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Solubilities of *N*-phenylacetamide, 2-methyl-*N*-phenylacetamide and 4-methyl-*N*-phenylacetamide in supercritical carbon dioxide

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Abstract

The solubilities of *N*-phenylacetamide, 2-methyl-*N*-phenylacetamide and 4-methyl-*N*-phenylacetamide in supercritical carbon dioxide were measured using a semi-flow apparatus. The experimental data were taken at 308.2, 318.2 and 328.2 K, and over the pressure range from 10 to 22 MPa. A plug flow fluid–solid mass transfer model was applied under the experimental conditions, and it showed that the corresponding solid solubility data were measured in the steady state region with low mass transfer effects. The experimental solid solubility data were then correlated using the Peng–Robinson and the Soave–Redlich–Kwong equations of state with van der Waals mixing rules. These data were also correlated with the semi-empirical equation presented by Chrastil, or that presented by Mendez-Santiago and Teja. The solid solubility data calculated from all the correlation models with optimally fitted parameters yielded absolute average deviation of 6%.
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Keywords: Solid solubility; Supercritical CO_2; Experimental data

1. Introduction

Supercritical fluid technology is becoming increasingly important in diversified fields of extraction, reaction, particle formation and materials processing [1,2]. Solid solubility data in supercritical fluids are among the most important thermophysical properties that are essential to the efficient design of supercritical processes. Solid solubility data in supercritical CO_2 have been reviewed by several authors [3–6], who have concluded that more experimental data and proper correlation models for specialty chemicals are still needed.

We have measured the solid solubility of various aromatic compounds in supercritical CO_2 [7]. In this study, we used the similar semi-flow apparatus to measure the equilibrium solubility of *N*-phenylacetamide, 2-methyl-*N*-phenylacetamide and 4-methyl-*N*-phenylacetamide in supercritical CO_2 at temperatures of 308.2, 318.2 and 328.2 K over the pressure range 10–22 MPa. 2-Methyl-*N*-phenylacetamide and 4-methyl-*N*-phenylacetamide are isomers which were used as dyestuff. *N*-Phenylacetamide was used in organic synthesis and the pharmaceutical industry. All three selected polar compounds consist

of the $NHCOCH_3$ functional group. As far as we know, no solid solubility data regarding these compounds have yet been reported in literature. In this study, we therefore report novel data for further applications and modeling. A fluid–solid mass transfer model investigated by Abaroudi et al. [8] was applied under our experimental conditions. It was used to examine whether the measured solid concentration in the fluid at the exit of the experimental cell approached the equilibrium solubility. The measured solid solubility data were then correlated using the Soave–Redlich–Kwong [9] and the Peng–Robinson [10] equations of state (EOS) with van der Waals (VDW2) mixing rules that included two adjustable parameters. Correlation results from the EOS models were then compared with those from the semi-empirical equations presented by Chrastil [11], or Mendez-Santiago and Teja [6].

2. Experimental

2.1. Chemicals

Carbon dioxide was supplied by San-Fu Chemical Co. (Taiwan) with a minimum purity of 99.8%. 2-Methyl-*N*-phenylacetamide and 4-methyl-*N*-phenylacetamide were purchased from Merck Co. *N*-Phenylacetamide was purchased

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Table 1
Physical properties of the pure compounds used in this study

