J. Chem. Eng. Data **2010,** *55,* 2333–2337

Solubility of Softisan 100 in Ethanol + Water and Acetone + Water Solutions

Qiang Lei, Songhong Zhang, Junxian Yun, Shaochuan Shen, and Kejian Yao*

State Key Laboratory Breeding Base of Green Chemistry Synthesis Technology, College of Chemical Engineering and Materials Science, Zhejiang University of Technology, Hangzhou 310014, China

Softisan 100 is a triglyceride mixture consisting of saturated vegetable fatty acids. Its solubility in two binary mixtures, that is, ethanol + water and acetone + water, was investigated experimentally at the temperature range from (279.95 to 304.45) K. The melting temperature and enthalpy of fusion of Softisan 100 were determined by differential scanning calorimetry (DSC). The Wilson and nonrandom two-liquid (NRTL) models were employed to correlate the experimental data, and the obtained results were compared. The calculated results by the Wilson model with a model parameter (Λ_{ij}) independent of the temperature were found to have a good agreement with the experimental data.

Introduction

Solid lipid nanoparticles (SLNs) are considered as an alternative colloidal drug delivery system compared to conventional emulsions, liposomes, and polymeric nanosized particles. It has attracted attention because of its many advantages, for example, controlled release, long-term stability, good tolerability, and so forth.[1−4] Chemicals like physiological and biodegradable lipids, the triglycerides, partial glycerides, fatty acids, steroids, and waxes are often used as matrix materials to prepare SLNs.[2] Among them, Softisan 100 has been used for manufacturing SLNs as one of the most important solid lipids.[5−7]

Softisan 100 is specified as hydrogenated coco-glycerides consisting of a triglyceride mixture of natural, saturated, even-numbered, and unbranched fatty acids with a chain length from C_{10} to C_{18}. Many methods are employed to prepare Softisan 100 nanoparticles based on the antisolvent precipitation, such as solvent injection,[8] particle formation by liquid flow-focusing,[9,10] and particle formation by liquid flow-focusing and gas displacing.[11] In these methods, the pharmaceutically acceptable organic solvents (such as acetone, ethanol, isopropanol, and ethyl acetate) are used as solvents, and water is used as an antisolvent. First, the Softisan 100 is dissolved in the organic solvent as a homogeneous liquid phase, and then a large amount of water is rapidly mixed with the solution of Softisan 100. The homogeneous liquid phase quickly becomes a two-liquid phase, and finally, SLNs are formed. Obviously, to determine the proper solvent and choose an optimum operate condition for manufacturing the Softisan 100 nanoparticles, it is necessary to know the solubility characteristics of the Softisan 100 in different solvent mixtures at different temperatures. However, from a review of the literature, the experimental solubility data of Softisan 100 in organic solvent + water solutions is lacking. In this work, the solubility of the Softisan 100 in ethanol + water and acetone + water solutions at different temperatures was measured, and the experimental solubility data were correlated with the Wilson and nonrandom two-liquid (NRTL) models.

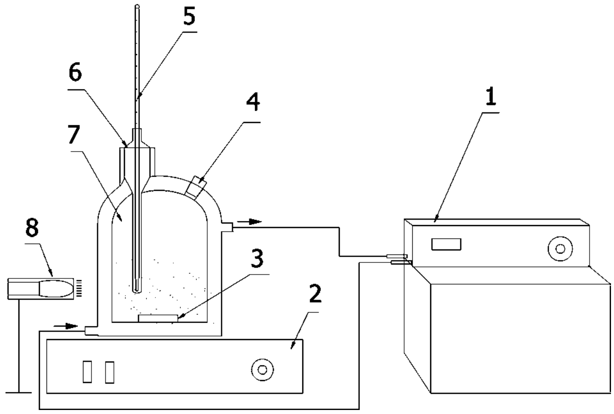

Figure 1. Experimental setup used for measuring solubility: (1) thermostatic bath; (2) magnetic stirrer; (3) stir bar; (4) inlet of solute; (5) thermometer; (6) thermometer jacket; (7) jacketed thermostat cell; (8) focus light.

Experimental Section

Materials. Softisan 100 was supplied by Sasol Chemical Co. Ltd. (Nanjing, China). Ethanol (99.7 %) and acetone (99.7 %) were used without further purification. The deionized water used had an electrical resistivity of 18.2 MΩ·cm at 298.15 K.

