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Measurement and Correlation for the Solubilities of Dihydrocapsaicin in *n*-Heptane, *n*-Hexane, *n*-Pentane, Ethyl Acetate, Acetone, Ethanol, and Water

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ABSTRACT: Using the dynamic method of a laser detecting system, the solubilities of dihydrocapsaicin in *n*-heptane, *n*-hexane, *n*-pentane, ethyl acetate, acetone, ethanol, and water from (298.43 to 329.84, 296.14 to 327.57, 297.26 to 306.45, 302.07 to 327.58, 299.49 to 319.77, 301.79 to 328.84, and 324.67 to 331.49) K, respectively, were measured. The experimental data were correlated with the Wilson model, a polynomial empirical equation, and the Apelblat equation. The calculations show that the data correlated with the Wilson model for the former three weak polar solvents have less deviations than those correlated with the polynomial empirical equation and the Apelblat equation, while the data correlated with the polynomial empirical equation for the latter four strong polar solvents have less deviations than those correlated with the Apelblat equation and the Wilson model.

■ INTRODUCTION

Capsaicinoids are an important raw material which are widely used as intermediate products in medicine, pesticides, heath care, foodstuffs, feedstuffs, dope, and military affairs. Especially in the field of medicine, capsaicinoids can be used to lose weight, invigorate the stomach, ease pain, detoxify drugs, and combat cancer.[1−4] Nowadays, the method of extracting and separating capsaicinoids from capsicum has been applied in industry. Therefore, the solubilities of dihydrocapsaicin, which is the second largest component of capsaicinoids, are an important reference for the extraction and separation of capsaicinoids from capsicum and the separation of dihydrocapsaicin from capsaicinoids in industry. However, systematic solubility data of dihydrocapsaicin have not been reported. In this study, the solubilities of dihydrocapsaicin in *n*-heptane, *n*-hexane, *n*-pentane, ethyl acetate, acetone, ethanol, and water have been measured. The experimental data were correlated with the Wilson model, the polynomial empirical equation, and the Apelblat equation.

■ EXPERIMENTAL SECTION

Materials. Dihydrocapsaicin, separated from *Guangxi capsicum* and appraised with nuclear magnetism, was further purified by recrystallization from organic solutions. (Dihydrocapsaicin was dissolved in ethanol, and the solution was filtrated to get rid of the indissolvable impurities and then recrystallized and dried. The sample was recrystallized several times by *n*-heptane for further purification.) Its purity was determined by reverse phase high-performance liquid chromatography (RP-HPLC) spectrometry (Waters 510, Shimadzu Co. Ltd.) to be 0.998 in mass fraction. Water (99.9 %), ethanol (99.7 %), acetone (99.5 %), ethyl acetate (99.5 %), *n*-pentane (99.6 %), *n*-hexane (99.7 %), and *n*-heptane (99.6 %) were obtained from the Guangdong Xilong Chemical Co., Ltd., China.

Apparatus and Procedure. The experimental apparatus included a solution equilibrium still (made by the Chongqing Tuo Xin Glassware Co., Ltd., China.), a magnetic stirring system, a temperature-controlling system, a temperature-measuring system, and a laser detecting system (made by the Changchun Bosheng Electron Co., Ltd., China). The solution equilibrium still includes an inside still and an outside still which share the same neutral axis. The inside still has two mouths in the upper extreme, while the outside still has a mouth in the upper and lower side, respectively. The mixer system is constituted by a stirring rod in the inside still and a magnetic agitator (made by the Zhengzhou Great Wall Industry and Commerce Co., Ltd., China) to guarantee the solute and the solvent in the inside still be mixed and heated evenly. The temperature-controlling system is made up of a constant temperature circulator (made by the Beijing Fortunejoy Science Technology Co., Ltd., China) connected to the outside still and a condenser connecting with the inside still, which is used to control the temperature of the solution equilibrium still system. The temperature-measuring system is a digital precision thermometer (made by the Shanghai Hua Chen Medical Instruments Co., Ltd., China) which lies inside the inside still from the upper mouth with an uncertainty of the thermocouple of ± 0.1 K to measure the temperature of the solution equilibrium still. The laser detecting system is constituted by a laser generator and a laser receiver. The laser generator is installed at one side of the solution equilibrium still to provide a laser beam through the equilibrium still, while the laser receiver is installed at the opposite side to detect the degree of the laser light and then to convert it into electrical signal. As the solid dissolves, the electrical signal strengthens. When the last piece of the solid dissolves, the laser power reaches its maximum value, and the temperature corresponding to the maximum value of the detector is the solid−liquid equilibrium temperature of the sample.

