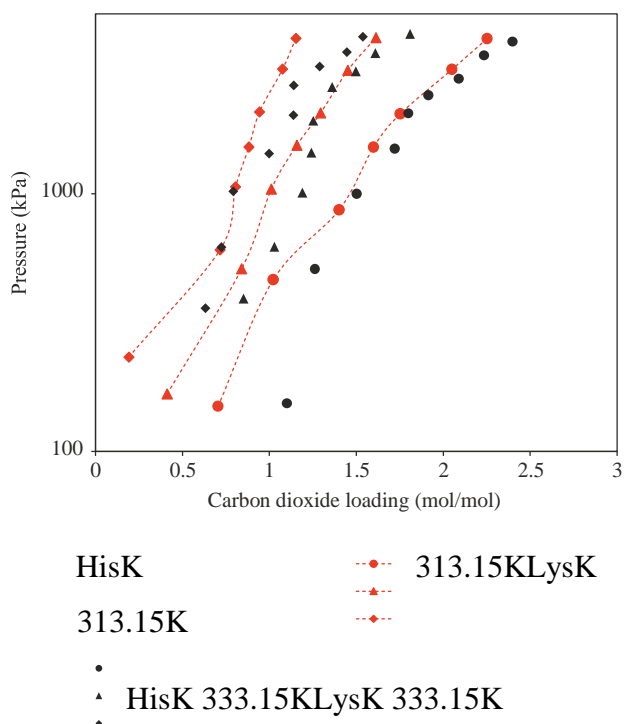


Figure 3: Experimental solubility behaviour of carbon dioxide in 2.5 M aqueous potassium salt of *L*-histidine and data of 2.5 monoethanolamine [45].



HisK 353.15KLysK 353.15K

Figure 4: Experimental solubility behaviour of carbon dioxide in 1 M aqueous potassium salt of *L*-histidine and data of 1 M aqueous potassium salt of lysinate [7].

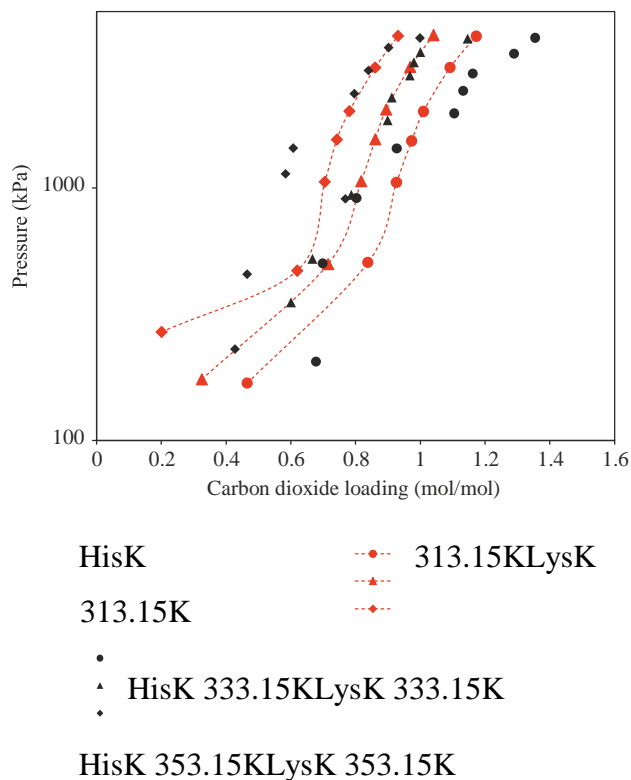


Figure 5: Experimental solubility behaviour of carbon dioxide in 2.5 M aqueous potassium salt of *L*-histidine and data of 2.5 M aqueous potassium salt of lysinate [7].

Table 1: Sources of experimental data for carbon dioxide solubility in various aqueous amino acid salt solutions.

Amino acid	Counterion	P (kPa)	T (K)	C (M)	Source
<i>L</i> -lysine	Potassium	150–4040	313.15–	1.0–2.5	[7] [8]
	Potassium	10	353.15	2.0–8.0	[9]
	Potassium	0.1–100	298.15–	0.2–3.0	[10]
	Potassium	0–45	323.15	0.5–2.5	
			298.15–		
			348.15		
			298.15–		
			313.15		
	Potassium	0.21–20.52	323.15–	2.317	[11]
			343.15		
	Potassium	0.47–115.26	298.15–	0.50–2.50	[12]
			353.15		
Potassium	0.21–20.81	313.15–	1.08–2.28	[13]	
		343.15			
Potassium	10	298.15–	2.0–8.0	[8] [9]	
Potassium	0.1–100	323.15	0.2–	[14]	
Potassium		298.15–	3.0	[15]	
		70	348.15	2.5	
			298.15–	0.5–3.0	
			313.15		
			285.15–		
<i>L</i> -proline			323.15		
	Potassium	2.90–928.60	313.15–	0.50–2.00	[16]
			353.15		
	Potassium	5.20–2583.90	293.15–	0.07–	[17]
			323.15	0.066	
	3-(methylamino)propylamine	10 0.20–	313.15–	2.5	[18]
<i>L</i> -alanine	Potassium	1041.70	353.15	1.50	[19]
			313.15–		
			353.15		
	Potassium	1–	313.15–	2.0–6.0	[20]
<i>L</i> -taurine	Potassium	1000	353.15	2.0–8.0	[8]
		10	298.15–		
			323.15		
	Sodium	100–2500	298.15–	1.0–3.0	[21]
	Sodium	0.1–200	313.15	1.0–2.0	[22]