Apparatus and Procedure. In this work, the synthetic method[12−16] was employed for determining the solubility data. The setup used for the solubility measurements is shown in Figure 1. The jacketed glass cell for the measurement of Softisan 100 solubility was maintained at a desired temperature by water circulating from a thermostatic bath (type SC-15, Ningbo Tianheng Instrument Factory, China). Continuous stirring was achieved with a magnetic stir bar in the jacketed glass cell. The jacketed temperature was maintained within ± 0.05 K. A mercury-in-glass thermometer was inserted into the inner chambers of the cell for measurements of the temperature. The thermometer had an uncertainty of ± 0.05 K. Solubilities were determined by visual observation. An intense focus light was used for visual monitoring. To resist the external light interference and improve the observation accuracy, all of the measurements were carried out in the dark.

In the procedure, a mixture of Softisan 100 and solvent (or solvent + water mixtures) with a fixed composition was

---

* Corresponding author. Phone: +86 571 88320951. Fax: +86 571 88033331. E-mail: yaokj@zjut.edu.cn.

10.1021/je900754a

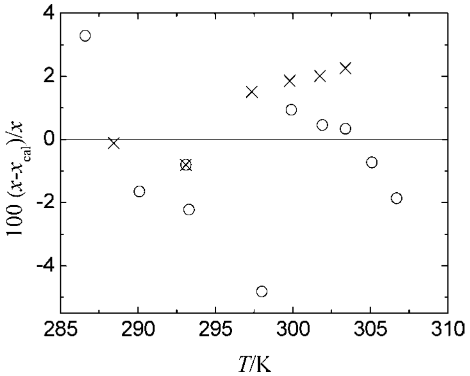

Figure 2. Deviation plot of solubility for lauric acid in acetone. x_{cal} is calculated from the van't Hoff equation.[17] x is the experimental solubility data: ○, ref 17; ×, this work.

prepared. The preweighed amount of the samples and solvents were determined using an analytical balance with an uncertainty of ± 0.0001 g. The mixtures were initially placed into the jacketed thermostat cell and heated quickly to achieve a homogeneous liquid phase. Then the solutions were cooled significantly below the dissolution temperature to make a slurry, which was kept at a constant temperature for 1 h. The temperature of the mixtures was increased slowly in a stepwise fashion until the temperature was reached at which all of the Softisan 100 was dissolved. Near the dissolution point, the temperature was increased less than 0.1 K every 20 min. All experiments were made at least twice, and the obtained data were averaged.

For some measurements, instead of starting with a fresh feed of Softisan 100 and solvent mixtures, an new predetermined amount of Softisan 100 was added into the cell with Softisan 100 and solvent mixture (or solvent + water mixtures), and the equilibrium temperature at this new composition was measured. This reduced the amount of Softisan 100 required to perform a series of solubility measurements at different concentrations for a particular solvent or solvent + water mixture.

The melting temperature and enthalpy of fusion were measured with differential scanning calorimetry (DSC; type Q100, TA Instrument Co., America) at a rate of 5 K·min^{-1}. Measurements were performed twice.

Reliability Analysis. To verify the validity of the experimental method for measuring the solubility of Softisan 100, contrastive experiments were carried out. Figure 2 shows a comparison of the solubility of lauric acid in acetone by using the present method with those given in the literature.[17] As can be seen, the experimental data showed good agreement with the literature. The relative deviation of the solubility is less than 2 %. Therefore, the procedures used in this work are valid, and the present method can provide accurate solubility measurements.

Table 1. Experimental Mass Fraction Solubilities of Softisan 100 (1) in Binary Water (2) + Ethanol (3) Solvent Mixtures

