Bubble-point measurement for the CO_2+diethylene glycol diacrylate and CO_2+diethylene glycol dimethacrylate systems at high pressure

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Abstract−Pressure-composition isotherms are measured by using a static apparatus for the phase behavior data for the CO_2+diethylene glycol diacrylate (DEGDA) and CO_2+diethylene glycol dimethacrylate (DEGDMA) systems. The experiments are performed at five temperatures of (313.2 to 393.2) K and pressures up to 28.3 MPa. The solubility of CO_2 for the two systems decreases as the temperature increases at a fixed pressure. The CO_2+DEGDA and CO_2+DEGDMA systems exhibit type-I phase behavior. The experimental results for the CO_2+DEGDA and CO_2+DEGDMA systems are correlated with Peng-Robinson equation of state using a mixing rule.

Key words: Carbon Dioxide, Diethylene Glycol Diacrylate, Diethylene Glycol Dimethacrylate, Peng-Robinson EOS, Phase Behavior

INTRODUCTION

Diethylene glycol diacrylate (DEGDA) and diethylene glycol dimethacrylate (DEGDMA) have characteristics such as adhesive force, chemical resistance, low viscosity and low volatility. Therefore, both are mainly used as an adhesive, sealant, coating, elastomer, photoresist and solder resist in the fields utilizing those characteristics [1], while ethylene glycol dimethacrylate is used as a functional monomer for polymers and as a crosslinking agent between the molecular chains of polymers [2].

Supercritical carbon dioxide ($scCO_2$) has become a focus of attention as a useful alternative to toxic or volatile organic solvents for polymer synthesis and processing [3-5]. The $scCO_2$ possesses many advantages, such as being an environment friendly solvent due to its lower toxicity, lower inflammability, chemically inert nature, and natural abundance. It also possesses high diffusivity and low solubility for high molar mass or polar monomeric materials due to its low dielectric constant and lack of dipole moment [6]. In addition, $scCO_2$ causes polymer to swell. Therefore, a separation process using $scCO_2$ can be used to remove the residual and unreacted monomers on the inside of the synthesis polymer. Particularly, high pressure phase behavior data of binary mixtures containing $scCO_2$ are required to design a plant and operate the supercritical fluid extraction process.

The phase behavior experimental data for the ethylene glycol dimethacrylate in supercritical carbon dioxide were reported at 313.2 K and 393.2 K and pressure up to 22 MPa by Kim et al. [7]. The phase behavior of CO_2+neopentyl glycol diacrylate and CO_2+neopentyl glycol dimethacrylate systems were studied by Jang et al. [8]. Recently, the phase behavior for CO_2+tri-ethylene glycol dimethacrylate and CO_2+tetra-ethylene glycol dimethacrylate has been reported at temperatures ranging from 313.2 to 363.2 K and at pressures from 4 to 27 MPa by Cho et al. [9]

The purpose of this research was to obtain the experimental data

of (CO_2+DEGDA) and (CO_2+DEGDMA) mixture, by looking into mixtures of carbon dioxide with two components in high pressures. The experimental data of (CO_2+DEGDA) and (CO_2+DEGDMA) systems obtained in this work were correlated with the Peng-Robinson equation of state (PR-EOS) [10] using a van der Waals one-fluid mixing rule that includes two adjustable parameters. The critical pressure, critical temperature and acentric factor of two components were estimated by the Joback-Lyderson method [11] with group-contributions, while the vapor pressure is estimated by the Lee-Kesler method [11].

EXPERIMENTAL SECTION

1. Materials

The diethylene glycol diacrylate (DEGDA) [mass fraction purity >0.900, CAS RN 4074-88-8, $(H_2C=CHCO_2CH_2CH_2)_2O$] and diethylene glycol dimethacrylate (DEGDMA) [mass fraction purity>0.950, CAS RN 2358-84-1, $(H_2C=C(CH_3)CO_2CH_2CH_2)_2O$] used in this work were obtained from Scientific Polymer Products, Inc. Both components were used without further purification in the experiments. Carbon dioxide (mass fraction purity>0.998) was obtained from Daesung Industrial Gases Co. and used as received.