The normal melting temperature T_m and enthalpy of fusion $\Delta_{fus}H$ of dihydrocapsaicin were determined by differential scanning calorimetry (DSC, NETZSCH, type STA409PC/PG) in the presence of nitrogen with a heating speed of $5\ K\cdot min^{-1}$. The normal melting temperature of dihydrocapsaicin is (332.5 ± 0.5) K, and its enthalpy of fusion is $(61.8 \pm 0.1)\ J\cdot g^{-1}$, that is, $(19002 \pm 31)\ J\cdot mol^{-1}$.

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Table 1. Experimental Solubility Data and Correlation Results of the Wilson Model

T/K	x	x^{calcd}	dev/%[a]	T/K	x	x^{calcd}	dev/%[a]
			Dihydrocapsaicin + n-Heptane				
298.43	$2.286 \cdot 10^{-4}$	$2.288 \cdot 10^{-4}$	0.1062	315.46	$6.223 \cdot 10^{-4}$	$6.219 \cdot 10^{-4}$	−0.06029
300.59	$2.604 \cdot 10^{-4}$	$2.598 \cdot 10^{-4}$	−0.2169	317.55	$7.016 \cdot 10^{-4}$	$7.036 \cdot 10^{-4}$	0.2805
302.85	$2.986 \cdot 10^{-4}$	$2.969 \cdot 10^{-4}$	−0.5830	318.84	$7.650 \cdot 10^{-4}$	$7.638 \cdot 10^{-4}$	−0.1533
304.03	$3.176 \cdot 10^{-4}$	$3.173 \cdot 10^{-4}$	−0.09406	320.08	$8.222 \cdot 10^{-4}$	$8.227 \cdot 10^{-4}$	0.06263
305.69	$3.494 \cdot 10^{-4}$	$3.494 \cdot 10^{-4}$	0	321.72	$9.077 \cdot 10^{-4}$	$9.096 \cdot 10^{-4}$	0.2064
307.08	$3.780 \cdot 10^{-4}$	$3.786 \cdot 10^{-4}$	0.1600	323.23	$9.966 \cdot 10^{-4}$	$9.993 \cdot 10^{-4}$	0.2754
308.84	$4.223 \cdot 10^{-4}$	$4.208 \cdot 10^{-4}$	−0.3451	325.05	0.001127	0.001126	−0.04514
309.97	$4.508 \cdot 10^{-4}$	$4.496 \cdot 10^{-4}$	−0.2742	326.86	0.001279	0.001274	−0.4164
311.04	$4.795 \cdot 10^{-4}$	$4.786 \cdot 10^{-4}$	−0.1906	328.37	0.001405	0.001403	−0.1242
313.41	$5.493 \cdot 10^{-4}$	$5.497 \cdot 10^{-4}$	0.07869	329.84	0.001558	0.001554	−0.2582
			Dihydrocapsaicin + n-Hexane				
296.14	$1.361 \cdot 10^{-4}$	$1.359 \cdot 10^{-4}$	−0.1272	314.74	$4.451 \cdot 10^{-4}$	$4.459 \cdot 10^{-4}$	0.1878
298.73	$1.587 \cdot 10^{-4}$	$1.594 \cdot 10^{-4}$	0.4609	316.54	$5.018 \cdot 10^{-4}$	$5.032 \cdot 10^{-4}$	0.2760
300.87	$1.815 \cdot 10^{-4}$	$1.823 \cdot 10^{-4}$	0.4489	317.91	$5.556 \cdot 10^{-4}$	$5.551 \cdot 10^{-4}$	−0.08721
