

**Modeling of Solid Liquid Equilibrium
for Tertiary Mixtures of Fatty Acid by Wilson Model**

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Abstract

Pure and eutectic mixtures of fatty acids are desirable phase change materials (PCMs) for low/medium thermal energy storage (TES) applications because of their high density of energy storage, biodegradability, sustainability, and compatibility with existing systems. In the current study, thermodynamics and the experimental standpoint of phase equilibrium for 10 ternary mixtures of fatty acids were considered. In this regard, an approach based on the Wilson model was developed to predict the melting temperature of fatty acids to predict the eutectic points of ternary mixtures including Capric acid, Undecanoic acid, pentadecanoic acid, Margaric and Stearic acid. It indicated that the eutectic points were close to the melting temperature of lower density compounds and for Capric+Undecanoic+Pentadecanoic the melting point has the minimum values among the other nine mixtures and equals 281.0 °C. A comparison of the derivate activity model with the experimental data represented deviations of less than 1% between experimental and predicted values.

Keywords: fatty acid; activity model; melting; ternary mixture; eutectic temperature

1. Introduction

Because of the increasing complexity and evolution of the international community, energy in the present century plays a key role in the economics and politics of a country, and accurate forecasting of the energy sector outlook and adopting appropriate solutions are key to maintaining political and economic stability. Over the past three decades, energy shortages and high prices as well as concerns about environmental problems have made it necessary to avoid energy waste. In addition, the need for additional TES and eliminating the interval between consumption and energy production has been increasingly addressed [1]. PCMs are one of the most efficient tools for TES [2-8]. By changing the phase of these materials, the thermal energy can be stored as latent heat. In studies on phase change materials, pure and eutectic mixtures of fatty acids have received greater attention due to their premiere properties. An important advantage of fatty acids is that they are the derivative of common animal oils and vegetables which, despite the scarcity of fuel sources, makes it possible to provide a safe and continuous supply. Ease of use according to the requirements is another feature of these materials [3-8]. On the other hand, fatty acid melting points for some applications like heating and cooling are very high and can be up to 30 degrees above the optimal temperature in the building [9]. Therefore, saturated fatty acid mixtures with lower temperatures have been considered [10]. For example, the melting temperatures of myristic acids and palmitic are 61 and 52 °C, respectively, which is a high temperature for storage. The temperature of melting for the eutectic mixture, however, is about 42 °C, which is suitable for solar energy storage [11].

Overall, it can be said that the thermodynamic and kinetic criteria of this group of materials are suitable for the storage of latent heat at low temperatures [6, 11, 12]. Therefore, the increasing use of the fatty acids eutectic mixture for TES necessitates further and more serious studies. In most cases with three-component mixtures, the melting temperature at the eutectic point is lower than the melting temperature of not only each of the pure materials but also the eutectic points of all binary compounds of these three substances. Therefore, three-component mixtures (due to the low melting point of their mixture) can be much more functional than two-component and single-component mixtures.

To apply these materials in the industry, quantities such as melting point and the fusion latent heat must be determined. Because of the differences between experimental results [14, 15] reported in different articles and the limited information on the thermal properties of eutectic mixtures [6], accurate and reliable experiments are needed. The development of thermodynamic activity models can aid the estimation of thermal properties and phase behavior of fatty acid mixtures [16, 17].

Most thermodynamic models have been improved to predict only the eutectic point [17-19], yet it is crucial to predict the pre-eutectic point, too, where the component is formed in the solid phase [20, 21].

Many investigations have been done on preparing and characterizing the binary mixture of phase change materials [22-28], but studies on the ternary mixture of fatty acids are still limited [29, 30].

Mirpoorian et al. studied the S-L phase equilibrium for binary mixtures of a group of fatty acids. They developed NRTL, UNIQUAC, and Wilson activity models to determine eutectic points and estimate melting temperature as functions of mole fraction [31, 32]. They found a good agreement between predictions from thermodynamic models and experimental results.

Parveen et al [33] developed thermochemical characterizing and considered the eutectic mixture biological safety of fatty acids as a new form for temperature sensitive potential of drug release because of their attractive and inimitable characteristics like consistency, safety, and facility of accessibility. Zhou et al [34] prepared some binary eutectic mixtures of fatty acids by use decanoic acid, dodecanoic acid, tetradecanoic acid, hexadecanoic acid, and octadecanoic acid as raw materials for latent heat TES. Results showed that reported fatty acid binary eutectic mixtures were worthy as TES materials for systems with low temperatures. Fan et al [35] studied the thermophysical properties, consistency, and dependability of dodecanoic acid binary eutectic mixtures for the efficiency of building energy. They reported that dodecanoic acid binary eutectic phase change materials showed great thermal properties and chemical structure after five hundred cold and hot cycles. Ma et al [36], because of the prompt need for latent heat TES in the field of cryogenic and the application of renewable energy resources, predicted the eutectic mass ratios and thermophysical properties of three novel eutectic PCMs (methyl dodecanoic/dodecanoic acid, methyl dodecanoic/tetradecanoic acid, and methyl dodecanoic/ hexadecanoic acid) which are validated and determined through the hot disk method and DSC (differential scanning calorimetry).

