Short Articles

Measurement and Correlation of Vapor−Liquid Equilibrium for the Carbon Dioxide + 1-Butoxy Butane System

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In this paper, 1-butoxy butane was proposed as a novel absorbent for carbon dioxide capturing from the process gas stream with rich carbon dioxide, and the feasibility for further research and development was investigated through the study on the vapor−liquid equilibrium (VLE) for the carbon dioxide + 1-butoxy butane system. The VLE measurements were carried out with a set of high pressure devices connected online to a gas chromatograph under a range from (263.15 to 309.15) K and (0.5 to 3.0) MPa. The experimental results were given with expanded uncertainties, which were δ 0.03 K and δ 0.006 MPa. Then, on the basis of the Peng−Robinson (PR) equation of state (EoS), an isothermal correlation for experimental data and the interaction parameter k_{ij} was obtained. The average liquid absolute deviation is 0.0159, and the average vapor absolute deviation is 0.0025. It proves the validity to use the PR EoS for describing the VLE behavior for 1-butoxy butane + carbon dioxide system.

1. Introduction

The emission of carbon dioxide has been identified as the main contributor to global warming and climate change. Reduction of carbon dioxide emissions can be achieved by a variety of means. The challenge for modern industry is to find cost-effective solutions that will reduce the release of carbon dioxide into the atmosphere. At present, physical absorption has less energy consumption and is considered as an effective method.[1] However, in the recent decade, many scientists have being studying to search for new absorbents for improving the performance of the absorption process.[2−4] On the basis of the excess Gibbs function criterion for absorbent selection,[5] binary systems involving many kinds of solvents and carbon dioxide have been investigated in this work. The carbon dioxide + 1-butoxy butane system was chosen for this study.

The vapor−liquid equilibrium (VLE) behavior of the absorbent and carbon dioxide system might give information about whether the absorbent is suitable for carbon dioxide capture. However, the VLE data of carbon dioxide + dimethyl,[6] carbon dioxide + ethyl ether,[7] and carbon dioxide + isopropyl ether[8] had been published, respectively. Though the VLE data of carbon dioxide + 1-butoxy butane[9] had been reported at (312.65, 338.15, and 366.15) K, the VLE data of carbon dioxide + 1-butoxy butane has not been seen below 312.65 K.

The aim of this work is to investigate the feasibility for using 1-butoxy butane as a novel absorbent for carbon dioxide capture. The VLE data were measured at five temperatures of (263.15, 273.25, 289.35, 298.55, and 309.15) K, with the pressure range from (0.442 to 2.818) MPa. Experimental data were correlated with the Peng−Robinson (PR) equation of state (EoS).

2. Experimental Section

2.1. Chemicals. Carbon dioxide with a purity greater than mass fraction, which was 0.999, was purchased from Zhaoge Gas Co. 1-Butoxy butane was purchased from Tianjin Jinke Fine Chemical Co.; the purity was greater than mass fraction, which was 0.99. These chemicals were used without further purification.

2.2. Apparatus. A detailed description of the VLE experimental apparatus is presented in an earlier paper.[8] The apparatus used in this work was based on the static−analytical method with liquid and vapor phase sampling of the online mode. However, some improvements have been done in this study. The schematic diagram of the experiment apparatus is shown in Figure 1. A six-way valve was used to control the injection volume. As a result, the repeatability is significantly improved. The volume of the stainless steel equilibrium cell was changed from (120 to 160) mL to improve the equilibrium performance while sampling; a thermal regulator (model LC-6) was used, which was supplied by Julabo Co. The temperature uncertainty of the bath was upgraded from (0.1 to 0.03) K; a chilled unit (Eyela Co.) was used to ameliorate low temperature performance of the experimental system.

2.3. Reliability Validation of Improved Apparatus. The phase behavior of the carbon dioxide + ethanol system was experimentally obtained. The results compare very well with those obtained by Secuianu et al.[10] The average relative deviation is 0.0033, and the maximum relative deviation is 0.0161, which shows that the reliability of the apparatus is confirmed. The experimental data is shown in Table 1.