301.98	$1.956 \cdot 10^{-4}$	$1.958 \cdot 10^{-4}$	0.1153	319.95	$6.376 \cdot 10^{-4}$	$6.386 \cdot 10^{-4}$	0.1592
303.09	$2.098 \cdot 10^{-4}$	$2.100 \cdot 10^{-4}$	0.1070	321.02	$6.887 \cdot 10^{-4}$	$6.896 \cdot 10^{-4}$	0.1341
305.04	$2.382 \cdot 10^{-4}$	$2.379 \cdot 10^{-4}$	−0.1133	322.07	$7.425 \cdot 10^{-4}$	$7.438 \cdot 10^{-4}$	0.1767
307.13	$2.693 \cdot 10^{-4}$	$2.707 \cdot 10^{-4}$	0.5169	324.02	$8.615 \cdot 10^{-4}$	$8.618 \cdot 10^{-4}$	0.03630
309.25	$3.091 \cdot 10^{-4}$	$3.104 \cdot 10^{-4}$	0.4093	325.18	$9.436 \cdot 10^{-4}$	$9.432 \cdot 10^{-4}$	−0.04366
310.68	$3.402 \cdot 10^{-4}$	$3.410 \cdot 10^{-4}$	0.2272	326.37	0.001043	0.001040	−0.2777
312.02	$3.743 \cdot 10^{-4}$	$3.736 \cdot 10^{-4}$	−0.1999	327.57	0.001153	0.001149	−0.3815
			Dihydrocapsaicin + n-Pentane				
297.26	$1.150 \cdot 10^{-4}$	$1.147 \cdot 10^{-4}$	−0.2437	302.58	$1.649 \cdot 10^{-4}$	$1.646 \cdot 10^{-4}$	−0.1630
298.19	$1.225 \cdot 10^{-4}$	$1.222 \cdot 10^{-4}$	−0.2724	303.63	$1.775 \cdot 10^{-4}$	$1.771 \cdot 10^{-4}$	−0.2303
299.27	$1.300 \cdot 10^{-4}$	$1.308 \cdot 10^{-4}$	0.5806	304.76	$1.899 \cdot 10^{-4}$	$1.906 \cdot 10^{-4}$	0.3825
300.43	$1.424 \cdot 10^{-4}$	$1.421 \cdot 10^{-4}$	−0.1881	305.61	$2.025 \cdot 10^{-4}$	$2.027 \cdot 10^{-4}$	0.1079
301.54	$1.525 \cdot 10^{-4}$	$1.529 \cdot 10^{-4}$	0.2440	306.45	$2.149 \cdot 10^{-4}$	$2.151 \cdot 10^{-4}$	0.08446

[a] dev = $(x - x^{\text{calcd}})/(x)$, where x^{calcd} is the value correlated with Wilson model.

The solubility was measured by a dynamic method.[5] A predetermined sample, after weighing by a precision balance (type AR2130, produced by Adventurer Group) with an accuracy of 0.0001 g, was heated by a speed of less than 0.1 K·h^{-1}; therefore, the systematic temperature was close to the solid—liquid equilibrium temperature. The dihydrocapsaicin in the solution dissolved as the temperature increased, and the temperature at which the last piece of the solid dissolved was the solid—liquid equilibrium temperature of the dihydrocapsaicin.