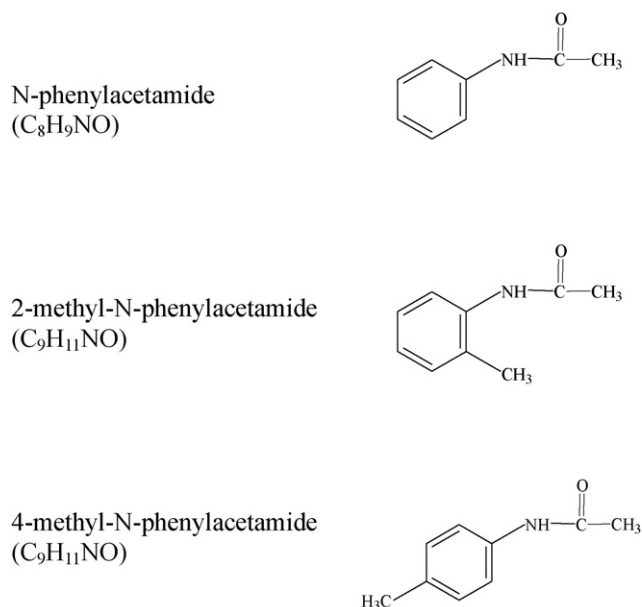| Compound	Mw ($\times 10^{-3}$ kg/mol)	T_m (K)	V_s ($\times 10^{-3}$ m^3/mol)	T_c (K)	P_c (MPa)	ω
Carbon dioxide	44.01			304.19 [15]	7.382 [15]	0.228 [15]
N-Phenylacetamide (C$_8$H$_9$NO)	135.17	387.5 [14]	0.1109 [14]	735.85 [12]	4.011 [12]	0.577 [13]
2-Methyl-N-phenylacetamide (C$_9$H$_{11}$NO)	149.19	383.2 [14]	0.1277 [14]	761.01 [12]	3.501 [12]	0.625 [13]
4-Methyl-N-phenylacetamide (C$_9$H$_{11}$NO)	149.19	421.7 [14]	0.1231 [14]	761.01 [12]	3.501 [12]	0.625 [13]

Fig. 1. Structures of three organic compounds in this study.

from Acros Co. All three pure compounds had a minimum purity of 99%, and were used without further purification. The properties of the pure compounds used in this study are tabulated in Table 1. However, the critical constants and acentric factors for pure solid compounds were not available in literature. The critical temperature and pressure were estimated using the correlation equation of Joback [12], and the acentric factors were estimated from by Ambrose method [13]. The structures of these pure compounds used for experiments are illustrated in Fig. 1.

2.2. Experimental apparatus and procedures

A semi-flow type apparatus used in this study for measuring the solid solubility in supercritical CO$_2$ is shown in Fig. 2. The experimental system consisted of three sections: (1) the supply of supercritical CO$_2$, (2) the equilibrium between solid and supercritical phases and (3) the analysis of experimental results.

The experimental procedures were similar to those described in our previous study [7]. Pure CO$_2$ was liquefied to 272.2 K and then was compressed to the desired pressure by a HPLC pump (Thermo Separation Product). The pressure was controlled by a back pressure regulator. The high pressure CO$_2$ passed through a pre-heating coil that was immersed in a water bath. It was then charged into the pre-equilibrium and equilibrium cells. The pre-equilibrium cell had a volume of 150 cm^3 and 25 g solid sample was then distributed into five layers packed with glass beads. The main equilibrium cell had a volume of 300 cm^3 and 50 g solid sample was distributed into 10 layers packed also with glass beads. The equilibrium cells were equipped with filters to prevent any physical entrainment. The temperature and pressure were measured using a calibrated quartz thermocouple and a calibrated Heise gauge, respectively. The temperature and pressure measurements displayed accuracy of ±0.1 K and ±0.03 MPa, respectively in this study.

After flowing through the equilibrium cell, the supercritical CO$_2$ was expanded to atmospheric pressure through a needle valve wrapped with heating tape. The heating tape was kept in the temperature range of 20–30 K above the melting point of the solid solute in order to avoid any precipitation in the line. After the expansion, solid was separated from the gas phase and then was dissolved in a flask with organic solvent. The volume of CO$_2$
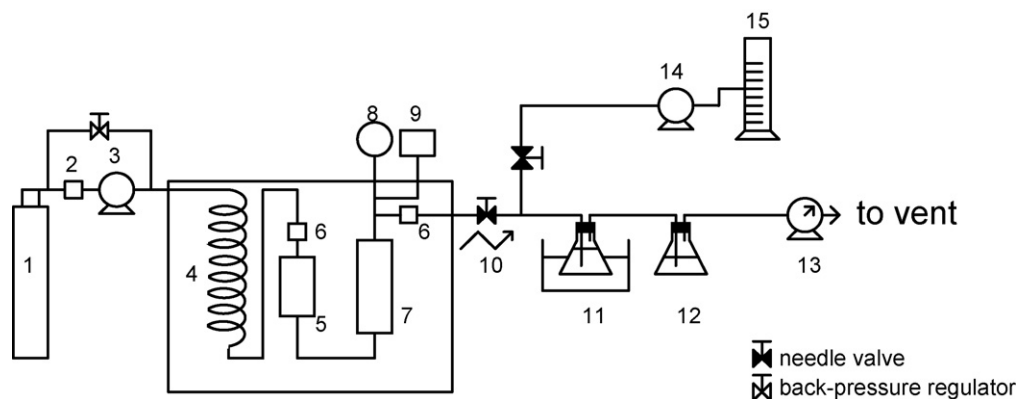