w_1	T/K	w_1	T/K	w_1	T/K
		$w_2 = 0.000$			
0.00027	279.95	0.00223	293.65	0.00843	300.05
0.00058	285.15	0.00291	294.85	0.01057	301.05
0.00079	287.90	0.00390	296.05	0.01363	302.05
0.00121	290.60	0.00527	297.75	0.01760	303.15
0.00165	292.25	0.00673	299.10	0.02234	304.25
		$w_2 = 0.0205$			
0.00020	281.20	0.00163	294.75	0.00664	301.25
0.00036	286.05	0.00232	296.25	0.00970	302.80
0.00066	289.45	0.00329	297.95	0.01274	304.25
0.00108	293.00	0.00474	299.95		
		$w_2 = 0.0404$			
0.00016	281.05	0.00107	294.40	0.00361	300.45
0.00030	285.65	0.00166	296.55	0.00536	302.30
0.00061	290.85	0.00241	298.35	0.00838	304.45
		$w_2 = 0.0626$			
0.00013	282.55	0.00073	294.25	0.00321	302.75
0.00019	286.15	0.00111	297.05	0.00424	304.15
0.00027	288.35	0.00171	299.35		
0.00048	291.75	0.00244	301.35		
		$w_2 = 0.0809$			
0.00012	283.45	0.00061	294.75	0.00170	300.65
0.00026	289.65	0.00084	296.55	0.00238	302.70
0.00044	292.75	0.00121	298.55	0.00314	304.35

Table 2. Experimental Mass Fraction Solubilities of Softisan 100 (1) in Binary Water (2) + Acetone (3) Solvent Mixtures

w_1	T/K	w_1	T/K	w_1	T/K
		$w_2 = 0.000$			
0.00175	282.65	0.02515	294.55	0.17309	299.25
0.00373	286.65	0.03479	295.45	0.23275	299.65
0.00578	288.75	0.04822	296.55	0.30568	299.95
0.00837	290.25	0.06720	297.45	0.39930	300.25
0.01193	291.65	0.09320	298.15		
0.01704	292.85	0.12727	298.85		
		$w_2 = 0.0202$			
0.00141	284.55	0.01125	294.15	0.09598	300.55
0.00212	286.65	0.01807	296.05	0.17031	301.05
0.00304	288.25	0.02843	297.75	0.26241	301.35
0.00452	290.35	0.04342	299.05	0.41511	301.55
0.00729	292.55	0.06505	299.85		
		$w_2 = 0.0401$			
0.00076	283.65	0.00858	295.75	0.07744	302.45
0.00161	287.45	0.01226	297.15	0.12408	302.65
0.00238	289.55	0.01898	298.75	0.22437	302.95
0.00387	292.45	0.03249	300.55		
0.00628	294.65	0.05549	301.95		
		$w_2 = 0.0605$			
0.00056	284.75	0.00295	293.70	0.01204	299.50
0.00074	285.65	0.00395	294.75	0.02082	301.65
0.00111	288.65	0.00615	296.45	0.03273	303.05
0.00222	292.05	0.00838	297.85		
		$w_2 = 0.0818$			
0.00033	283.85	0.00226	295.30	0.01206	302.65
0.00065	288.10	0.00331	297.15	0.01866	304.00
0.00103	291.00	0.00505	299.45		
0.00155	293.55	0.00780	300.95		

Results and Discussion

Softisan 100 is composed of different triglycerides. It can be considered as composed of one single triglyceride because these different triglycerides have very similar physicochemical characterizations. Its solubility in organic solvent + water solutions can also be considered as one pseudo-solubility. The mass fraction experimental solubility data of Softisan 100 in ethanol + water and acetone + water solutions are listed in Tables 1 and 2, where T is the measured absolute temperature, w_1 the mass fraction solubility, and w_2 the mass fraction of water solute-free, respectively. Figures 3 and 4 show the plot of mole fraction solubility x_1 of Softisan 100 versus temperature at different w_2 for ethanol + water and acetone + water systems, respectively. The mass fraction solubility w_1 and the mole fraction solubility x_1 of Softisan 100 were calculated by:

$$w_1 = \frac{m_1}{m_1 + m_2 + m_3} \tag{1}$$

$$x_1 = \frac{m_1/M_1}{m_1/M_1 + m_2/M_2 + m_3/M_3} \tag{2}$$

where m_1, m_2, and m_3 are the mass of Softisan 100, water, and organic solvent, M_2 and M_3 are the molecular weight of water

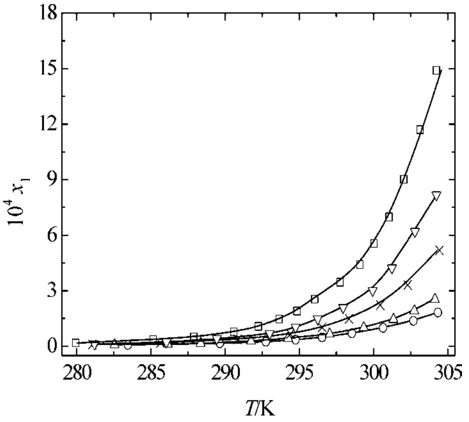

Figure 3. Mole fraction solubilities x_1 of Softisan 100 in binary ethanol + water solvent mixtures. The mass fraction of solute-free water is: □, $w_2 = 0$; ▽, $w_2 = 0.0205$; ×, $w_2 = 0.0404$; △, $w_2 = 0.0626$; ○, $w_2 = 0.0809$; solid line, solubility curve calculated from the NRTL model.