RESULTS AND DISCUSSION

Experimental Results. With dihydrocapsaicin as the solute, relatively weak polar *n*-heptane, *n*-hexane, and *n*-pentane and relatively strong polar ethyl acetate, acetone, ethanol, and water as the solvents, the experiment measures the solubilities of dihydrocapsaicin in the seven solvents which are divided into two groups. The solubilities are listed in Tables 1 and 2 according to the degree of the polarity of the solvents, in which x is the mole fraction of the dihydrocapsaicin in the solution. Each measurement was performed more than five times, and the data reported are the average values. At the equilibrium temperature the maximum measurement deviation of the solubilities of the dihydrocapsaicin was ± 0.5 %, ± 0.6 %, ± 0.5 %, ± 0.8 %, ± 0.9 %, ± 0.7 %, and ± 1.0 % in *n*-heptane, *n*-hexane, *n*-pentane, ethyl acetate, acetone, ethanol, and water, respectively.

Figures 1, 2, and 3 show the experimental results of the binary systems of the seven solvents. The solubility data of dihydrocapsaicin in *n*-pentane, ethyl acetate, acetone, ethanol, and water rise smoothly when the temperature increases across the whole temperature range studied. The solubilities of dihydrocapsaicin in *n*-heptane and *n*-hexane also increased smoothly at low temperatures but then rapidly above a temperature of about 311 K. The solubilities of dihydrocapsaicin in ethyl acetate, acetone, and ethanol are higher than those in *n*-heptane, *n*-hexane, *n*-pentane, and water. So *n*-heptane and *n*-hexane may be chosen as the appropriate solvents during the process of recrystallization purification. At the temperature of 325 K, the solubilities of dihydrocapsaicin in ethyl acetate, acetone, and ethanol are many times those in water. Meanwhile, the solubilities of dihydrocapsaicin in water are very low. When the temperature rises to 329.17 K, the solubilities are nearly invariant. Therefore, water may not be a suitable solvent for extracting capsaicinoids from capsicum, whereas ethyl acetate, acetone, and ethanol may be suitable solvents for this porpose.

Wilson Model. Suppose the dihydrocapsaicin is a pure solute, and the liquid phase does not get into the solid phase during dissolution; then in the binary system, the Wilson model[6] correlates the solid—liquid equilibrium of dissolution as follows:

$$\ln \gamma_1 = \ln\left(\frac{1}{x_1 + \Lambda_{12}x_2}\right) + x_2\left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1}\right) \tag{1a}$$

$$\ln \gamma_2 = \ln\left(\frac{1}{x_2 + \Lambda_{21}x_1}\right) + x_1\left(\frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} - \frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2}\right) \tag{1b}$$

in which γ_1 and γ_2 are activity coefficients of the solvent and dihydrocapsaicin and x_1 and x_2 are the mole fractions of the solvent and dihydrocapsaicin, respectively. The parameters

Table 2. Experimental Solubility Data and Correlation Results of the Polynomial Empirical Equation