In the current study, the thermodynamic and experimental aspects of S-L phase equilibrium for 10 tertiary mixtures of five fatty acids, comprising capric acid, undecanoic acid, pentadecanoic acid, heptadecanoic (margaric) acid, and octadecanoic (stearic) acid, using the DSC technique studied. The mixtures of Fatty acids PA+MA+SA, UA+MA+SA, UA+PA+SA, UA+PA+MA, CA+MA+SA, CA+PA+SA, CA+PA+MA, CA+UA+SA, CA+UA+MA and CA+UA+PA were investigated, and the experimental results of the 10 mixtures were correlated by using the Wilson [37] activity model.

2. Materials and methods

2.1. Materials

All materials were purchased from Merck Company with more than 98% purity.

The thermophysical properties of the fatty acids were measured by DSC (DSC-60 Shimadzu, Japan), illustrated in Table 1 as mentioned in previous work [38]

Table 1: fatty acid thermal properties

Material	T_{melt} (K)	λ^* (J/mol)
Capric acid	304.8	27.79
Undecylenic acid	301.7	25.98
Pentadecanoic acid	325.7	41.53
Margaric acid	334.2	51.33
Stearic acid	342.7	61.21

* λ : latent heat

2.2. Preparation of ternary mixtures

In this study, pseudo-binary mixtures were considered ternary mixtures. A binary eutectic mixture of two fatty acids (A&B, for example) and another fatty acid (C, for example) were considered as the pseudo-first and pseudo-second component, respectively. The mass ratio of A and B in the pseudo-first components (binary mixtures of four considered fatty acids) as well as latent heat and melting temperature in eutectic points were obtained from Mirpoorian et al. and shown in Table 2 [31, 32].

Table2: Thermophysical properties of binary fatty acid system [31, 32]

Mixtures		Mass ratio	$T_{eutectic}$ (K)	λ (kJ/mol)
Comp. 1	Comp. 2	Comp.1:Comp2		
capric acid(CA)	Undecylenic acid(UA)	0.457:0.543	284.7	25.04
capric acid(CA)	Pentadecanoic acid(PA)	0.764:0.236	297.5	30.29
capric acid(CA)	Margaric acid(MA)	0.869:0.131	300.9	30.53
Undecylenic acid(UA)	Pentadecanoic acid(PA)	0.794:0.206	295.0	27.92
Undecylenic acid(UA)	Margaric acid(MA)	0.889:0.111	298.2	27.91
Pentadecanoic acid(PA)	Margaric acid(MA)	0.643:0.357	316.5	43.30

Initially, binary mixtures were prepared as pseudo-first components according to the ratios listed in Table 2 and then mixed with third components in different combination ratios. For example, CA and UA were blended in a 0.457:0.543 ratio; then this pseudo-single component was mixed with PA in different compositions.

The thermal properties of the prepared mixtures were measured by DSC tests performed by use of Diamond DSC (Perkin Elmer, USA), under N₂, with the heating and cooling rate of 10 °C/min, in the range of 268-323 K. The peak of DSC curves represents the melting point of the materials, and the λ was measured using the area below each peak.

2.3. Eutectic point determination

In the DSC heating curve of eutectic mixtures, only one peak appears, while non-eutectic binary mixtures have two separate peaks, each corresponding to one of the components of the mixture. As mentioned above, pseudo-binary mixtures with different ratios were synthesized, and their DSC heating curves were plotted.

To determine the pseudo-binary mixture eutectic point, the temperature changes of these two peaks (T₁ and T₂) versus the mass ratio of the pseudo-second component (X) were plotted on a graph. The intersection of these two curves gave the X in the eutectic mixture.

For all pseudo-binary (ternary) mixtures, the composition of the components at the eutectic point was obtained using the method presented in Table 3.

