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Theoretical Prediction and Experimental Research of the Thermal Properties of Fatty Acid Mixtures

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Abstract. The theoretical calculation formula was used to predict the phase transition temperature and latent heat of the binary mixtures. Phase transition temperature and latent heat were experimentally studied by differential scanning calorimeter and compared with theoretical and experimental values. It is proved that the theoretical calculation formula was feasible to predict the phase change temperature and latent heat of fatty acid mixtures. Capric acid, stearic acid, myristic acid, palmitic acid and lauric acid organic phase-change materials were mixed to prepare binary mixtures. The results showed that the experimental data of phase transition temperature and latent heat of the binary mixtures were in good agreement with the theoretical ones. The results provide a reference and basis for the theoretical prediction of phase transition temperature and latent heat of phase transition for fatty acid mixtures.

1. Introduction

The application of phase change materials in the field of energy storage has broad prospects, and a single phase change material cannot meet people's needs in many cases. Composite phase change materials formed by mixing different phase change materials can increase the latent heat of phase change, lower the melting point and improve the heat storage performance. Therefore, the application of composite phase change materials is more universal. When phase change materials are used in practice, the selection of phase transition temperature and latent heat is a key issue. We test the phase transition temperature and latent heat of the composite phase change material by experimental methods, which will be affected by the purity of the sample, the error of the instrument, the time consumption of the experiment, and the investment. If the phase change temperature can be calculated with a suitable formula and the calculation of latent heat has an irreplaceable advantage.

Professor Zhang Yiping [1] provides a method for the theoretical calculation of composite phase change materials based on the second law of thermodynamics and the theoretical calculation method of melting point and heat of fusion of the (quasi) eutectic system. Che Deyong [2] et al. theoretically deduced the phase transition temperature and latent heat of binary nitrate and compared it with the experimental values. Prove the feasibility of the theoretical formula. Liu Wei [3] theoretically predicted the phase transition temperature and latent heat of quaternary mixed nitrate, and used the differential scanning calorimeter to carry out experimental tests. Compared with the theoretical values, the correctness of the theoretical formula was verified. The research provides reference value. Yuan Yanping [4] and others selected a mixture of six fatty acids, such as capric acid, stearic acid, palmitic acid, myristic acid, lauric acid and butyl stearate, to prepare a mixture of dibasic fatty acids. The formula and experimental methods were used to analyze the phase transition temperature and latent heat of the dibasic fatty acids. The results show that the calculated values of the theoretical formula



agree well with the experimental values. Liu Cheng [5] et al. prepared a mixture of ternary fatty acids with lauric acid, myristic acid and palmitic acid, and calculated the phase transition temperature and latent heat of the ternary fatty acid according to the formula of the mixture of dibasic fatty acids, and the experimental values. In contrast, the results show that the theoretical calculation formula is feasible for the calculation of ternary fatty acids and expands the choice of fatty acid mixture.

In this paper, four kinds of fatty acid organic phase change materials were selected and mixed into two kinds of fatty acid mixtures according to different ratios. A total of 20 binary mixture samples were obtained, and the phase transition temperature and latent heat of phase change were obtained by solid-liquid phase change mixture. The theoretical calculation formula is used for calculation, and the phase transition temperature and latent heat of the prepared binary mixture sample are experimentally tested by differential scanning calorimetry (DSC) to obtain experimental values. The theoretical value is compared with the experimental value to verify the feasibility of the formula.

2. Experimental Test and Results

2.1 Experimental Equipment and Materials

The experimental equipment and instruments include the 200PC type differential scanning calorimeter (DSC), analytical balance, beaker, infrared lamp, enamel, glass rod, etc. of the German NETZSCH.

The experimental materials were all from Beijing Guoyao Group Chemical Reagent Co., Ltd., and the heat storage performance is shown in Table 1.