T/K	x	x^{calcd}	dev/%[a]	T/K	x	x^{calcd}	dev/%[a]
Dihydrocapsaicin + Ethyl Acetate							
302.07	0.3069	0.3065	0.1303	314.85	0.4310	0.4317	−0.1624
304.12	0.3304	0.3303	0.03027	317.08	0.4476	0.4489	−0.2904
305.29	0.3424	0.3431	−0.2044	319.24	0.4638	0.4643	−0.1078
306.48	0.3540	0.3556	−0.4520	321.58	0.4804	0.4795	0.1873
307.69	0.3686	0.3679	0.1899	323.85	0.4937	0.4924	0.2633
308.81	0.3793	0.3788	0.1318	325.04	0.4969	0.4983	−0.2817
310.65	0.3970	0.3959	0.2771	326.35	0.5047	0.5042	0.09907
312.79	0.4155	0.4147	0.1925	327.58	0.5086	0.5089	−0.05899
Dihydrocapsaicin + Acetone							
299.49	0.1928	0.1921	0.3631	309.82	0.2957	0.2959	−0.06764
300.47	0.2026	0.2037	−0.5429	310.89	0.3042	0.3051	−0.2959
302.34	0.2244	0.2244	0	312.85	0.3216	0.3214	0.06219
303.46	0.2361	0.2361	0	314.88	0.3364	0.3370	−0.1784
304.58	0.2487	0.2474	0.5227	315.91	0.3451	0.3443	0.2318
305.69	0.2564	0.2581	−0.6630	316.95	0.3519	0.3512	0.1989
306.75	0.2691	0.2682	0.3344	318.17	0.3577	0.3585	−0.2237
308.78	0.2874	0.2867	0.2436	319.77	0.3665	0.3664	0.02729
Dihydrocapsaicin + Ethanol							
301.79	0.1841	0.1835	0.3259	316.25	0.2869	0.2880	−0.3834
303.35	0.1961	0.1965	−0.2040	317.93	0.2970	0.2969	0.03367
305.54	0.2132	0.2144	−0.5629	319.62	0.3050	0.3050	0
307.86	0.2328	0.2325	0.1289	321.41	0.3132	0.3128	0.1277
309.95	0.2492	0.2480	0.4815	323.25	0.3210	0.3201	0.2804
311.23	0.2580	0.2570	0.3876	324.83	0.3247	0.3259	−0.3696
312.98	0.2678	0.2686	−0.2987	326.47	0.3320	0.3314	0.1807
314.44	0.2775	0.2776	−0.03604	328.84	0.3388	0.3390	−0.05903
Dihydrocapsaicin + Water							
324.67	$4.806 \cdot 10^{-5}$	$4.846 \cdot 10^{-5}$	−0.8323	327.96	$1.020 \cdot 10^{-4}$	$1.016 \cdot 10^{-4}$	0.3922
325.03	$5.237 \cdot 10^{-5}$	$5.183 \cdot 10^{-5}$	1.031	328.53	$1.090 \cdot 10^{-4}$	$1.087 \cdot 10^{-4}$	0.2752
325.66	$6.136 \cdot 10^{-5}$	$6.099 \cdot 10^{-5}$	0.6030	329.17	$1.141 \cdot 10^{-4}$	$1.143 \cdot 10^{-4}$	−0.1753
326.29	$7.190 \cdot 10^{-5}$	$7.242 \cdot 10^{-5}$	−0.7232	329.85	$1.172 \cdot 10^{-4}$	$1.178 \cdot 10^{-4}$	−0.5119
326.81	$8.167 \cdot 10^{-5}$	$8.227 \cdot 10^{-5}$	−0.7347	330.68	$1.204 \cdot 10^{-4}$	$1.199 \cdot 10^{-4}$	0.4153
327.37	$9.263 \cdot 10^{-5}$	$9.234 \cdot 10^{-5}$	0.3131	331.49	$1.219 \cdot 10^{-4}$	$1.220 \cdot 10^{-4}$	−0.08203

[a] dev = $(x - x^{\text{calcd}})/(x)$, where x^{calcd} is the value correlated with polynomial empirical equation.

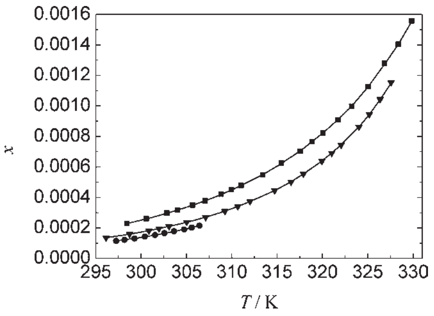

Figure 1. Solubilities of dihydrocapsaicin in n-heptane, n-hexane, and n-pentane. ■, dihydrocapsaicin + n-heptane; ▼, dihydrocapsaicin + n-hexane; ●, dihydrocapsaicin + n-pentane; —, Wilson model.