Table 3: the composition of the eutectic Pseudo binary mixtures

Pseudo-binary mixture		mass ratio %
Comp.1	Comp.2	Comp.1:Comp.2
(CA+UA)	PA	90.0:10.0
(CA+UA)	MA	96.3:3.7
(CA+UA)	SA	98.0:2.0
(CA+PA)	MA	91.4:8.6
(CA+PA)	SA	95.5:0.045
(CA+MA)	SA	94.3:5.7
(UA+PA)	MA	92.6:7.4
(UA+PA)	SA	96.2:3.8
(UA+MA)	SA	95.3:4.7
(PA+MA)	SA	84.5:15.5

Eutectic pseudo-binary (ternary) mixtures based on the ratios shown in Table 3 were prepared, and DSC tests were carried out on them using the previously explained procedure.

3. Thermodynamic model

3.1. General model for liquid phase

For the binary mixture of fatty acids, the T-x diagram, which represents the solid-liquid equilibrium, consisted of three regions.

Region I is illustrated by the liquid line, where the second component is the solid phase; Region II is formed when the first component is in the solid phase; and Region III, if any, is where the solid phase is the compound of components 1 and 2. In this study, no presence of a component in the solid phase was observed. Thus, Region III was ignored.

The following equations show the S-L phase equilibrium for fatty acid binary or pseudo-binary mixtures [39]:

Region I

The melting temperature of mixture in region I is presented in Eq (1):

$$T = \frac{\Delta h_{f2}}{\frac{\Delta h_{f2}}{T_{f2}} - R \cdot \ln [(1 - x_1) \cdot \gamma_2^l]} \quad (1)$$

Region II

The melting temperature of mixture in region II is presented in Eq (2):

$$T = \frac{\Delta h_{f1}}{\frac{\Delta h_{f1}}{T_{f1}} - R \cdot \ln [x_1 \cdot \gamma_1^l]} \quad (2)$$

where ΔH_{fi} is latent heat of fusion, T_{fi} is melting temperature, γ_i^l is activity coefficient of component i in the liquid phase; x_1 is the molar fraction of first component, and T is the mixture melting temperature.

In the above equations, activity coefficients γ_i^l are a function of T and x_i^l . Therefore, temperature is implicit and should be found using the iterative approach.

3.1.3. Latent heat of fusion for pseudo-binary blends

Latent heat of fusion for the mixtures of fatty acids can be achieved by using the Eq(3) [36]:

$$H_m = T_m \sum_{i=1}^n \left[\frac{X_i H_i}{T_i} + X_i (C_{PLi} - C_{PSi}) \ln \frac{T_m}{T_i} \right] \quad (3)$$

wherein H_m is the latent heat of fusion for the binary blends in J/mol and C_{PSi} and C_{PLi} are the specific heat at constant pressure of component i at solid and liquid phases, respectively. For long-chain fatty acid compounds, it can be ignored from $(C_{PLi} - C_{PSi})$ versus sensible heat term, therefore H_m is (Eq(4)):

$$H_m = T_m \left[\frac{x_1 \Delta h_{f1}}{T_{f1}} + \frac{(1-x_1) \Delta h_{f2}}{T_{f2}} \right] \quad (4)$$

3.2. Wilson model for liquid phase

Wilson [37] proposed the following equation for the excess Gibbs free energy of a binary mixtures as dedicated in Eq(5).

$$\frac{g^E}{RT} = -x_1 \ln(x_1 + \Lambda_{12}x_2) - x_2 \ln(x_2 + \Lambda_{21}x_1) \quad (5)$$

The derivative activity coefficients from Wilson equation are presented in Eqs (6)&(7):

$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12}x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right) \quad (6)$$

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21}x_1) - x_1 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right) \quad (7)$$

In this study, according to Eqs (1), (2), (6), and (7), the liquefied phase is modeled on the basis of the Wilson model for two different equilibrium regions (Eqs (8)&(9)).

3.2.1. Region I

$$T_1 = \frac{\Delta h_{f2}}{\frac{\Delta h_{f2}}{T_{f2}} - R \left[\ln(1-x_1) - \ln(x_2 + \Lambda_{21}x_1) - x_1 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right) \right]} \quad (8)$$

3.2.2. Region II

$$T_2 = \frac{\Delta h_{f1}}{\frac{\Delta h_{f1}}{T_{f1}} - R \left[\ln x_1 - \ln(x_1 + \Lambda_{12}x_2) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + x_2} \right) \right]} \quad (9)$$

3.2.3. Eutectic point

Because of no existence of Region III in the investigated mixtures ($v_1 < 0$, $v_2 < 0$ and $\Delta G_R^\circ \geq 0$), the mole fraction of the eutectic point can be achieved by using Eq(10).

$$\frac{\Delta h_{f1}}{T_{f1}} - R \left[\ln x_1 - \ln(x_1 + \Lambda_{12}(1-x_1)) + x_2 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}(1-x_1)} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + (1-x_1)} \right) \right] = \frac{\Delta h_{f2}}{T_{f2}} - R \left[\ln(1-x_1) - \ln(x_2 + \Lambda_{21}x_1) - x_1 \left(\frac{\Lambda_{12}}{x_1 + \Lambda_{12}(1-x_1)} - \frac{\Lambda_{21}}{\Lambda_{21}x_1 + (1-x_1)} \right) \right] \quad (10)$$

4. Results and discussions

In this study, ten ternary mixtures as pseudo-binary mixtures of fatty acids were considered.