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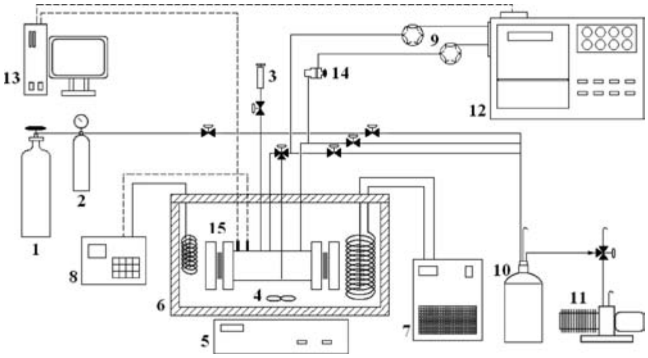

Figure 1. Schematic diagram of the experimental apparatus: 1, gas cylinder; 2, gas storage tank; 3, liquid injector; 4, rotor magnetic stirrer; 5, magnetism mixer; 6, constant temperature water bath; 7, refrigerator; 8, temperature controller; 9, six-way valve; 10, cushion tank; 11, vacuum pump; 12, gas chromatography; 13, computer; 14, decompression valve; 15, equilibrium cell.

Table 1. Experimental Mole Fraction of Component 1 in the Liquid Phase, x_1, and in the Vapor Phase, y_1, at the Pressure, *P*, and Temperature, *T*, for the Binary System Carbon Dioxide (1) + Ethanol (2)

item	$T = 293.15$ K			$T = 303.15$ K		
p^{exp}/MPa	0.75	1.60	2.22	0.95	2.00	3.05
x_1^{exp}	0.0555	0.1292	0.1755	0.0606	0.1355	0.2185
y_1^{exp}	0.9886	0.9948	0.9972	0.9879	0.9940	0.9972

3. Equation of State

The PR EoS[11] has been widely used and regarded as a better way to the system at high pressure. It was also adopted in this work, using the classical and Wong−Sandler[12] mixing rule. The critical properties and acentric factors used in the PR EoS were selected from literature.[13]

4. Results and Discussion

4.1. Experimental Data. In this work, the $p-T-x-y$ data for the carbon dioxide + 1-butoxy butane system were measured at five temperatures (263.15, 273.25, 289.35, 298.55, and 309.15) K, and six pressures (0.5, 1.0, 1.5, 2.0, 2.5, and 3.0) MPa. The measured equilibrium compositions at various temperature and pressure states for this binary mixture are shown in the columns of Table 2 with the symbols x_1^{exp} and y_1^{exp}.

The results of the liquid and vapor experimental data are also illustrated in Figures 2 and 3, respectively. It can be found from Figure 2 that the liquid mole fraction of carbon dioxide in 1-butoxy butane increases significantly with increased pressure and increases with decreased temperature. In the range of experimental temperature, the liquid mole fraction of carbon dioxide changes greatly in a range of 0.11 to 0.70, especially under low temperatures. For example, when the pressure is changed from (0.5 to 2.0) MPa, the liquid mole fraction of carbon dioxide is changed from 0.11 to 0.33 at high temperatures, but it is changed from 0.15 to 0.54 at low temperatures.

It can be found from Figure 3 that the vapor mole fraction of 1-butoxy butane is very small; it changes from 0.002 to 0.006 in the experimental condition. The variation general trend of the vapor mole fraction of carbon dioxide is similar with Figure 2, but the vapor mole fraction of carbon dioxide changes a little, from about 0.994 to 0.998 in the experimental condition.

4.2. VLE Deviation. The deviations of the calculated results by the PR EoS from the experimental data are shown in Figures 2 and 3. It can be seen that the calculation data agree well with the experimental results. The average liquid absolute deviation is 0.0159, and the average vapor absolute deviation is 0.0025. So, the PR EOS is appropriate to describe the VLE data of the carbon dioxide + 1-butoxy butane system.