Λ_{12} and Λ_{21} can be obtained by the following equations.

$$\Lambda_{12} = \frac{V_2^{\text{L}}}{V_1^{\text{L}}} \exp\left(\frac{g_{11} - g_{12}}{RT}\right) \tag{2a}$$

$$\Lambda_{21} = \frac{V_1^{\text{L}}}{V_2^{\text{L}}} \exp\left(\frac{g_{22} - g_{21}}{RT}\right) \tag{2b}$$

in which V_1^{L} and V_2^{L} are the mole volumes of the solvent and dihydrocapsaicin, respectively. Using regression with MATLAB, $(g_{12} - g_{11})$ and $(g_{21} - g_{22})$ can be calculated. On the basis of the Wilson model, the optimized parameters of the solubility of dihydrocapsaicin in the seven solvents are listed in Table 3.

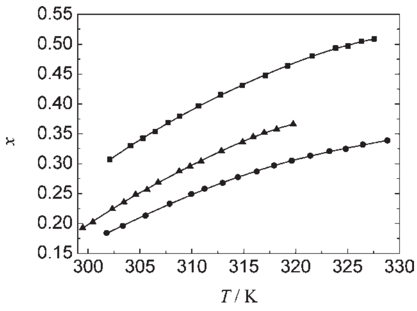

Figure 2. Solubilities of dihydrocapsaicin in ethyl acetate, acetone and ethanol. ■, dihydrocapsaicin + ethyl acetate; ▲, dihydrocapsaicin + acetone; ●, dihydrocapsaicin + ethanol; —, polynomial empirical equation.

By using the Table 3 data in the above equations, the x^{calcd} values calculated by the Wilson model correlate with the solubilities of dihydrocapsaicin in the three weak polar solvents n-heptane, n-hexane, and n-pentane. The x^{calcd} values are listed in Table 1. The deviations given in Table 1 are calculated by dev = $(x - x^{\text{calcd}})/(x)$. Therefore, the calculations show that the calculated mole fraction of the dihydrocapsaicin of the three

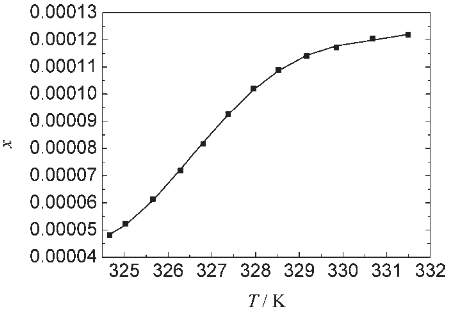

Figure 3. Solubilities of dihydrocapsaicin in water. ■, dihydrocapsaicin + water; —, polynomial empirical equation.

Table 3. Data of Dual Correlation Parameters of the Wilson Model for Different Systems[a]

system	$(g_{12} - g_{11})$ J·mol^{-1}	$(g_{21} - g_{22})$ J·mol^{-1}
dihydrocapsaicin + *n*-heptane	7691.0	21242
dihydrocapsaicin + *n*-hexane	5475.0	20506
dihydrocapsaicin + *n*-pentane	4040.0	19371
dihydrocapsaicin + ethyl acetate	4291.6	−312.3
dihydrocapsaicin + acetone	2252.9	−1908.0
dihydrocapsaicin + ethanol	4409.5	−923.00
dihydrocapsaicin + water	17405	25560

[a] The mole volume of dihydrocapsaicin is 274.5 mL·mol^{-1}. The mole volume was calculated with the data of mole quality and density of dihydrocapsaicin, which were obtained from Sigma Co., Ltd.

weak polar solvents *n*-heptane, *n*-hexane, and *n*-pentane is nearly identical with x values of the experiment.

At the same time, the Wilson model correlation with the solubilities of dihydrocapsaicin in ethyl acetate, acetone, ethanol, and water has a much wider deviation since the dihydrocapsaicin is a nonelectrolyte solute, and the four solvents are strongly polar. These results are in accordance with Muir's discovery[7] of the Wilson model that there is a wide deviation of nonelectrolyte solutes in strong polar systems.

Polynomial Empirical Equation. The polynomial empirical equation[8,9] has the characteristic of easy operation when it is used to correlate solubility data, so it is often used in engineering design and practical application.