Figure 1 shows the DSC curves of heating for these eutectic mixtures.

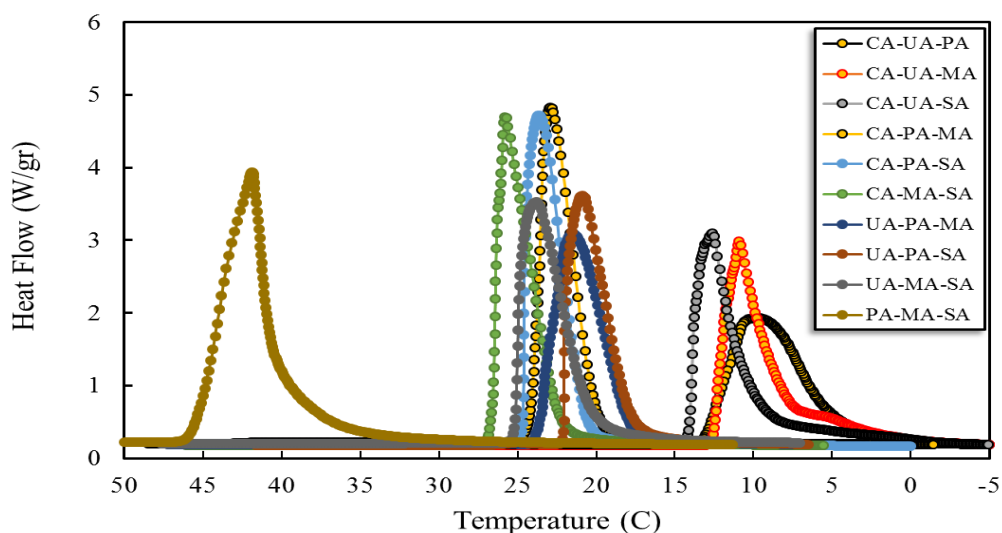


Figure 1: DSC curves of heating for ten ternary components

As can be seen from Figure 1, for all ternary mixtures of fatty acids, only one long peak appeared in the DSC curve.

Applying the Wilson activity equation to the ternary (pseudo binary) systems of fatty acids, the eutectic temperatures and the corresponding mixing proportions of (CA + UA): PA, (CA + UA): MA, (CA + UA): SA, (CA + PA): MA, (CA + PA): SA, (CA + MA): SA, (UA + PA): MA, (UA + PA): SA, (UA + MA): SA and (PA + MA): SA mixtures were obtained. Table 4 shows the comparisons between the calculated and experimental results.

Table 4: The theoretical (Wilson) and experimental eutectic points of ternary fatty acid system.

Tertiary mixture			Ternary mass ratio %	Theoretical eutectic points (K)	Experimental eutectic points (K)
Comp.1	Comp.2	Comp.3	Comp1:Comp2:Comp3		
CA	UA	PA	41.1:48.9:10	282.2	281.0
CA	UA	MA	44.0:52.3:3.7	283.7	282.4
CA	UA	SA	44.8:53.2:2.0	284.4	283.5
CA	PA	MA	69.8:21.7:8.6	295.0	294.0
CA	PA	SA	72.9:22.9:4.5	296.5	295.1
CA	MA	SA	82.0:12.4:5.7	299.7	298.5
UA	PA	MA	73.9:18.7:7.4	294.2	295.3
UA	PA	SA	76.8:19.4:3.8	294.4	296.2
UA	MA	SA	85.2:10.1:4.7	297.8	298.5
PA	MA	SA	54.8:29.7:15.5	313.7	315.1