2. Apparatus and Procedure

Fig. 1 shows a schematic diagram of the experimental apparatus, variable-volume view cell used for the phase equilibrium measurement [12]. It is used to obtain the bubble point, critical point and dew point of CO_2+DEGDA and CO_2+DEGDMA binary mixture systems. The high-pressure phase behavior data obtained from this experiment have been reported [13,14].

The main components of the experimental systems are high-pressure generator, variable volume view cell and visual apparatus. The variable volume view cell (6.2 cm O.D×1.59 cm I.D, a working volume of ~28 cm³) at a high-pressure is capable of operating up to 70 MPa pressure. A sapphire window was fitted in the front part of the cell to observe the phases. Before the monomer is loaded into the cell to within ±0.001 g using a syringe, the cell is purged several times with nitrogen and carbon dioxide to remove trace of air and

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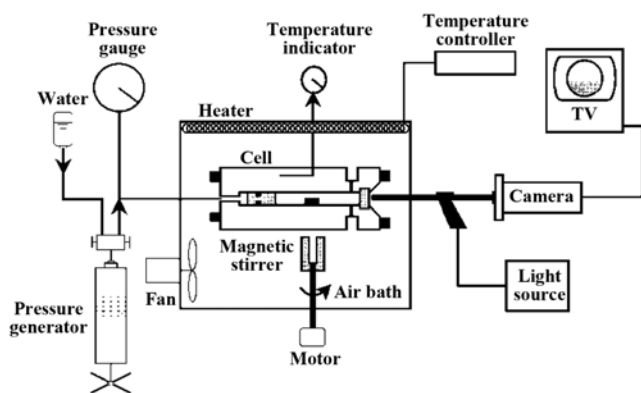E-mail: hsbyun@chonnam.ac.kr

Fig. 1. Schematic diagram of the experimental apparatus.

organic solvents. Typically, supercritical carbon dioxide is added to the cell to within ±0.002 g using a high pressure bomb. The mixture in the view cell was compressed to the desired pressure by moving a piston located within the cell. The piston (2.54 cm length) was moved using water pressure by a high pressure generator (HIP, model 37-5.75-60). The pressure of mixture was measured by a Heise gauge (Dresser Ind., model CM-53920, 0 to 34.0 MPa) accurate to ±0.02 MPa. The temperature in the cell, which is maintained to within ±0.2 K, was measured using a platinum-resistance thermometer (Thermometrics Corp., Class A) connected to a digital multimeter (Yokogawa, model 7563, accurate to within ±0.005%). The mixture inside the cell was viewed on a video monitor using a camera coupled to a borescope (Olympus Corp., model F100-038-000-50) placed against the outside of the sapphire window.

At the desired temperature and pressure, the mixture in the cell was compressed to a single phase at high-pressure, and it was maintained in the single phase for at least 30-40 min for the cell to reach phase equilibrium. A bubble point pressure is obtained when small bubbles appear first in the cell, while a dew point is obtained if a fine mist appears in the cell. Critical points are obtained by adjusting the temperature and pressure of the mixture until critical opalescence is observed along with equal liquid and vapor volume upon the formation of the second phase. The vicinity region of mixture-critical point is sensitive to a slight change in either pressure or temperature. A slight change in pressure (or temperature) for the mixture-critical point causes a dramatic change in the amount of one phase or two phases present in the cell [6].

THERMODYNAMIC MODELS

In this study, the experimental phase behavior data are correlated

with the Peng-Robinson equation of state (PR-EOS) [10]. PR-EOS is expressed as follows:

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

$$a(T) = 0.457235 \frac{R^2 T_c^2}{p_c} \alpha(T) \tag{2}$$

$$b(T_c) = 0.077796 \frac{RT_c}{p_c} \tag{3}$$

$$\alpha(T) = [1 + K(1 - T_r^{0.5})]^2 \tag{4}$$

$$K = 0.37464 + 1.54226\omega - 0.26992\omega^2 \tag{5}$$

where, p_c and T_c are the critical pressure and temperature of pure components, and ω is the acentric factor. The van der Waals one-fluid mixed rules are expressed as follows:

$$a_m = \sum_i \sum_j x_i x_j a_{ij} \tag{6}$$

$$a_{ij} = \sqrt{a_{ii} a_{jj}}(1 - k_{ij}) \tag{7}$$

$$b_m = \sum_i \sum_j x_i x_j b_{ij} \tag{8}$$

$$b_{ij} = \frac{b_{ii} + b_{jj}}{2}(1 - \eta_{ij}) \tag{9}$$

These two binary interaction parameters (k_{ij}, η_{ij}) were determined by regressing experimental data from the PR-EOS. Objection function (OBF) [15] and root mean squared relative deviation (RMSD) percent of this calculation were defined as follows:

$$OBF = \sum_i^N \left(\frac{p_{exp} - p_{cal}}{p_{exp}} \right)^2 \tag{10}$$

$$RMSD(\%) = \sqrt{\frac{OBF}{ND}} \times 100 \tag{11}$$

ND in Eq. (11) means the number of data points. We used the Marquardt algorithm [15] to optimize objection function. All isotherms were included for calculation. Critical constants (T_c, P_c) and acentric factor [11] for PR-EOS are listed in Table 1. In the case of DEGDA and DEGDMA, T_c and P_c were estimated with Joback-Lyderson [11] method, and acentric factor (ω) was estimated with Lee-Kesler method [11]. The boiling points of DEGDA [16] and DEGDMA were obtained from the literature [17].

RESULTS AND DISCUSSION

High pressure phase behavior data of binary for the CO_2+DEGDA

Table 1. Pure component properties for the Peng-Robinson equation of state

Compounds	M_w	Structure	T_b/K	T_c/K	p_c/MPa	ω
Carbon dioxide	44.01	O=C=O		304.2	7.38	0.225
Diethylene glycol diacrylate	214.24		564.1	745.6	2.27	0.797
Diethylene glycol dimethacrylate	242.27		596.0	775.4	1.92	0.818

Table 2. Experimental data of bubble-point, critical-point and dew-point for the CO$_2$+diethylene glycol diacrylate system

Diethylene glycol diacrylate mole fraction	p/MPa	Transition[a]
T=313.2 K		
0.044	11.09	BP
0.059	11.14	BP
0.077	11.14	BP
0.091	11.05	BP
0.115	11.07	BP
0.133	10.83	BP
0.189	10.21	BP
0.259	9.84	BP
0.333	8.97	BP
0.401	8.22	BP
0.455	7.67	BP
0.528	6.91	BP
0.594	6.31	BP
T=333.2 K		
0.044	16.72	BP
0.059	17.07	BP
0.077	17.00	BP
0.091	17.11	BP
0.115	16.86	BP
0.133	16.24	BP
0.189	14.24	BP
0.259	13.25	BP
0.333	11.28	BP
0.401	10.24	BP
0.455	9.48	BP
0.528	8.17	BP
0.594	7.76	BP
T=353.2 K		
0.044	21.55	DP
0.059	21.89	CP
0.077	21.89	BP
0.091	21.83	BP
0.115	21.48	BP
0.133	21.00	BP
0.189	18.52	BP
0.259	16.67	BP
0.333	13.41	BP
0.401	12.10	BP
0.455	10.93	BP
0.528	9.41	BP
0.594	8.66	BP

Table 2. Continued

Diethylene glycol diacrylate mole fraction	p/MPa	Transition[a]
T=373.2 K		
0.044	25.07	DP
0.059	25.35	DP
0.077	25.41	BP
0.091	25.41	BP
0.115	25.14	BP
0.133	24.83	BP
0.189	22.21	BP
0.259	19.76	BP
0.333	15.85	BP
0.401	13.86	BP
0.455	12.45	BP
0.528	10.45	BP
0.594	9.21	BP
T=393.2 K		
0.044	27.90	DP
0.059	28.26	DP
0.077	28.31	CP
0.091	28.17	BP
0.115	28.07	BP
0.133	27.66	BP
0.189	25.48	BP
0.259	22.03	BP
0.333	18.14	BP
0.401	15.59	BP
0.455	13.76	BP
0.528	11.55	BP
0.594	10.10	BP

[a]BP: Bubble-point, CP: Critical-point, DP: Dew-point

and CO$_2$+DEGDMA systems were measured and are presented in Table 2 and Table 3. The experimental uncertainty was estimated to within ±0.03 MPa and ±0.2 K for a given loading of the cell. The combined expanded uncertainties of DEGDA and DEGDMA mole fractions are estimated to be ±0.0008 (coverage factor, k=2) [18].