The polynomial empirical equation used to correlate with the solubility data is based on the following situations:

1 The variable factors such as the solvent, solute, and pressure are a function of temperature.
2 The solubility is also a function of temperature, and the solubility is supposed to change when the temperature changes.

The solubility can be described by a polynomial equation of temperature as in the following equation:

$$x = A + BT + CT^2 + DT^3 + ET^4 \tag{3}$$

in which x is the mole fraction of the dihydrocapsaicin; T is the absolute temperature; and A, B, C, D, and E are constants. On the basis of the polynomial empirical equation, the optimized parameters of solubilities of dihydrocapsaicin in the seven measured solvents are listed in Table 4.

By using the Table 4 data in eq 3, the x^{calcd} values calculated by the polynomial empirical equation correlate with the solubilities of dihydrocapsaicin in the four strong polar solvents ethyl acetate, acetone, ethanol, and water. The x^{calcd} values and deviations are given in Table 2. Thus the calculations show that the calculated mole fraction of the dihydrocapsaicin in the four strong polar solvents ethyl acetate, acetone, ethanol, and water is nearly identical with that of the experiment.

The x^{calcd} values of the polynomial empirical equation which correlates with the solubilities of dihydrocapsaicin in the three weak polar solvents *n*-heptane, *n*-hexane, and *n*-pentane are also consistent with the x values of the experiment, but the x^{calcd} values of the Wilson model for these weak polar solvents are more consistent with the x values of the experiment.

Apelblat Equation. The modified Apelblat equation[10,11] can also be used to correlate the solubilities of dihydrocapsaicin in the seven solvents. The modified Apelblat equation can be expressed as:

$$\ln x = A + \frac{B}{T} + C \ln T \tag{4}$$

in which x is the mole fraction of dihydrocapsaicin; T is the absolute temperature; and A, B, and C are constants. On the basis of the modified Apelblat equation, the optimized parameters of the solubilities of dihydrocapsaicin in the seven solvents are listed in Table 5.

By using the Table 5 data in eq 4, the x^{calcd} values of the modified Apelblat equation which correlates with the solubilities of dihydrocapsaicin in the three weak polar solvents *n*-heptane, *n*-hexane, and *n*-pentane are in accordance with the x values of the experiment, but the x^{calcd} values of the Wilson model for these weak polar solvents are more consistent with the x values of the experiment. The x^{calcd} values of the modified Apelblat equation which correlates with the solubilities of dihydrocapsaicin in the four strong polar solvents ethyl acetate, acetone, ethanol, and water are also in accordance with the x values of the experiment, but the x^{calcd} values of the polynomial empirical equation for these strong polar solvents are more consistent with the x values of the experiment.

Comparison of the Three Models. The objective function in the simplex method was calculated by using eq 5, which gives the absolute average relative deviation between the experiment and the calculated mole fraction of the dihydrocapsaicin.

$$F = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{x_i^{\text{calcd}} - x_i}{x_i}\right| \tag{5}$$

in which x_i and x_i^{calcd} are the experiment and the calculated mole fraction of the dihydrocapsaicin; and N is the number of experiments.

The absolute value of the relative average deviation of each thermodynamic model is listed in Table 6 according to the weak and strong polar solvents, respectively. For the three weak polar solvents *n*-heptane, *n*-hexane, and *n*-pentane, the calculation shows that the Wilson model has an average deviation of 0.2402 %, while the polynomial empirical equation and the Apelblat equation have bigger average deviations of 0.4095 % and 0.7094 %. Therefore, the x^{calcd} values which use the Wilson model to calculate the solubilities of dihydrocapsaicin in the three weak polar solvents *n*-heptane, *n*-hexane, and *n*-pentane are most consistent with the x values of the experiment. For the four strong polar solvents ethyl acetate, acetone, ethanol, and water, the calculation shows that the polynomial empirical equation has an average deviation of 0.2968 %, while the Apelblat equation and