Fig. 2. Schematic diagram of the experimental apparatus: 1, CO$_2$ cylinder; 2, cooler; 3, HPLC pump; 4, pre-heater; 5, pre-equilibrium cell; 6, filter; 7, equilibrium cell; 8, pressure transducer; 9, thermometer; 10, heating tape; 11, ice bath; 12, saturator; 13, wet test meter; 14, solvent delivery pump; 15, solvent reservoir.

flow was measured by a wet test meter (Ritter TG1). A UV–vis spectrometer (Jasco UV-975) was used to analyze the compositions of the organic solution in the flask. The organic solution in the collection flask was sonicated for 10 min to ensure complete dissolution before it was analyzed using the UV–vis spectrometer. In this study, ethyl acetate was chosen as the solvent. A sharp absorption peak in the UV–vis spectrometer for both 2-methyl-N-phenylacetamide and 4-methyl-N-phenylacetamide was observed at the band of 263 nm. The optimal absorption band for N-phenylacetamide was also observed at 261 nm. Calibrations for the UV analyses were made before the experiments using standard solutions of known concentrations. The experimental data were taken after CO_2 flowed through the equilibrium cell for 30 min. In each experiment, at least three measurements were taken at a given temperature and pressure. The reproducibility of the solid solubility measurements was observed at ±5%, and the accuracy of the solid solubility data was estimated as ±0.002 mol fraction.

3. Results and discussion

A fluid–solid mass transfer model presented by Abaroudi et al. [8] was solved in this study under our experimental conditions. The purpose of solving this model was to ensure that the mass transfer effects were insignificant to our measurements. In this model, the supercritical CO_2 was assumed to pass through the packed equilibrium cell in a one-dimensional plug flow. A mass balance over a differential bed length (z) in the cell was written as

$$\varepsilon \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial z} = k_g a_s (C_{sat} - C) \tag{1}$$

where C is the solid concentration in the fluid phase, ε the porosity of the equilibrium cell, a_s the mass transfer area, k_g the solid to fluid mass transfer coefficient and u is the interstitial fluid velocity in the equilibrium cell. The initial and boundary conditions were:

$$t = 0, \qquad C = 0 \quad \text{for any } z > 0 \tag{2}$$

$$z = 0, \qquad C = 0 \quad \text{for any } t > 0 \tag{3}$$

The Laplace transform method was applied to solve Eq. (1) and the following dimensionless groups were introduced:

$$X = \frac{C}{C_{sat}}, \quad \tau = \frac{L\varepsilon}{u}, \quad \theta = \frac{t}{\tau}, \quad \xi = \frac{z}{L}, \quad St' = \frac{k_g a_s L}{u} \tag{4}$$

where X is the ratio of the solid solute concentration in supercritical fluid phase (C) to its saturated solubility (C_{sat}) and L is the length of the equilibrium cell. It was solved as a function of the dimensionless mean residence time θ, the dimensionless bed distance ξ and the modified Stanton's number St'. The solution for Eq. (1) yielded:

$$X = [1 - \exp(-\xi St')][1 - \exp(-\theta St')] \quad \text{for} \quad \theta > St' \tag{5}$$

$$X = 1 - \exp(-St' \theta) \quad \text{for} \quad St' > \theta > 0 \tag{6}$$

Table 2
Properties and approach to equilibrium for CO_2 (1) + N-phenylacetamide (2) at various operation conditions