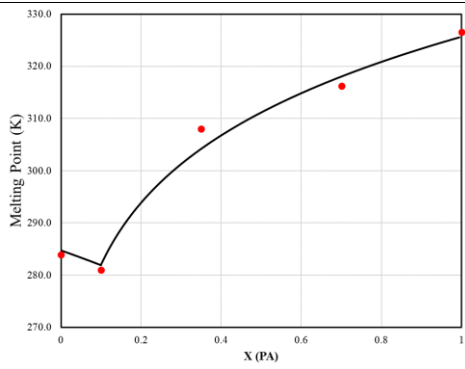
The ratio of components in the ternary mixture, shown in Table 4, is as follows; for example, as indicated in Table 2, the mass fraction at the eutectic temperature of CA - UA binary blend is 45.7:54.3. Hence, for the pseudo-binary mixture of (CA-UA) and PA, the experimental mass fraction at the eutectic temperature was 90:10 (CA + UA: PA), which is equivalent to the mass fraction of 41.1:48.9:10 for the ternary system of CA: UA: PA

The characteristics of the ternary mixture were similar to those of the pseudo-binary blend through the mentioned analysis, so the Wilson activity equation was applied to the tertiary fatty acid mixtures. According to the experimental data, the Wilson activity equation estimated the S-L equilibrium phase transition. The Wilson model parameters for phase diagrams are presented in Table 5.

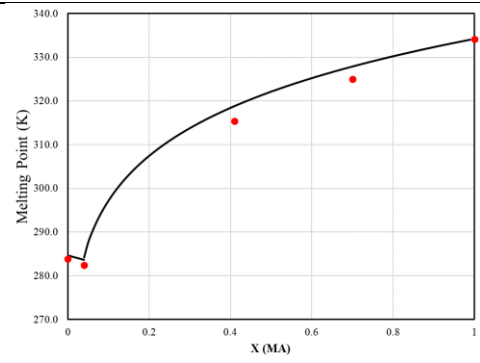
Table 5: Computed parameters of Wilson for ten investigated binary mixtures of fatty acids

<i>pseudo -binary mixture</i>		Eq (8)		Eq (9)	
<i>Comp.1</i>	<i>Comp.2</i>	Λ_{12}	Λ_{21}	Λ_{12}	Λ_{21}
(CA+UA)	PA	1.0154	0.983	0.983	1.0194
(CA+UA)	MA	1.0267	0.974	0.973	1.0271
(CA+UA)	SA	1.0215	0.991	0.982	1.0259
(CA+PA)	MA	1.0214	0.962	0.966	1.0321
(CA+PA)	SA	1.0254	0.971	0.978	1.0211
(CA+MA)	SA	1.0277	1.008	1.015	0.994
(UA+PA)	MA	0.997	1.011	1.009	1.024
(UA+PA)	SA	1.0357	0.973	0.974	1.0269
(UA+MA)	SA	0.989	0.952	1.052	1.0061
(PA+MA)	SA	1.019	0.992	0.984	1.0212

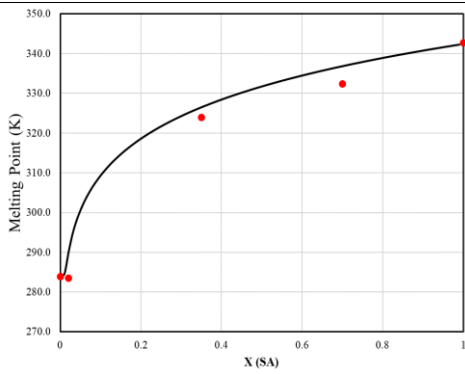
Figure 2(a-j) shows the results of comparisons of computed values using Eq. (8) and (9) for the Wilson equation along with the experimental data for CA + UA): PA, (CA + UA): MA, (CA + UA): SA, (CA + PA): MA, (CA + PA): SA, (CA + MA): SA, (UA + PA): MA, (UA + PA): SA, (UA + MA): SA and (PA + MA): SA pseudo-binary blends, respectively. In these phase diagrams, X1 is the molar ratio of the pseudo-first component (the mixture in the eutectic composition of x1 and x2) and T is the melting temperature in Kelvin.