Fig. 2 shows the experimental pressure- composition (P-x) isotherms at T=313.2, 333.2, 353.2, 373.2 and 393.2 K, and pressure up to 28.3 MPa for the CO$_2$+DEGDA and CO$_2$+DEGDMA systems. Three phases were not observed at any five temperatures. The P-x isotherms shown in Fig. 2 are consistent with those expected for a type-I system where a maximum occurs in the critical mixture curve. The solubility of CO$_2$ in the liquid phase decreases as temperatures shift higher under constant pressure.

The experimental data obtained in this study were correlated with the PR-EOS using the van der Waals one-fluid mixing rule including two binary interaction parameters (k$_{ij}$, η_{ij}).

Fig. 3 represents the comparison between experimental data and calculated values obtained using PR-EOS of CO$_2$+DEGDA (the top) and CO$_2$+DEGDMA (the bottom) systems at a temperature of 353.2 K. The binary interaction parameters of PR-EOS were fitted by the experimental data at 353.2 K. The values of optimized parameters of PR-EOS for the CO$_2$+DEGDA (the top) and CO$_2$+DEGDMA (the bottom) systems are k$_{ij}$=0.035 and η_{ij}=−0.035 (RMSD=2.87%, data point no.=13), and k$_{ij}$=0.028 and η_{ij}=−0.031 (RMSD=2.53%, data point no.=14), respectively.

Fig. 2 (the top) compares the experimental data with calculated pressure-composition (P-x) isotherms at temperatures of (313.2, 333.2, 353.2, 373.2 and 393.2) K for the CO$_2$+DEGDA system using

Table 3. Experimental data of bubble-point, critical-point and dew-point for the CO₂+diethylene glycol dimethacrylate system

Diethylene glycol dimethacrylate mole fraction	p/MPa	Transition[a]
T=313.2 K		
0.045	10.21	BP
0.061	10.45	BP
0.072	10.52	BP
0.091	10.56	BP
0.106	10.59	BP
0.121	10.24	BP
0.150	10.10	BP
0.175	9.62	BP
0.247	9.03	BP
0.319	8.24	BP
0.403	7.55	BP
0.470	6.93	BP
0.542	6.34	BP
0.617	5.80	BP
T=333.2 K		
0.045	15.55	DP
0.061	15.83	DP
0.072	16.07	BP
0.091	16.21	BP
0.106	15.94	BP
0.121	15.48	BP
0.150	14.62	BP
0.175	13.55	BP
0.247	11.66	BP
0.319	10.29	BP
0.403	9.14	BP
0.470	7.97	BP
0.542	7.21	BP
0.617	6.35	BP
T=353.2 K		
0.045	19.83	DP
0.061	20.41	DP
0.072	20.48	BP
0.091	20.66	BP
0.106	20.41	BP
0.121	19.79	BP
0.150	18.79	BP
0.175	17.17	BP
0.247	14.79	BP
0.319	12.66	BP
0.403	10.55	BP
0.470	9.24	BP
0.542	8.17	BP
0.617	6.86	BP

Table 3. Continued

Diethylene glycol dimethacrylate mole fraction	p/MPa	Transition[a]
T=373.2 K		
0.045	23.38	DP
0.061	23.97	DP
0.072	24.28	CP
0.091	24.21	BP
0.106	24.00	BP
0.121	23.52	BP
0.150	22.45	BP
0.175	21.00	BP
0.247	17.79	BP
0.319	14.66	BP
0.403	12.31	BP
0.470	10.59	BP
0.542	9.21	BP
0.617	7.38	BP
T=393.2 K		
0.045	26.03	DP
0.061	26.66	DP
0.072	26.79	DP
0.091	26.97	CP
0.106	26.83	BP
0.121	26.57	BP
0.150	25.41	BP
0.175	23.83	BP
0.247	19.56	BP
0.319	16.86	BP
0.403	13.69	BP
0.470	11.83	BP
0.542	10.10	BP
0.617	7.83	BP