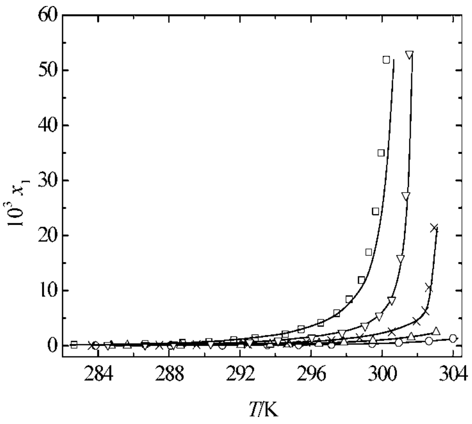

Figure 4. Mole fraction solubilities x_1 of Softisan 100 in binary acetone + water solvent mixtures. The mass fraction of solute-free water is: □, $w_2 = 0$; ▽, $w_2 = 0.0202$; ×, $w_2 = 0.0401$; △, $w_2 = 0.0605$; ○, $w_2 = 0.0818$; solid line, solubility curve calculated from the Wilson model with Λ_{ij} independent of the temperature.

and organic solvent, and M_1 is the average molecular weight of Softisan 100. The value of M_1 is 705 $\text{g}\cdot\text{mol}^{-1}$, which was calculated by the saponification value of Softisan 100 (the saponification value is 237 mg KOH/g obtained from the producer).

In this work, the highest measured temperature was 304.45 K, and it has already approached the melting point. As shown in Figures 3 and 4, the solubility of Softisan 100 in ethanol + water and acetone + water increases dramatically with the increase of the temperature and decreases significantly with the increase of the water content. Therefore, in the precipitation process of Softisan 100, temperature plays an important role, and water can be used as an excellent antisolvent. For the Softisan 100 + water + acetone system, the solubility of Softisan 100 with low water content at 304.45 K cannot be obtained, because the liquid−liquid−solid three-phase equilibrium temperature has already reached before the temperature was close to 304.45 K. Meanwhile, for the Softisan 100 + water + ethanol system, the liquid−liquid−solid three-phase equilibrium temperature did not reach 304.45 K. Compared with the solubilities of Softisan 100 in acetone, the solubilities of Softisan 100 in ethanol were much smaller. These differences were ascribed to the differences in solvent−solute interactions and polarity.

Correlation of Solid−Liquid Equilibrium. The solid−liquid equilibrium can be calculated by the following equation:[18]

$$-\ln(\gamma_1 x_1) = \frac{\Delta H_t}{RT_{tp}}\left(\frac{T_{tp}}{T} - 1\right) - \frac{\Delta C_p}{R}\left(\frac{T_{tp}}{T} - 1\right) + \frac{\Delta C_p}{R}\ln\left(\frac{T_{tp}}{T}\right) \qquad (3)$$

where γ_1, x_1, ΔH_t, T_{tp}, and ΔC_p are the activity coefficient of solute, the mole fraction of solute in the liquid phase, the molar enthalpy of fusion of the solute, the triple-point temperature, and the difference in solute heat capacity between the solid and the liquid at the melting point, respectively. For most substances, there is a little difference between the triple-point temperature and the normal melting point temperature and also a negligible difference between the enthalpies of fusion at these two temperatures. Thus, as a good approximation, the enthalpy and temperature at the triple point can be substituted by its values at the normal melting temperature. In addition, the two terms of eq 3 containing ΔC_p almost cancel each other. Therefore, in the case that a solid−solid phase transition does not occur, a simplified form of this equation can be used:

$$-\ln(\gamma_1 x_1) = \frac{\Delta H_f}{RT_f}\left(\frac{T_f}{T} - 1\right) \qquad (4)$$

where ΔH_f is the enthalpy of fusion at the normal melting point T_f. The melting temperature and fusion enthalpy of Softisan 100 were observed to be 305.6 K and 126.6 $\text{J}\cdot\text{g}^{-1}$, respectively. These data have small discrepancies with the results reported by Schubert and Müller-Goymann[8] because of the differences in purity of the used components.