Table 4. Parameters of the Polynomial Empirical Equation for Seven Systems

system	polynomial				
	A	*B*	*C*	*D*	*E*
dihydrocapsaicin + *n*-heptane	49.751	−0.65932	0.00328	$-7.24 \cdot 10^{-6}$	$6.00 \cdot 10^{-9}$
dihydrocapsaicin + *n*-hexane	10.411	−0.13652	$6.72 \cdot 10^{-4}$	$-1.47 \cdot 10^{-6}$	$1.21 \cdot 10^{-9}$
dihydrocapsaicin + *n*-pentane	7.5002	−0.09838	$4.84 \cdot 10^{-4}$	$-1.06 \cdot 10^{-6}$	$8.72 \cdot 10^{-10}$
dihydrocapsaicin + ethyl acetate	−1343.0	17.009	−0.08096	$1.72 \cdot 10^{-4}$	$-1.37 \cdot 10^{-7}$
dihydrocapsaicin + acetone	−4265.5	55.191	−0.26795	$5.78 \cdot 10^{-4}$	$-4.69 \cdot 10^{-7}$
dihydrocapsaicin + ethanol	−1121.4	−14.323	0.06842	$-1.45 \cdot 10^{-4}$	$1.15 \cdot 10^{-7}$
dihydrocapsaicin + water	74761	−910.24	4.1558	−0.00843	$6.42 \cdot 10^{-6}$

Table 5. Parameters of the Modified Apelblat Equation for Seven Systems

system	Apelblat		
	A	*B*	*C*
dihydrocapsaicin + *n*-heptane	−491.06	16409	74.946
dihydrocapsaicin + *n*-hexane	−831.23	32549	125.20
dihydrocapsaicin + *n*-pentane	−563.63	20818	85.200
dihydrocapsaicin + ethyl acetate	630.56	−31055	−92.621
dihydrocapsaicin + acetone	1137.0	−54838	−167.58
dihydrocapsaicin + ethanol	811.19	−39755	−119.29
dihydrocapsaicin + water	37359	−1817163	−5494.2

Table 6. Comparison of Absolute Average Relative Deviation for Different Models

system	*F*/%		
	Wilson	polynomial	Apelblat
dihydrocapsaicin + *n*-heptane	0.2071	0.3067	0.6692
dihydrocapsaicin + *n*-hexane	0.2361	0.5492	1.092
dihydrocapsaicin + *n*-pentane	0.2774	0.3727	0.3670
total average deviation of the three weak polar solvents	0.2402	0.4095	0.7094
dihydrocapsaicin + ethyl acetate	4.777	0.1912	0.2841
dihydrocapsaicin + acetone	2.487	0.2472	0.4261
dihydrocapsaicin + ethanol	4.029	0.2413	0.4634
dihydrocapsaicin + water	1.762	0.5074	1.406
total average deviation of the four strong polar solvents	3.264	0.2968	0.6449

the Wilson model have 0.6449 % and 3.264 %, respectively. Therefore, the x^{calcd} values which use the polynomial empirical equation to calculate the solubilities of dihydrocapsaicin in the four strong polar solvents ethyl acetate, acetone, ethanol, and water are most consistent with the x values of the experiment.

■ CONCLUSION

The solubilities of dihydrocapsaicin of the seven solvents have been measured by a dynamic method, and the experimental data were correlated with the Wilson model, the polynomial empirical equation, and the Apelblat equation. The calculations show that the correlation of the Wilson model for the solubilities of dihydrocapsaicin in the three weak polar solvents *n*-heptane, *n*-hexane, and *n*-pentane systems has less deviation than that of the polynomial empirical equation and the Apelblat equation, while the correlation of the polynomial empirical equation for the solubilities of dihydrocapsaicin in the four strong polar solvents ethyl acetate, acetone, ethanol, and water systems has less deviation than that of the Apelblat equation and the Wilson model.

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