[a]BP: Bubble-point, CP: Critical-point, DP: Dew-point

the optimized values k_{ij}=0.035 and η_{ij}=−0.035 determined at 353.2 K. As shown in Fig. 2, experimental data were obtained with the PR-EOS using adjustable mixture parameters for the CO₂+DEGDA

system (RMSD=7.42%, data point no.=65). Fig. 2 (bottom) plotted the experimental data to show the comparison of calculated P-x isotherms at temperatures of (313.2, 333.2, 353.2, 373.2 and 393.2) K for the CO₂+DEGDMA system using the optimized values k_{ij}=0.028 and η_{ij}=−0.031 determined at 353.2 K, which were obtained with the PR-EOS using adjustable mixture parameters for the CO₂+DEGDMA system (RMSD=8.32%, data point no.=70). The calculations have high error. However, the optimum parameters of two systems were correlated at each temperature as shown in Fig. 4.

Fig. 4 plots the pressures against mole fraction to illustrate the comparison of the experimental data (symbols) of CO₂+DEGDA (the top) and CO₂+DEGDMA (the bottom) systems with calculations (solid lines) obtained with the PR-EOS at each temperature. As shown in Fig. 4, the calculated curves were plotted using optimized values determined at each temperature. RMSD at five temperatures (313.2, 333.2, 353.2, 373.2 and 393.2) K for the CO₂+DEGDA (the top) system was 4.67%, 2.04%, 2.87%, 2.44% and 2.05%, respectively. And RMSD at five temperatures (313.2, 333.2, 353.2, 373.2 and 393.2) K for the CO₂+DEGDMA (the bottom)
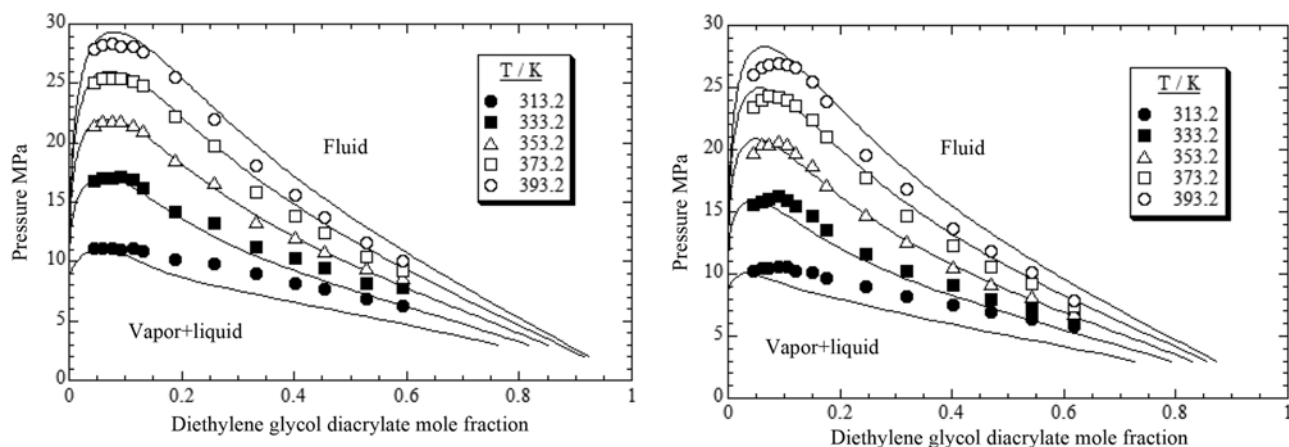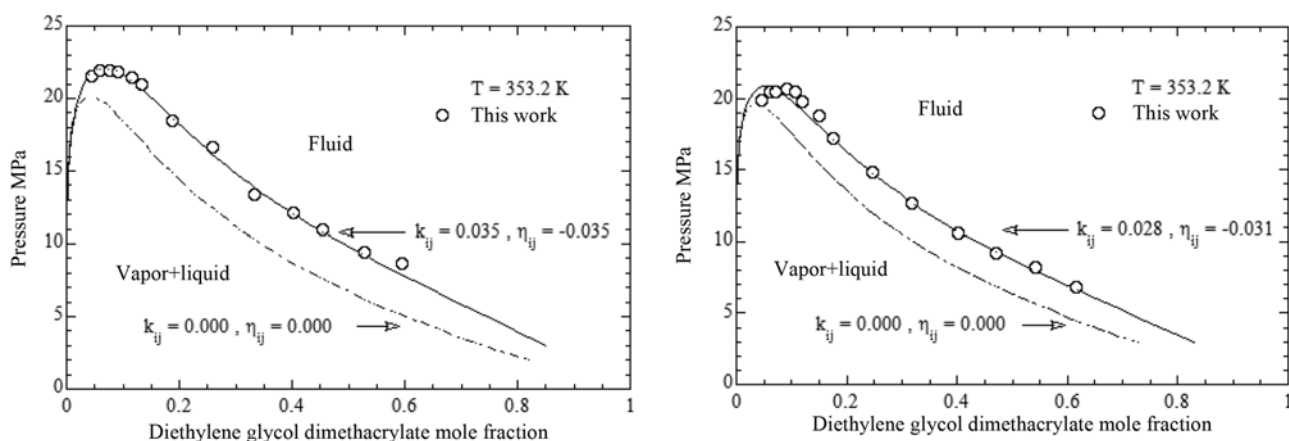
Fig. 2. Plot of pressure against mole fraction to illustrate the comparison of the experimental data (symbols) for the CO₂+diethylene glycol diacrylate (the top) and CO₂+diethylene glycol dimethacrylate (the bottom) systems with calculations (solid lines) obtained with the Peng-Robinson equation of state k_{ij} equal to 0.033 and η_{ij} equal to −0.035 (CO₂+diethylene glycol diacrylate), and k_{ij} equal to 0.028 and η_{ij} equal to −0.031 (CO₂+diethylene glycol dimethacrylate). ●, 313.2 K; ■, 333.2 K; △, 353.2 K; □, 373.2 K; ○, 393.2 K.