In eq 4, the key variable is the solute activity coefficient. In this work, the Wilson model of two versions and the NRTL model were chosen to describe the activity coefficient.

Wilson Model. Wilson[19] expressed the activity coefficient for component i in a mixture as follows:

$$\ln\gamma_i = 1 - \ln\left(\sum_{j=1}^{n} x_j\Lambda_{ij}\right) - \sum_{k=1}^{n}\left(\frac{x_k\Lambda_{ki}}{\sum_{j=1}^{n} x_j\Lambda_{kj}}\right) \qquad (5)$$

where Λ_{ij} is the model parameter. There were two versions to be used to describe the solid−liquid equilibrium. In the first version, it was assumed that Λ_{ij} is temperature-independent.[20−22] In the second version, Λ_{ij} is expressed as a function of temperature, and the energy parameter $(g_{ij} - g_{ii})$ is considered independent of the temperature. Thus, the model parameter of the second version can be expressed as:

$$\Lambda_{ij} = \frac{V_j}{V_i}\exp\left(-\frac{(g_{ij} - g_{ii})}{RT}\right) = \frac{V_j}{V_i}\exp\left(-\frac{A_{ij}}{RT}\right) \qquad (6)$$

where V_i is the mole volume of the pure i component in the liquid phase, which is given in Table 3. A_{ij} is a constant.

Table 3. Physical Properties of Softisan 100,[a] Organic Solvents,[b] and Water[b]

substance	mol wt	ρ / $\text{g}\cdot\text{cm}^{-3}$	V / $\text{cm}^3\cdot\text{mol}^{-1}$	T / K
water	18	0.998	18.06	293
ethanol	46	0.789	58.39	293
acetone	58	0.790	73.52	293
Softisan 100	705	0.859	820.72	333

[a] The mole volume of Softisan 100 was calculated with the data of average molecular weight and density which was obtained from the experiment. [b] The density data of organic solvents and water were obtained from the literature.[24]

Table 4. Parameters for the Wilson and NRTL Models for Softisan 100 + Water + Ethanol and Softisan 100 + Water + Acetone

system		Wilson				NRTL	
i	j	Λ_{ij}	Λ_{ji}	A_{ij}/J·mol^{-1}	A_{ji}/J·mol^{-1}	A_{ij}/J·mol^{-1}	A_{ji}/J·mol^{-1}
Softisan 100	water	0	0	132741	69958.5	−683.984	34013.8
Softisan 100	ethanol	0.000412	0.6706	12177.8	7754.01	−896.534	4494.63
water	ethanol	4.9720	26.4285	−2072.18	−12516.3	−1254.78	1426.46
Softisan 100	water	0	0	212067	32532.5	−23.0919	31720.6
Softisan 100	acetone	0.001514	1.1125	9546.34	5728.11	−632.993	2804.06
water	acetone	3.3346	11.2523	−75166	−9894.44	−1060.99	1744.19

Table 5. Root-Mean-Square Deviations from the Description by the Wilson and NRTL Models

system	$\sigma_{\text{w1}}{}^{a}$/K	$\sigma_{\text{w2}}{}^{b}$/K	σ_{N}/K
Softisan 100 + water + ethanol	0.22	0.27	0.12
Softisan 100 + water + acetone	0.25	0.28	0.35

[a] The Wilson model with Λ_{ij} independent of the temperature. [b] The Wilson model with Λ_{ij} dependent on the temperature.

NRTL Model. In the NRTL model,[23] the activity coefficient for component i can be calculated by:

$$\ln \gamma_i = \frac{\sum_{j=1}^{\delta} \tau_{ji} G_{ji} x_j}{\sum_{j=1}^{\delta} G_{ji} x_j} + \sum_{j=1}^{\delta} \frac{x_j G_{ij}}{\sum_{k=1}^{\delta} x_k G_{kj}} \left[\tau_{ij} - \frac{\sum_{k=1}^{\delta} x_k \tau_{kj} G_{kj}}{\sum_{k=1}^{\delta} x_k G_{kj}} \right] \tag{7}$$

where G_{ij} and τ_{ij} are the model parameters, and they are expressed as follows:

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij}) \qquad \tau_{ij} = \frac{g_{ij} - g_{jj}}{RT} = \frac{A_{ij}}{RT} \tag{8}$$

where the nonrandomness parameter α_{ij} was set as 0.3.