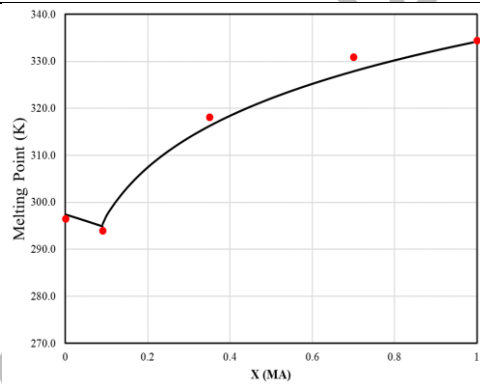
2a) $(CA+UA)_{(1)} + PA_{(2)}$



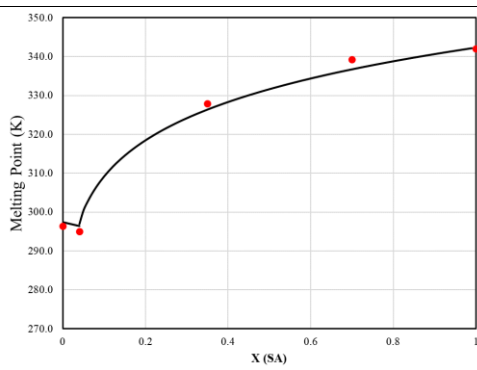
2b) $(CA+UA)_{(1)} + MA_{(2)}$



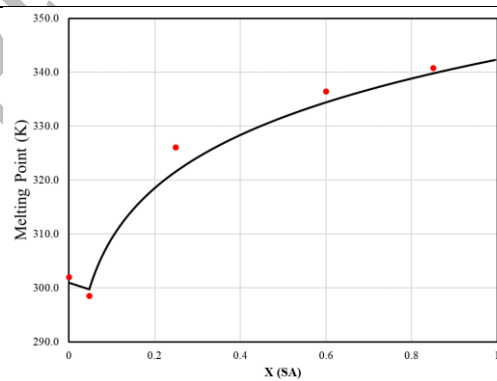
2c) $(CA+UA)_1 + SA_2$



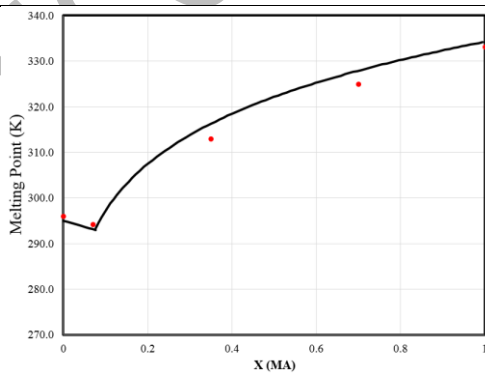
2d) $(CA+PA)_1 + MA_2$



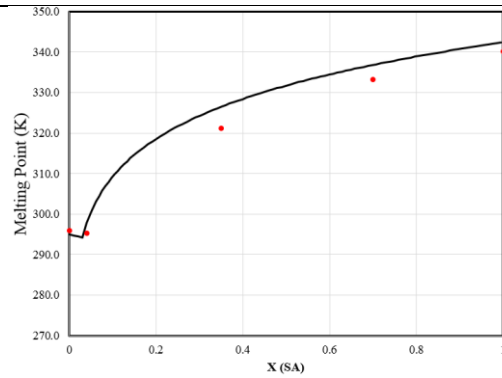
2e) $(CA+PA)_1 + SA_2$



2f) $(CA+MA)_1 + SA_2$



2g) $(UA+PA)_1 + MA_2$



2h) $(UA+PA)_1 + SA_2$

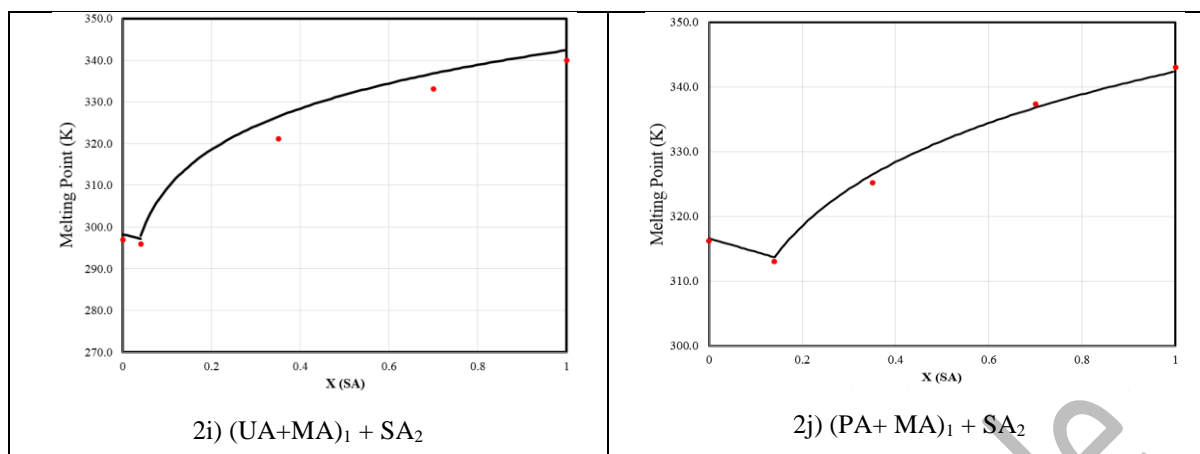


Figure 2: Diagram for solid - liquid equilibrium of pseudo-binary blends

Case study 1 (Figure 2a) is the pseudo-binary blend of (CA: UA): PA in saturation form. The eutectic points of CA: UA as the pseudo-single component were retrieved from previous work [31] and equaled 284.7 K. The ternary melting temperature of CA: UA: PA is equal to 282.2 K at the eutectic point. As shown in Figure 2a, the existence of the eutectic point was predicted at 0.900 for $x_1(\text{CA: UA})$ by Wilson.