Fig. 3. Plot of pressure against mole fraction to illustrate the comparison of experimental data (symbols) for the CO₂+diethylene glycol diacrylate (the top) and CO₂+diethylene glycol dimethacrylate) (the bottom) with calculation obtained from the Peng-Robinson equation of state by k_{ij} and η_{ij} set equal to zero (dashed lines), and k_{ij}=0.033 and η_{ij}=−0.035 (CO₂+diethylene glycol diacrylate) and k_{ij}=0.028 and η_{ij}=−0.031 (CO₂+diethylene glycol dimethacrylate) (solid lines) at 353.2 K.

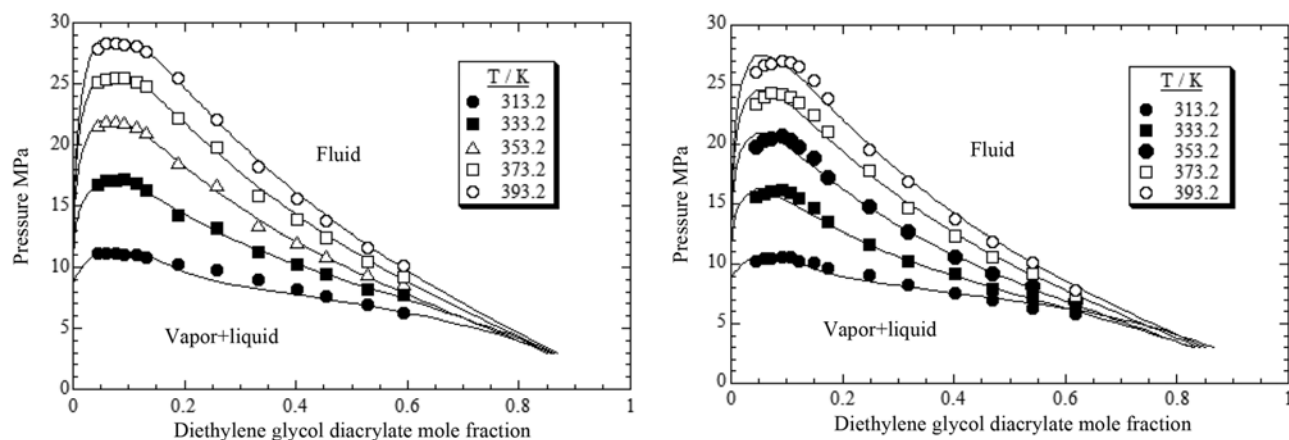**Fig. 4. Plot of pressure against mole fraction that compares the experimental data (symbols) of the CO₂+diethylene glycol diacrylate (the top) and CO₂+diethylene glycol dimethacrylate (the bottom) systems with calculations (solid lines) obtained with the Peng-Robinson