In this work, the global optimization algorithm and Levenberg−Marquardt algorithm were employed to perform a nonlinear curve fitting. The model parameters were fitted by optimization of the following objective function:

$$F = \sum_{i=1}^{n} [\ln(\gamma_{i,\text{exp}} x_i) - \ln(\gamma_{i,\text{cal}} x_i)]^2 \tag{9}$$

where n is the number of experimental data, $\gamma_{i,\text{exp}}$ and $\gamma_{i,\text{cal}}$ are the experimental and calculated activity coefficients, respectively. For all the models, the root-mean-square deviation of temperature was used as a measure of the goodness of the fit of the solubility curves:

$$\sigma = [\sum_{i=1}^{n} (T_{i,\text{exp}} - T_{i,\text{cal}})^2/(n-1)]^{1/2} \tag{10}$$

where $T_{i,\text{exp}}$ is the experimental temperature and $T_{i,\text{cal}}$ is the calculated temperature.

The curve-fitting parameters are listed in Table 4. For the Wilson model with Λ_{ij} independent of the temperature, all of the optimized binary parameters for water and Softisan 100 are zero. Therefore, the Wilson model with Λ_{ij} independent of the temperature can provide a more simple mathematical expression for the solubility phenomena. The root-mean-square deviations of temperature for all of the models are listed in Table 5. According to the calculated results, the Wilson model with Λ_{ij} independent of the temperature gave a better description than the Λ_{ij} dependent on the temperature. The NRTL model gave the best description for Softisan 100 + water + ethanol system, while the worst description was for the Softisan 100 + water + acetone system. All in all, the root-mean-square deviations of temperature for all of the models ranged from (0.12 to 0.35) K; therefore, both the Wilson and the NRTL models can give a good description for all of the solubility data.

Conclusions

The solubility of Softisan 100 has been measured in binary ethanol + water and acetone + water mixtures between (279.95 and 304.45) K. For both of the systems, the solubility increases dramatically with the increase of the temperature and decreases significantly with the increase of the water content. Acetone is the expected solvent for dissolving the Softisan 100, and water is an excellent antisolvent in the precipitation process. The solubility data were correlated by the Wilson and NRTL models, and the calculated solubilities show a good agreement with the experimental values. The Wilson model parameter Λ_{ij} expressed as a function of temperature does not improve the accurate mathematical description for the solubility phenomena.

Literature Cited

(1) Müller, R. H.; Mäder, K.; Gohla, S. Solid lipid nanoparticles (SLN) for controlled drug delivery - a review of the state of the art. *Eur. J. Pharm. Biopharm.* **2000**, *50*, 161–177.

(2) Mehnert, W.; Mäder, K. Solid lipid nanoparticles: Production, characterization and applications. *Adv. Drug Delivery Rev.* **2001**, *47*, 165–196.

(3) Wissing, S. A.; Kayser, O.; Müller, R. H. Solid lipid nanoparticles for parenteral drug delivery. *Adv. Drug Delivery Rev.* **2004**, *56*, 1257–1272.

(4) Gasco, M. R. Lipid nanoparticles: perspectives and challenges. *Adv. Drug Delivery Rev.* **2007**, *59*, 377–378.

(5) Date, A. A.; Naik, B.; Nagarsenker, M. S. Novel drug delivery systems: Potential in improving topical delivery of antiacne agents. *Skin Pharmacol. Physiol.* **2006**, *19*, 2–16.

(6) Friedrich, I.; Reichl, S.; Müller-Goymann, C. C. Drug release and permeation studies of nanosuspensions based on solidified reverse micellar solutions (SRMS). *Int. J. Pharm.* **2005**, *305*, 167–175.

(7) Cole, E. T.; Cad, D.; Benameur, H. Challenges and opportunities in the encapsulation of liquid and semi-solid formulations into capsules for oral administration. *Adv. Drug Delivery Rev.* **2008**, *60*, 747–756.

(8) Schubert, M. A.; Müller-Goymann, C. C. Solvent injection as a new approach for manufacturing lipid nanoparticles - evaluation of the method and process parameters. *Eur. J. Pharm. Biopharm.* **2003**, *55*, 125–131.