Case study 2 (Figure 2b) is the pseudo-binary blend of (CA: UA): MA in saturation form. The eutectic points of CA: UA equaled 284.7 K. The ternary melting temperature of CA:UA: MA is equal to 283.7 K at the eutectic point. As shown in Figure 2b, the existence of the eutectic point was predicted at 0.963 for $x_1(\text{CA: UA})$ by Wilson.

Case study 3 (Figure 2c) is the pseudo-binary blend of (CA: UA): SA in saturation form. The eutectic points of CA: UA equaled 284.7 K. The ternary melting temperature of CA:UA: SA is equal to 284.4 K at the eutectic point. As shown in Figure 2c, the existence of the eutectic point was predicted at 0.980 for $x_1(\text{CA: UA})$ by Wilson.

Case study 4 (Figure 2d) is the pseudo-binary blend of (CA: PA): MA in saturation form. The eutectic points of CA: PA equaled 297.5 K. The ternary melting temperature of CA:PA: MA is equal to 295.0 K at the eutectic point. As shown in Figure 2d, the existence of the eutectic point was predicted at 0.914 for $x_1(\text{CA: PA})$ by Wilson.

Case study 5 (Figure 2e) is the pseudo-binary blend of (CA: PA): SA in saturation form. The eutectic points of CA: PA equaled 297.5 K. The ternary melting temperature of CA:PA: SA is equal to 296.5 K at the eutectic point. As shown in Figure 2e, the existence of the eutectic point was predicted at 0.955 for $x_1(\text{CA: PA})$ by Wilson.

Case study 6 (Figure 2f) is the pseudo-binary blend of (CA: MA): SA in saturation form. The eutectic points of CA: MA equaled 300.9 K. The ternary melting temperature of CA:MA: SA is equal to 279.7 K at the eutectic point. As shown in Figure 2f, the existence of the eutectic point was predicted at 0.943 for $x_1(\text{CA: MA})$ by Wilson.

Case study 7 (Figure 2g) is the pseudo-binary blend of (UA: PA): MA in saturation form. The eutectic points of UA: PA equaled 295.0 K. The ternary melting temperature of UA:PA: MA is equal to 294.2 K at the eutectic point. As shown in Figure 2g, the existence of the eutectic point was predicted at 0.926 for $x_1(\text{UA: PA})$ by Wilson.

Case study 8 (Figure 2h) is the pseudo-binary blend of (UA: PA): SA in saturation form. The eutectic points of UA: PA equaled 295.0 K. The ternary melting temperature of UA:PA: SA is equal to 294.4 K at the eutectic point. As shown in Figure 2h, the existence of the eutectic point was predicted at 0.962 for $x_1(\text{UA: PA})$ by Wilson.

Case study 9 (Figure 2i) is the pseudo-binary blend of (UA: MA): SA in saturation form. The eutectic points of UA: MA equaled 298.2 K. The ternary melting temperature of UA:MA: SA is equal to 297.8 K at the eutectic point. As shown in Figure 2i, the existence of the eutectic point was predicted at 0.953 for $x_1(\text{UA: PA})$ by Wilson.

Case study 10 (Figure 2j) is the pseudo-binary blend of (PA: MA): SA in saturation form. The eutectic points of PA: MA equaled 316.5 K. The ternary melting temperature of PA:MA: SA is equal to 313.7 K at the eutectic point. As shown in Figure 2j, the existence of the eutectic point was predicted at 0.845 for $x_1(\text{UA: PA})$ by Wilson.

The results indicate a good compromise for all ten case studies.

Since the correlation of the experimental measurements was performed using the Wilson model, the average absolute relative deviations (AARD) of melting temperature values of pseudo-binary blends calculated from the Wilson activity model can be achieved by using the Eq (11):

$$AARD = 100 \sum_{i=1}^N \frac{|T_{exp,i} - T_{calc,i}|}{T_{exp,i}} / N \quad (11)$$

where N is the number of data, T_{calc} and T_{exp} are the calculated and experimental temperatures, respectively. The deviation between the calculated and experimental data of melting temperatures for the ten investigated ternary mixtures by Wilson is presented in Table 6.