equation of state using optimum parameters (k_{ij} and η_{ij}) at each temperatures: ●, 313.2 K; ■, 333.2 K; △, 353.2 K; □, 373.2 K; ○, 393.2 K.**
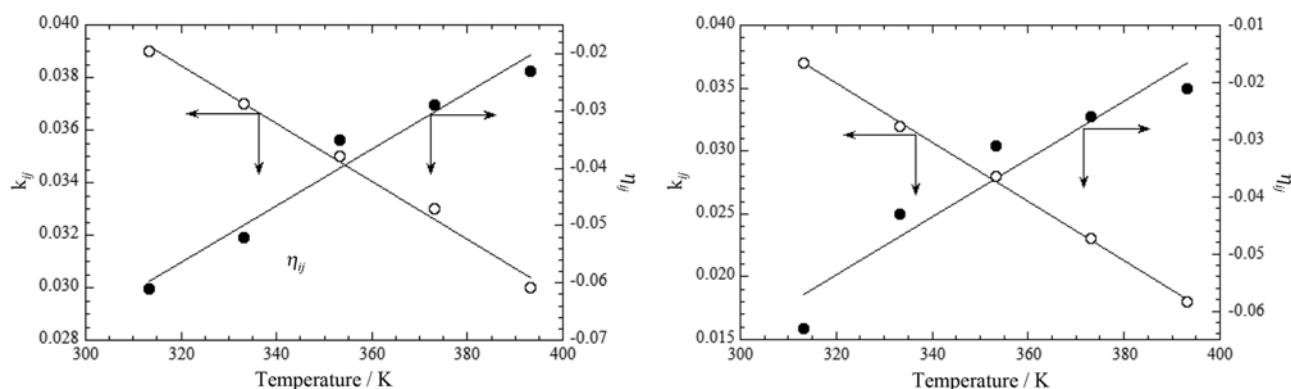
Fig. 5. Plot of k_{ij} and η_{ij} parameters against temperature for the CO_2+diethylene glycol diacrylate (the top) and CO_2+diethylene glycol dimethacrylate (the bottom) systems with the Peng-Robinson equation of state. The equation of the fitting line for the CO_2+diethylene glycol diacrylate (the top) and CO_2+diethylene glycol dimethacrylate (the bottom) is $k_{ij}=0.073652-0.00011T$ and $\eta_{ij}=-0.21483+0.000495T$ (313.2 K$\leq$T$\leq$393.2 K) [the top], and $k_{ij}=0.1106-0.000235T$ and $\eta_{ij}=-0.21517+0.000505T$ (313.2 K$\leq$T$\leq$393.2 K) [the bottom].
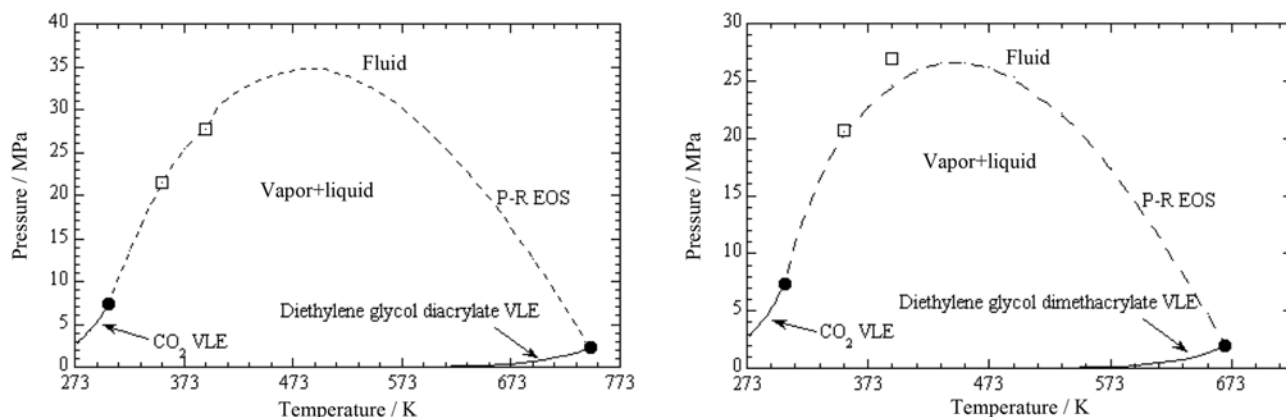