T (K)	P (MPa)	ρ_{CO_2} (kg/m^3)	μ_{CO_2} ($\times 10^5$ Pa s)	D_{12} ($\times 10^8$ m^2/s)	Sc	Re	St'	Minimum value of X ($=C/C_{sat}$)
308.2	10.44	671.80	6.25	1.83	5.09	2.70–8.11	136.9–405.6	1.00
	12.16	728.35	7.09	1.58	6.17	2.38–7.15	125.3–371.0	1.00
	13.89	769.00	7.80	1.41	7.17	2.17–6.50	116.5–345.0	1.00
	15.61	800.96	8.44	1.30	8.13	2.00–6.00	109.5–324.1	0.99
	17.33	827.64	9.06	1.20	9.09	1.87–5.60	103.5–306.2	0.99
	19.06	850.76	9.66	1.13	10.07	1.75–5.25	98.2–290.4	0.99
	20.78	871.02	10.26	1.06	11.07	1.65–4.94	93.5–276.5	0.99
	22.50	889.18	10.85	1.01	12.10	2.56–4.67	89.2–263.9	0.99
318.2	10.44	502.73	4.36	2.95	2.94	3.88–11.64	171.4–508.2	1.00
	12.30	615.88	5.58	2.19	4.15	3.03–9.08	151.1–447.7	1.00
	13.88	672.43	6.31	1.89	4.97	2.68–8.04	139.8–414.2	1.00
	15.61	717.69	6.97	1.67	5.80	2.43–7.28	130.3–386.1	1.00
	17.33	753.14	7.55	1.52	6.58	2.24–6.71	122.7–363.3	1.00
	19.05	782.59	8.11	1.41	7.36	2.08–6.25	116.1–343.8	1.00
	20.78	808.00	8.64	1.31	8.15	1.96–5.87	110.3–326.6	0.99
	22.50	830.18	9.17	1.23	8.95	1.84–5.53	105.2–311.4	0.99
328.2	10.44	356.70	3.14	4.64	1.89	5.39–16.16	194.4–576.2	1.00
	12.30	487.46	4.26	3.17	2.75	3.97–11.92	177.5–526.1	1.00
	14.02	572.26	5.13	2.53	3.55	3.30–9.89	162.6–482.1	1.00
	15.75	632.00	5.83	2.16	4.27	2.90–8.70	151.1–447.7	1.00
	17.47	677.17	6.42	1.92	4.93	2.63–7.90	141.8–420.2	1.00
	19.19	713.65	6.95	1.75	5.58	2.43–7.30	134.0–397.1	1.00
	20.92	744.46	7.45	1.61	6.22	2.27–6.81	127.3–377.0	1.00
	22.50	768.89	7.89	1.51	6.81	2.14–6.43	121.8–360.6	1.00

$X = C/C_{sat}$ was calculated at the outlet of the equilibrium cell, $t = 30$ min and CO_2 flow rates (coverted at the STP conditions) = 5–15 L/h.

The detail procedures for the determination of the modified Stanton's number, and the calculation of parameters in the mass transfer model have been presented in our previous study [7]. The flow rates of CO_2, converted to the values at the STP condition, ranged from 5 to 15 L/h in this study. The measured solid solubility at a given temperature and pressure should not vary with the CO_2 flow rates, according to the phase rule. We applied this criterion to examine if the correct experimental data were obtained. Following a similar approach and employing the same experimental conditions, the minimum values of X were also evaluated at various temperatures and pressures for each solid compound. Table 2 demonstrates an example for the 1calculated minimum relative saturation values in the solid solubility measurements of *N*-phenylacetamide.

Since the X values shown in Table 2 were very close to unity, it is verified that the mass transfer has negligible effect on all measured solid solubility data in supercritical CO_2. Similar results have been observed for the other two solids in this study.