Table 6: AARD% of ten considered ternary mixtures correlated by Wilson model

T_{exp}/K	X	T_{calc}/K	AARD %	T_{exp}/K	x	T_{calc}/K	AARD %
(Capric:Undecylenic) + Pentadecanoic				(Capric:Undecylenic) + Margaric			
283.9	0.00	284.5	0.21	283.9	0.00	284.5	0.21
281.0	0.10	282.2	0.43	282.4	0.04	283.7	0.46
308.0	0.35	304.2	1.23	315.4	0.41	308.6	2.16
316.2	0.70	318.1	0.60	325.0	0.70	319.7	1.63
326.5	1.00	325.6	0.28	334.2	1.00	334.5	0.09
Average			0.55	Average			0.91
(Capric:Undecylenic) + Stearic				(Capric: Pentadecanoic) + Margaric			
283.9	0.00	284.5	0.21	296.5	0.00	297.2	0.24
283.5	0.02	284.4	0.32	294.0	0.09	295.0	0.34
324.0	0.35	326.5	0.77	318.2	0.35	316.3	0.60
332.5	0.70	336.8	1.29	331.0	0.70	327.9	0.94
342.8	1.00	342.4	0.10	334.5	1.00	334.1	0.10
Average			0.54	Average			0.44
(Capric: Pentadecanoic) + Stearic				(Capric: Margaric) + Stearic			
296.5	0.00	297.2	0.24	302.0	0.00	300.4	0.53
295.1	0.04	296.5	0.47	298.5	0.05	299.7	0.40
328.0	0.35	326.5	0.46	326.0	0.25	321.5	1.38
339.3	0.70	336.8	0.74	336.4	0.60	334.6	0.54
342.1	1.00	342.4	0.09	340.8	0.85	342.3	0.44
Average			0.40	Average			0.66
(Undecylenic:Pentadecanoic) + Margaric				(Undecylenic:Pentadecanoic) + Stearic			
296.0	0.00	295.1	0.30	296.0	0.00	295.1	0.30
294.2	0.075	293.3	0.31	295.3	0.03	294.4	0.30
313.0	0.35	316.3	1.05	321.2	0.35	326.5	1.65
325.0	0.70	327.6	0.80	333.2	0.70	336.8	1.08
333.2	1.00	334.4	0.36	340.1	1.00	342.3	0.65
Average			0.56	Average			0.80
(Undecylenic:Margaric) + Stearic				(Pentadecanoic:Margaric) + Stearic			
297.0	0.00	298.2	0.40	316.2	0.00	316.5	0.09
296.0	0.04	297.8	0.61	313.0	0.14	313.8	0.26
321.2	0.35	326.5	1.65	325.2	0.35	326.5	0.40
333.2	0.70	336.8	1.08	337.4	0.70	337.0	0.12
340.1	1.00	342.3	0.65	343.0	1.00	342.3	0.20

Average	0.88	Average	0.21
Temperature measurement uncertainty : ± 0.5 K			

As can be observed from Table 6, the highest AARD% of the Wilson model is 0.91% for (Capric: Undecylenic) + Margaric acid ternary mixture.

Conclusion

In this study, the phase equilibrium of ten ternary mixtures of fatty acids for S-L phase equilibrium was determined. The equilibrium data and eutectic temperature of PA+MA+SA, UA+MA+SA, UA+PA+SA, UA+PA+MA, CA+MA+SA, CA+PA+SA, CA+PA+MA, CA+UA+SA, CA+UA+MA and CA+UA+PA ternary blends were measured. The eutectic and melting points were estimated from the obtained curves. The Wilson model was a derivation for estimating the melting temperature of fatty acid ternary blends as a function of the molar ratio. The experimental values of ten ternary blends were correlated using the Wilson activity equation. To compare the experimental data and melting point values of Wilson, the average absolute deviations were calculated. The approaches in this study are generalizable to other three-component mixtures of fatty acids. The results revealed that the eutectic points were close to the melting temperature of lower density compounds and for CA:UA: PA, the mixture melting point is 281.0 °C and has the minimum values among the other nine ternary mixtures. A comparison of the derivate activity model with the experimental data represented AARD=0.91% between experimental and predicted values. Some of these recommended materials can be utilized for medium-temperature energy storage applications. On the other hand, there is still a strong need for carrying out more research in this field for using PCMs in cold regions by using low melting temperature PCMs.

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