Fig. 6. Plot of pressure against temperature for the CO_2+diethylene glycol diacrylate (the top) and CO_2+diethylene glycol dimethacrylate (the bottom) systems. Solid lines and circles represent the vapor-liquid lines and critical points for pure CO_2 and diethylene glycol diacrylate (the top) or diethylene glycol dimethacrylate (the bottom). Open squares are critical points determined from isotherms measured in this work. Dashed lines represent calculations obtained using the Peng-Robinson equation of state with $k_{ij}=0.035$ and $\eta_{ij}=-0.035$ (the top), and $k_{ij}=0.028$ and $\eta_{ij}=-0.031$ (the bottom).

system was 3.60%, 2.84%, 2.53%, 2.30% and 4.26%, respectively. The comparison between the experimental data and calculated curves shows a good agreement at five temperatures. According to calculated results, the critical mixture curve is type-I.

Fig. 5 plots k_{ij} and η_{ij} parameters, which were obtained from PR-EOS against temperature for the CO_2+DEGDA (the top) and CO_2+DEGDMA (the bottom) systems at each temperature. The equations of parameter for the fitting line were $k_{ij}=0.073652-0.00011T$ and $\eta_{ij}=-0.21483+0.000495T$ from 313.2 K to 393.2 K in the case of CO_2+DEGDA (above) and $k_{ij}=0.1106-0.000235T$ and $\eta_{ij}=-0.21517+0.000505T$ at temperature range from 313.2 K to 393.2 K in the case of CO_2+DEGDMA (bottom) systems.

Fig. 6 compares the mixture-critical curves of the experimental data with calculated values by the PR-EOS for the CO_2+DEGDA (the top) and CO_2+DEGDMA (the bottom) systems using two interaction parameters (k_{ij} and η_{ij}) optimized at 353.2 K. The calculated mixture-critical curve is type-I region. As shown in Fig. 6, the solid lines signify the vapor pressure for pure carbon dioxide, DEGDA or DEGDMA. The vapor pressure of pure DEGDA and DEGDMA

was obtained by Lee-Kesler method. The solid circles signify the critical point for pure CO_2 and DEGDA, CO_2 and DEGDMA. The upper region of the dashed line is single phase (fluid), the lower region of it vapor-liquid (two phases). The dashed lines represent the calculated values obtained from the PR-EOS, with $k_{ij}=0.035$ and $\eta_{ij}=-0.035$ (CO_2+DEGDA) and $k_{ij}=0.028$ and $\eta_{ij}=-0.031$ (CO_2+DEGDMA), respectively. The open squares are for the mixture-critical points determined from isotherms measured in this experiment.

CONCLUSIONS

The pressure-composition (P-x) isotherm data of CO_2+DEGDA and CO_2+DEGDMA systems have been studied using a variable-volume view cell apparatus at temperatures ranging from 393.2 K to 313.2 and pressure up to 28.3 MPa. These two systems exhibit type-I phase behavior and do not exhibit three phase at any five temperatures. The PR-EOS is able to predict the phase behavior for the two systems using the binary mixture interaction parameters (k_{ij} and η_{ij}) obtained at 353.2 K. The comparison between experimen-

tal data and calculated curves reaches reasonably good agreement with PR-EOS using adjustable optimized parameters obtained at each temperature. RMSD at five temperatures for two systems shows the deviation ranging from 2.04% to 4.67% for the CO_2+DEGDA and from 2.30% to 4.26% for the CO_2+DEGDMA systems.

ACKNOWLEDGEMENTS

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