Table 3: Values of constants for equation (25).

Equilibrium constant	a	b	c	Reference
k_c	-12092.1	-36.7816	235.482	[40]
k_d	-1243.7	-35.4819	220.067	[40]
k_e	-13445.9	-22.4773	140.932	[40]

Table 4: Values of constants k_a k_b for equations

and (25) and (26).

Amino acid salt	Equilibrium constant for a_i	deprotonation, k_a c_i	Equilibrium constant reversion, for carbamate k_b a_i	c_i
HisK	-20325.2711	-29.5371	-8306.3479	-46.2272

 f_a and f_b for

Table 5: Values of constants equations (28) and (29).

Amino acid salt	Correction parameter s_1	meter for deprotonation, s_2	on, f_a s_3	Correction parameter for reversion, s_4	for carbamate reversion, f_b s_5	s_6
HisK	1.1343	-0.0900	-0.0139	-0.5817	0.0013	-0.0402

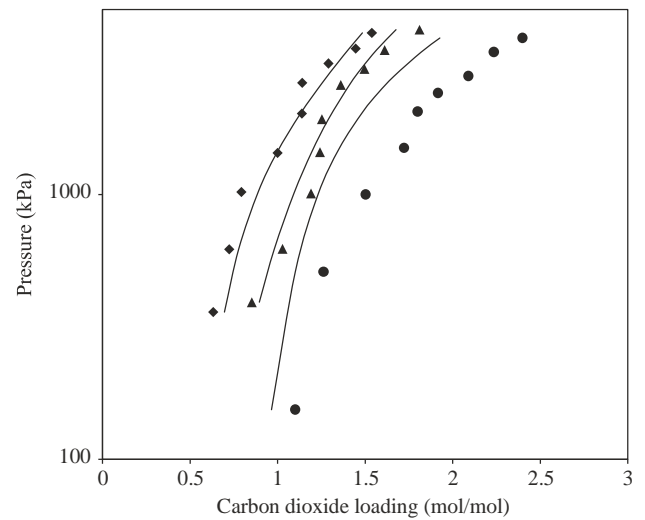
Table 6: Experimental carbon dioxide solubility in aqueous potassium salt of *L*-histidine.

Concentration (M)	Temperature (K)					
	313.15		333.15		353.15	
	P (kPa)	α (mol. (mol·HisK ⁻¹))	P (kPa)	α (mol. (mol·HisK ⁻¹))	P (kPa)	α (mol. (mol·HisK ⁻¹))
1.0	154.00	1.1007	392.60	0.8512	360.30	0.6319
	511.00	1.2621	623.90	1.0293	621.60	0.7239
	1001.0	1.5029	1011.7	1.1899	1023.4	0.7924
	1499.0	1.7222	1448.9	1.2419	1434.9	0.9988
	2055.0	1.8000	1923.9	1.2533	2021.6	1.1379
	2418.0	1.9153	2605.1	1.3601	2641.1	1.1405
	2801.0	2.0897	2992.6	1.4968	3123.5	1.2897
	3450.0	2.2356	3523.9	1.6111	3555.8	1.4457
	3901.0	2.3990	4192.6	1.8089	4078.9	1.5379
	2.5	205.10	0.6782	352.60	0.5996	230.10
502.60		0.6990	523.90	0.6665	455.10	0.4659
911.40		0.8031	942.60	0.7865	1136.4	0.5843
1432.6		0.9276	1861.4	0.8991	1436.4	0.6076

from these figures that carbon dioxide solubility in HisK solutions is higher when compared to LysK solutions at 313.15 K and almost similar at 353.15 K. Although amino acid salt of lysine was previously observed to have higher CO₂ absorption capacity than others in the group