The measured solid solubilities in supercritical CO_2 for *N*-phenylacetamide, 2-methyl-*N*-phenylacetamide and 4-methyl-*N*-phenylacetamide are presented in Tables 3–5, respectively. The densities of pure CO_2 shown in these tables were calculated using the Peng–Robinson EOS. The solubilities for three compounds increased with pressure at each isotherm. At the same temperature and pressure, the solid solubilities increased in an order of *N*-phenylacetamide > 4-methyl-*N*-phenylacetamide > 2-methyl-*N*-phenylacetamide. *N*-phenylacetamide had the lowest molecular weight and it showed the largest solubility in supercritical CO_2. Although we know 4-methyl-*N*-phenylacetamide and 2-methyl-*N*-phenylacetamide are isomers, it is still difficult to discuss the specific interactions

for these solid compounds with supercritical CO_2 since no dipole moments of these solids were available in literature. 4-Methyl-*N*-phenylacetamide had smaller solid molar volume than that of 2-methyl-*N*-phenylacetamide. The former solid was expected to have higher solubility upon extraction by CO_2, as the solid was surrounded by clusters of CO_2 molecules. The experimental solid solubility data were then correlated using either the equation of state or the semi-empirical equations.

Table 3
Solubilities of *N*-phenylacetamide (2) in supercritical carbon dioxide (1)

T (K)	P (MPa)	y_2 ($\times 10^4$)	ρ_1 (kg/m^3)
308.2	10.44	0.508	671.80
	12.16	0.794	728.35
	13.89	1.109	769.00
	15.61	1.246	800.96
	17.33	1.497	827.64
	19.06	1.695	850.76
	20.78	1.756	871.02
	22.50	2.025	889.18
318.2	10.44	0.410	502.73
	12.30	0.810	615.88
	13.88	1.224	672.43
	15.61	1.741	717.69
	17.33	2.386	753.14
	19.05	2.783	782.59
	20.78	3.124	808.00
	22.50	3.245	830.18
328.2	10.44	0.293	356.70
	12.30	0.782	487.46
	14.02	1.356	572.26
	15.75	2.376	632.00
	17.47	2.817	677.17
	19.19	3.487	713.65
	20.92	4.225	744.46
	22.50	4.562	768.89

Table 4
Solubilities of 2-methyl-*N*-phenylacetamide (3) in supercritical carbon dioxide (1)

T (K)	P (MPa)	y_3 ($\times 10^4$)	ρ_1 (kg/m^3)
308.2	12.16	0.358	728.35
	13.89	0.492	769.00
	15.61	0.708	800.96
	17.33	0.861	827.64
	19.06	1.163	850.76
	20.78	1.354	871.02
	22.50	1.676	889.18
318.2	12.30	0.301	615.88
	13.88	0.525	672.43
	15.61	0.931	717.69
	17.33	1.455	753.14
	19.05	1.997	782.59
	20.78	2.278	808.00
	22.50	2.762	830.18
328.2	12.30	0.197	487.46
	14.02	0.548	572.26
	15.75	1.042	632.00
	17.47	2.022	677.17
	19.19	2.912	713.65
	20.92	3.815	744.46
	22.50	4.633	768.89

Table 5
Solubilities of 4-methyl-*N*-phenylacetamide (4) in supercritical carbon dioxide (1)

T (K)	P (MPa)	y_4 ($\times 10^4$)	ρ_1 (kg/m^3)
308.2	12.16	0.527	728.46
	13.88	0.836	768.93
	15.61	1.022	800.97
	17.33	1.078	827.69
	19.06	1.221	850.72
	20.78	1.389	871.02
	22.50	1.664	889.21
318.2	12.16	0.480	609.89
	13.88	0.892	672.64
	15.61	1.344	717.69
	17.33	1.482	753.20
	19.06	1.997	782.69
	20.78	2.236	808.00
	22.50	2.452	830.22
328.2	12.16	0.384	479.18
	13.89	0.966	566.80
	15.61	1.222	627.82
	17.33	2.034	673.95
	19.06	2.947	711.06
	20.78	3.601	742.14
	22.50	4.802	768.93

Table 6
Correlated results of solid solubility data in supercritical carbon dioxide using various EOS and VDW2 mixing rules