(9) Zhang, S. H.; Shen, S. C.; Chen, Z.; Yun, J. X.; Yao, K. J.; Chen, B. B.; Chen, J. Z. Preparation of solid lipid nanoparticles in co-flowing microchannels. *Chem. Eng. J.* **2008**, *144*, 324–328.

(10) Zhang, S. H.; Yun, J. X.; Shen, S. C.; Chen, Z.; Yao, K. J.; Chen, J. Z.; Chen, B. B. Formation of solid lipid nanoparticles in a microchannel system with a cross-shaped junction. *Chem. Eng. Sci.* **2008**, *63*, 5600–5605.

(11) Yun, J. X.; Zhang, S. H.; Shen, S. C.; Chen, Z.; Yao, K. J.; Chen, J. Z. Continuous production of solid lipid nanoparticles by liquid flow-focusing and gas displacing method in microchannels. *Chem. Eng. Sci.* **2009**, *64*, 4115–4122.

(12) Privett, O.; Breault, E.; Covell, J.; Norcia, L.; Lundberg, W. Solubilities of fatty acids and derivatives in acetone. *J. Am. Oil Chem. Soc.* **1958**, *35*, 366–370.

(13) Roberts, K. L.; Rousseau, R. W.; Teja, A. S. Solubility of Long-Chain N-Alkanes in Heptane between 280 and 350 K. *J. Chem. Eng. Data* **1994**, *39*, 793–795.

(14) Jennings, D. W.; Weispfennig, K. Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd

versus even carbon number structures, and solvent chemistry on solubility. *Fluid Phase Equilib.* **2005**, *227*, 27–35.

(15) Ren, G. B.; Wang, J. K.; Yin, Q. X.; Zhang, M. J. Solubilities of Proxetine Hydrochloride Hemihydrate between 286 K and 363 K. *J. Chem. Eng. Data* **2004**, *49*, 1671–1674.

(16) Chen, S. N.; Xia, Q.; Lu, L. F.; Li, D.; Zhang, F. B.; Zhang, G. L. Solubility of Sebacic Acid in Binary Mixtures Containing Alcohols. *J. Chem. Eng. Data* **2009**, *54*, 776–780.

(17) Cepeda, E. A.; Bravo, R.; Calvo, B. Solubilities of Lauric Acid in n-Hexane, Acetone, Propanol, 2-Propanol, 1-Bromopropane, and Trichloroethylene from (279.0 to 315.3) K. *J. Chem. Eng. Data* **2009**, *54*, 1371–1374.

(18) Prausnitz, J. M.; Lichtenthaler, R. N.; de Azevedo, E. G. *Molecular Thermodynamics of Fluid-Phase Equilibria*, 3rd ed.; Prentice Hall PTR: Upper Saddle River, NJ, 1999.

(19) Wilson, G. M. Vapor-Liquid Equilibrium. XI. A New Expression for the Excess Free Energy of Mixing. *J. Am. Chem. Soc.* **1964**, *86*, 127–130.

(20) Morimi, J.; Nakanishi, K. Use of the Wilson equation to calculate solid-liquid phase equilibria in binary and ternary systems. *Fluid Phase Equilib.* **1977**, *1*, 153–160.

(21) Muir, R. F.; Howat, C. S., III. Predicting Solid-Liquid Equilibrium Data from Vapor-Liquid Data. *Chem. Eng.* **1982**, *89*, 89–92.

(22) Domanska, U. Solid-liquid phase relations of some normal long-chain fatty acids in selected organic one- and two-component solvents. *Ind. Eng. Chem. Res.* **1987**, *26*, 1153–1162.

(23) Renon, H.; Prausnitz, J. M. Estimation of Parameters for the NRTL Equation for Excess Gibbs Energies of Strongly Nonideal Liquid Mixtures. *Ind. Eng. Chem. Process Des. Dev.* **1969**, *8*, 413–419.

(24) Reid, R. C.; Prausnitz, J. M.; Poling, B. E. *The Properties of Gases and Liquids*, 4th ed.; McGraw-Hill Book Company: New York, 1987.

Received for review September 17, 2009. Accepted November 25, 2009. The authors gratefully appreciate the financial support by the Science Foundation of the National Natural Science Foundation of China (No. 20606031).

JE900754A