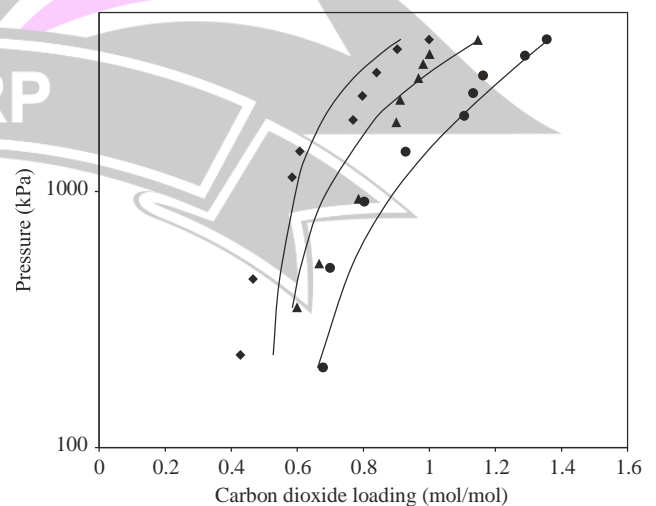
[7, 9, 46–48], it is explicated in this study that amino acid salt of histidine offered a comparable absorption capacity with the lysine. This can be attributed to the presence of an amide bond in the R-structure of *L*-histidine that presumably allows great capture of the carbon dioxide molecule. This means that *L*-histidine has comparatively high absorptive potential with lysine, allowing great separation of carbon dioxide in the carbon dioxide removal system. It is expected that the presence of amide bond shall also contribute to better kinetic rate for HisK solutions, since its structure resembles with piperazine-type promoters.

The modified Kent–Eisenberg model was used to correlate the experimental results of this study. Figure 6 shows the correlated CO₂ loading against the experimental results for carbon dioxide solubility in 1 molar HisK solutions. Similarly, Figure 7 illustrates the correlated CO₂ loading



HisK 313.15K HisK 353.15K
 • HisK 333.15K Model

Figure 6: Correlation of modified Kent–Eisenberg model against the experimental solubility of carbon dioxide in 1 M aqueous potassium salt of *L*-histidine (HisK).



HisK 313.15K HisK 353.15K
 • HisK 333.15K Model

Figure 7: Correlation of modified Kent–Eisenberg model against the experimental solubility of carbon dioxide in 2.5 M aqueous potassium salt of *L*-histidine (HisK).

against the experimental results for carbon dioxide solubility in 2.5 molar HisK solutions. The carbon dioxide loadings correlated by the model are slightly underpredicted at the low temperature (313.15 K) and overpredicted at the high temperature (353.15 K). This is attributed to the regression of temperature-dependent correction parameters (a_i and c_i) for equilibrium constants for deprotonation and carbamate formation and can be further improved by adding more correction factors by taking the square of temperature as the correction value. However, this will induce greater complexity in the model and tend to override the contribution of concentration and pressure-based correction factors. With respect to pressure, the model results are satisfactory as all the values along the pressure curve are well correlated. Similarly, the effect of concentration on the correlated values is well within the nonideality level assumed for the application of the Kent–Eisenberg model. Overall, the model results are in good agreement with the experimental CO₂

loading data. The results of the model are within the experimental errors of this study. The average absolute relative error (AARE%) was determined by
$$\text{AARE\%} = \frac{\sum_{i=1}^n |c_{\text{calc}} - c_{\text{expt}}|}{\sum_{i=1}^n c_{\text{expt}}} \cdot 100\% \quad (30)$$

The AARE% between the model predicted and experimental results was found to be 7.87%, indicating that the modified Kent–Eisenberg model shows satisfactory results and able to accurately predict the solubility of carbon dioxide at a wide range of process conditions with minimum computational complicity.

5. Conclusions

In this study, the VLE data of carbon dioxide-loaded aqueous solutions of potassium salt of *L*-histidine were measured using the HP-VLE apparatus. The experimental study was performed for a wide range of process parameters (temperature of 313.15 to 353.15 K, pressure of 150 to 4000 kPa, and solvent concentration of 1 and 2.5 molar). The experimental results show that the HisK solutions exhibited high absorption capacity of carbon dioxide, with intrinsic advantages of being negligibly volatile, resistant to degradation, and environmentally friendly. Moreover, a high carbon dioxide solubility

will limit the amount of solvent needed to capture a certain amount of carbon dioxide, thus reducing the amount of used pump power as well as decrease the heat requirements for regeneration [49, 50].

On the other hand, the HisK solutions also offered comparatively better carbon dioxide absorption potential than conventional solvent like MEA and potential amino acid salt solution like potassium lysinate. The experimental results provided a unique insight into the phase equilibrium behaviour of the studied $\text{CO}_2 + L\text{-histidine} + \text{H}_2\text{O}$ systems. The tested system has the ability to capture carbon dioxide and is a promising green solvent that can replace conventional alkanolamines. Moreover, the vapour-liquid equilibrium data for aqueous HisK solutions were correlated by a modified Kent–Eisenberg model. Remarkably, AARE% of 7.87% was generated. The model results were in excellent agreement with the experimental data of this study and indicate that the model can be effectually used for accurate prediction of VLE of the said system at other process conditions in simulation studies.

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