Peng–Robinson EOS			Soave–Redlich–Kwong EOS		
k_{1j}	l_{1j}	AADy$_j$ (%)	k_{1j}	l_{1j}	AADy$_j$ (%)
CO_2 (1) + *N*-phenylacetamide (2), ln P_2^{sat} (Pa) = 42.06 − 14036.33/*T* (K)					
0.036	0.001	6.54	0.045	0.018	7.03
CO_2 (1) + 2-methyl-*N*-phenylacetamide (3), ln P_3^{sat} (Pa) = 54.89 − 19570.25/*T* (K)					
−0.064	0.111	4.32	−0.060	0.120	4.71
CO_2 (1) + 4-methyl-*N*-phenylacetamide (4), ln P_4^{sat} (Pa) = 46.15 − 15826.82/*T* (K)					
0.088	0.126	6.21	0.088	0.118	6.40

AADy$_j$ (%) = $\frac{100}{n}\sum_{k=1}^{n}\frac{|y_{j,k}^{exp}-y_{j,k}^{cal}|}{y_{j,k}^{exp}}$, the summation was over all *k*th experimental points for solid *j*.

3.1. Equation of state method

At the phase equilibrium condition, the solid (component *j*) solubility in supercritical CO_2 (component 1) was calculated by

$$y_j = \frac{P_j^{sat}\exp((V_j^s(P-P_j^{sat}))/RT)}{\varphi_j^{SCF}P} \tag{7}$$

where V_j^s is the solid molar volume, P_j^{sat} the solid vapor pressure and φ_j^{SCF} is the fugacity coefficient of the solute in the supercritical phase. In this study, the vapor pressure of solute was expressed by the following empirical equation:

$$\ln P_j^{sat} = A - \frac{B}{T} \tag{8}$$

where *A* and *B* were two adjustable parameters that were optimally fitted into the solid solubility data. Two EOS with mixing rules were employed in this study to calculate the fugacity coefficient in the supercritical phases: the Soave–Redlich–Kwong EOS [9]:

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)} \tag{9}$$

and the Peng–Robinson EOS [10]:

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b)+b(v-b)} \tag{10}$$

The EOS parameters were evaluated from the critical constants of pure compounds.

The van der Waals mixing rules with two parameters were used to calculate the EOS parameters for fluid mixtures:

$$a_m = \sum\sum y_i y_j (a_i a_j)^{0.5}(1-k_{ij}) \tag{11}$$

$$b_m = \sum\sum y_i y_j \frac{(b_i+b_j)}{2}(1-l_{ij}) \tag{12}$$

where k_{ij} and l_{ij} were two adjustable binary interaction parameters, considered as temperature-independent in this study. The binary interaction parameters and the parameters in the solid vapor pressure equations were optimally fitted into the experimental solubility data by minimizing the following objective function:

$$obj = \sum \frac{|y_j^{exp}-y_j^{cal}|}{y_j^{exp}} \tag{13}$$

The correlation results using the EOS method are shown in Table 6. With the optimally fitted parameters (*A*, *B*, k_{1j} and l_{1j}), satisfactory accuracy for the calculated solid solubility was observed by the EOS method with an absolute average deviation around 6%.

3.2. Semi-empirical equation method

Two empirical equations presented by Chrastil [11] and by Mendez-Santiago and Teja [6] were commonly employed to correlate the solid solubility in supercritical CO_2. The Chrastil model was based on the hypothesis of molecular association. It expressed a linear relationship between the logarithm of the

Table 7
Correlated results of the solubility data in supercritical carbon dioxide using the Chrastil equation and the Mendez-Santiago and Teja equation

System	Chrastil equation				Mendez-Santiago and Teja equation			
	n	*C*	*D*	AADy$_j$ (%)	*E* (×10^4)	*F*	*G*	AADy$_j$ (%)
CO_2 (1) + *N*-phenylacetamide (2)	5.08	−7.44 × 10^3	−10.97	6.82	−1.22	2.85	26.07	4.82
CO_2 (1) + 2-methyl-*N*-phenylacetamide (3)	8.38	−1.13 × 10^4	−21.16	5.56	−1.69	4.30	36.83	7.33
CO_2 (1) + 4-methyl-*N*-phenylacetamide (4)	6.29	−9.07 × 10^3	−14.08	6.69	−1.39	3.38	29.82	6.42