Table 2. Mole Fraction of Component 1 in the Liquid Phase, x_1, and Mole Fraction of Component 1 in the Vapor Phase, y_1, at the Pressure, *p*, and Temperature, *T*, for the Binary System Carbon Dioxide (1) + 1-Butoxy Butane (2)

p/MPa	x_1^{exp}	y_1^{exp}
	$T = 263.15$ K	
0.442	0.1592	0.9966
0.771	0.2628	0.9968
1.192	0.3742	0.9969
1.652	0.4978	0.9972
2.002	0.6042	0.9975
2.322	0.7006	0.9977
	$T = 273.25$ K	
0.544	0.1539	0.9960
1.115	0.2858	0.9963
1.527	0.3878	0.9964
1.875	0.4669	0.9968
2.453	0.6069	0.9970
2.815	0.6897	0.9972
	$T = 289.35$ K	
0.506	0.1190	0.9955
1.003	0.2200	0.9957
1.472	0.3188	0.9959
2.002	0.4101	0.9961
2.310	0.4705	0.9962
2.685	0.5355	0.9964
	$T = 298.55$ K	
0.612	0.1235	0.9951
0.988	0.1977	0.9953
1.564	0.3172	0.9955
2.005	0.3908	0.9957
2.431	0.4415	0.9958
2.818	0.4989	0.9959
	$T = 309.15$ K	
0.663	0.1166	0.9945
1.318	0.2372	0.9947
1.488	0.2673	0.9949
1.934	0.3386	0.9951
2.395	0.3988	0.9952
2.810	0.4548	0.9955

4.3. Interaction Parameter. The interaction parameter k_{ij} was an important system characteristic parameter to predict and research the VLE behavior using the PR EoS. On the basis of the PR EoS, the VLE experimental data were fitted by computer programming using the least-squares method. The interaction parameter k_{ij} was obtained, which is 0.0418.

5. Conclusion

In this paper, the VLE behavior of carbon dioxide + 1-butoxy butane system was studied with a high-pressure static apparatus.

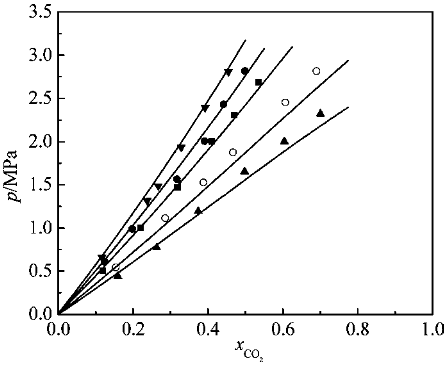

Figure 2. Variation of carbon dioxide in liquid phase at different temperatures: ▲, 263.15 K; ○, 273.25 K; ■, 289.35 K; ●, 298.55 K; ▼, 309.15 K; solid line, calculated results.

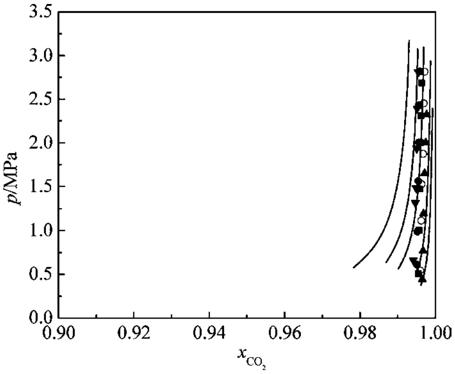

Figure 3. Variation of carbon dioxide in vapor phase at different temperatures: ▲, 263.15 K; ○, 273.25 K; ■, 289.35 K; ●, 298.55 K; ▼, 309.15 K; solid line, calculated results.

To verify the accuracy of the experimental equipment, the VLE data of carbon dioxide + ethanol binary system were measured. The maximum relative deviation and the average relative deviation between the literature data and the experimental data are 0.0161 and 0.0033, respectively.

A set of new VLE experimental data for the carbon dioxide + 1-butoxy butane system was measured at temperatures of (263.15, 273.25, 289.35, 298.55, and 309.15) K and pressures of (0 to 3) MPa.

The experimental equilibrium data for this system was correlated with the PR EoS using the Wong−Sandler mixing rules, and the interaction parameter k_{ij} was obtained, which is 0.0418. The average absolute deviations of liquid and vapor between the calculated results by the PR EoS and the experimental data are 0.0159 and 0.0025. It proves that the PR EoS is suitable to describe the VLE behavior of the carbon dioxide + 1-butoxy butane system.

The study result, for example, the liquid mole fraction of carbon dioxide, is 0.7006 at a temperature of 263.15 K and pressure of 2.322 MPa and shows that 1-butoxy butane has significant meaning for further research and development as a novel absorbent for carbon dioxide capturing.

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