AADy$_j$ (%) = $\frac{100}{n}\sum_{k=1}^{n}\frac{|y_{j,k}^{exp}-y_{j,k}^{cal}|}{y_{j,k}^{exp}}$, the summation is over all *k*th experimental points for solid *j*.
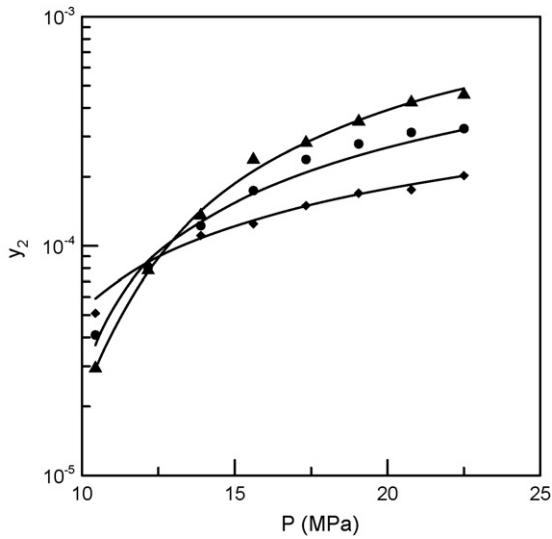
Fig. 3. Solubility for N-phenylacetamide (2) in supercritical carbon dioxide (1): ($\blacklozenge$) 308.2 K; ($\bullet$) 318.2 K; ($\blacktriangle$) 328.2 K; (—) Mendez-Santiago and Teja method.

solid solubility and the logarithm of the density of the pure CO_2 (component 1):

$$\ln S_j \ \text{(kg/m}^3) = n \ln \rho_1 \ \text{(kg/m}^3) + \frac{C}{T} + D \quad (14)$$

$$S_j = \frac{\rho_1 M_j y_j}{M_1(1 - y_j)} \quad (15)$$

where T is the temperature, n the association number and M is the molecular weight. The optimal values of n, and the other two parameters C and D were optimally fitted into the experimental data in this study. Mendez-Santiago and Teja proposed
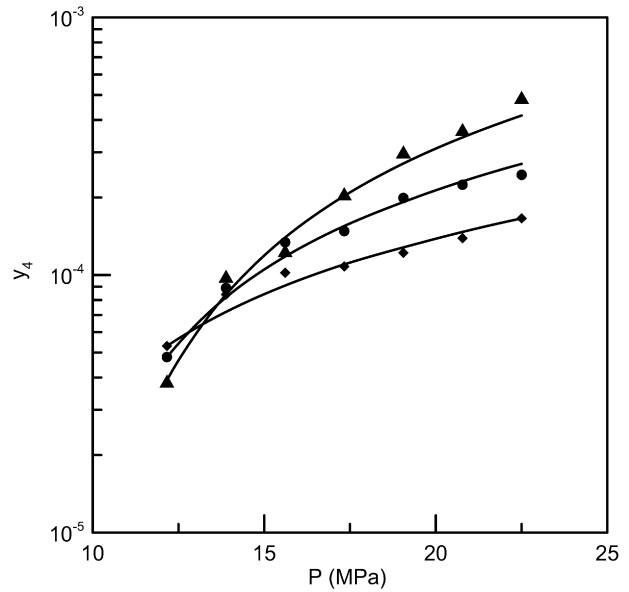

Fig. 5. Solubility for 4-methyl-N-phenylacetamide (4) in supercritical carbon dioxide (1): ($\blacklozenge$) 308.2 K; ($\bullet$) 318.2 K; ($\blacktriangle$) 328.2 K; (—) correlation results from the Mendez-Santiago and Teja equation.

an equation that also had three adjustable parameters:

$$T \ln(y_j P \ \text{(MPa)}) = E + F\rho_1 \ \text{(kg/m}^3) + GT \quad (16)$$

The empirical parameters (E, F and G) in Eq. (16) were also optimally fitted using the measured solid solubility data. The correlation results using the above two semi-empirical equations are shown in Table 7. Both equations yielded the absolute average deviation in solid solubility around 6%. Graphical presentations of the solid solubility data for various solid solutes are shown in Figs. 3–5, respectively. The cross-over pressures of the cor-
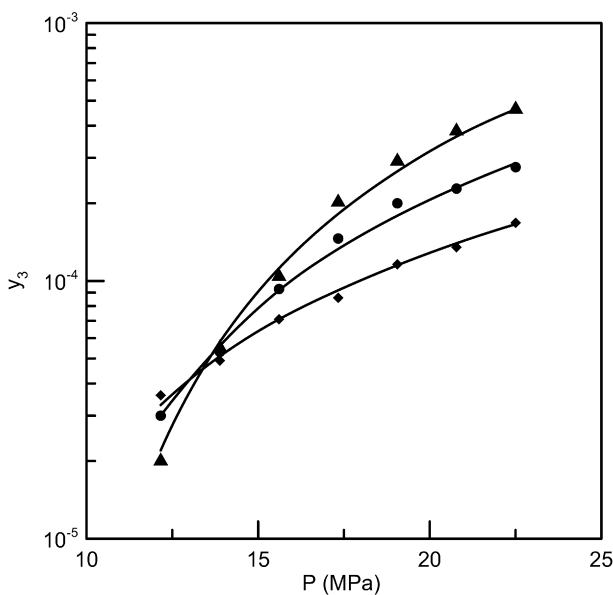

Fig. 4. Solubility for 2-methyl-N-phenylacetamide (3) in supercritical carbon dioxide (1): ($\blacklozenge$) 308.2 K; ($\bullet$) 318.2 K; ($\blacktriangle$) 328.2 K; (—) correlation results from the Mendez-Santiago and Teja equation.
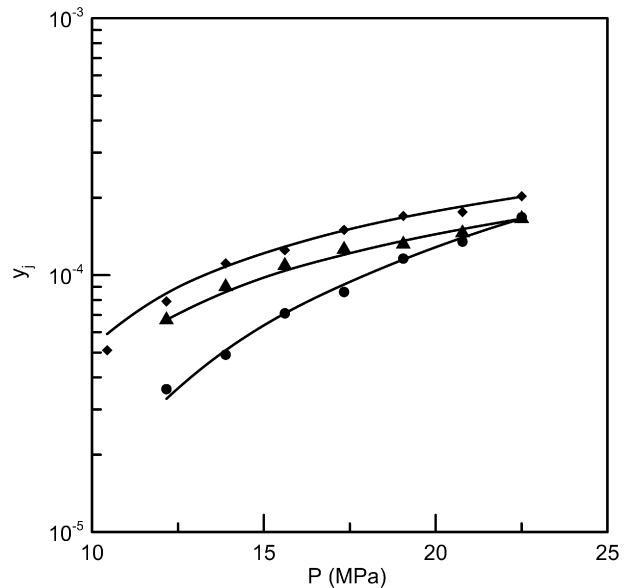
Fig. 6. Solubility of various compounds in supercritical CO_2 at 308.2 K: ($\blacklozenge$) N-phenylacetamide; ($\bullet$) 2-methyl-N-phenylacetamide; ($\blacktriangle$) 4-methyl-N-phenylacetamide; (—) correlation results from the Mendez-Santiago and Teja equation.

responding solids were between 12 and 14 MPa. The correlated results using the Mendez-Santiago and Teja equation with its optimally fitted parameters are also demonstrated in these figures. It is observed that the correlation results were satisfactory. Fig. 6 shows a typical plot of the comparison of the solid solubilities at 308.2 K and various pressures. The correlation results were again found satisfactory for all solid solutes.

4. Conclusion

In this study, new solid solubility data of *N*-phenylacetamide, 2-methyl-*N*-phenylacetamide and 4-methyl-*N*-phenylacetamide in supercritical carbon oxide are presented at 308.2, 318.2 and 328.2 K over the pressure range from 10 to 22 MPa. Subsequently, it was demonstrated that the mass transfer effects were negligible at the experimental conditions. Besides, in order to correlate the solubility data, the Peng–Robinson and the Soave–Redlich–Kwong EOS with VDW2 mixing rules, the Chrastil and the Mendez-Santiago–Teja semi-empirical equations were used. We further verified that all methods yielded satisfactory correlation results for solid solubility with absolute average deviation around 6%.

Acknowledgement

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