Table 1. Material heat storage performance

Experimental Materials	Phase transition temperature (°C)	Phase change latent heat (J/g)	Molecular weight
Capric acid (C ₁₀ H ₂₀ O ₂)	30.5	151.1	172.3
Myristic acid (C ₁₄ H ₂₈ O ₂)	52.7	217.6	228.4
Stearic acid (C ₁₈ H ₃₆ O ₂)	67.4	239.9	284.6
Palmitic acid (C ₁₆ H ₃₂ O ₂)	61.0	241.0	256.5
Lauric acid (C ₁₂ H ₂₄ O ₂)	42.8	222.3	200.3

2.2 Preparation of Samples

Four different kinds of fatty acids were mixed in two to two according to different mass ratios to prepare a binary mixture of fatty acids. According to the determined material mass ratio, the electronic balance is weighed and placed in a beaker, and then irradiated with an infrared lamp. When the solid acid is melted into a liquid, it is shaken and stirred until it is uniformly mixed. Subsequently, the infrared lamp was removed and the mixture was allowed to cool and solidify in a room temperature environment. Each experimental sample was numbered, the total weight was not more than 15 mg, and it was weighed in an aluminum crucible and pressed with a capping machine for use. Sample number and composition, as shown in Table 2.

Table 2. Sample number and composition

Numbering	ingredient	Mass ratio	Numbering	ingredient	Mass ratio	Numbering	ingredient	Mass ratio
1	capric acid: palmitic acid	1: 9	8	capric acid: myristic acid	8: 2	15	Stearic acid: palmitic acid	5: 5
2	capric acid: palmitic acid	6: 4	9	capric acid: lauric acid	1: 9	16	Stearic acid: palmitic acid	9: 1
3	capric acid: palmitic acid	7: 3	10	capric acid: lauric acid	6: 4	17	Stearic acid: myristic acid	1: 9
4	capric acid: palmitic acid	8: 2	11	capric acid: lauric acid	7: 3	18	Stearic acid: myristic acid	4: 6
5	capric acid: myristic acid	1: 9	12	capric acid: lauric acid	8: 2	19	Stearic acid: myristic acid	5: 5
6	capric acid: myristic acid	6: 4	13	Stearic acid: palmitic acid	1: 9	20	Stearic acid: myristic acid	9: 1
7	capric acid: myristic acid	7: 3	14	Stearic acid: palmitic acid	4: 6			

2.3 Experimental Process

Each sample was sequentially tested using a differential scanning calorimeter (DSC), and the phase transition temperature and latent heat of phase change of the sample were determined by software. Each sample was subjected to three sampling tests, and the average of three test results was taken as the final experimental result. During the use of DSC, liquid nitrogen is used for cooling. Both the shielding gas and the purge gas are made of high-purity nitrogen, wherein the shielding gas has a gas flow rate of 65 ml/min and the purge gas has a gas flow rate of 15 ml/min. The temperature control range is from -100 to -150°C.

2.4 Experimental Results

The experimental results of the phase transition temperature and latent heat of phase change of the 20 experimental samples prepared are shown in Figures 1 to 5.

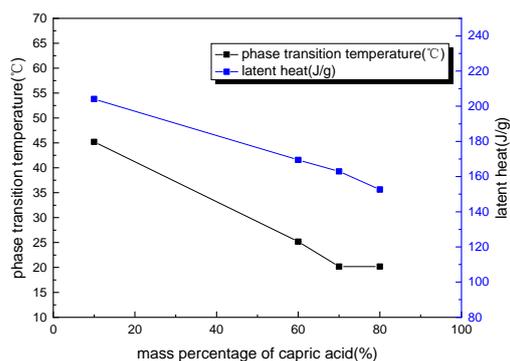


Figure 1. Capric acid in different ratios with myristic acid, experimental values of phase transition temperature and latent heat

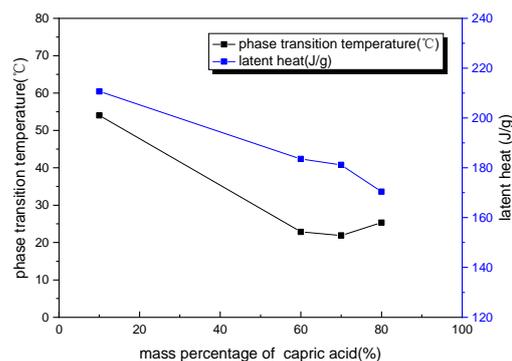


Figure 2. Capric acid in different ratios with palmitic acid, Experimental values of phase transition temperature and latent heat

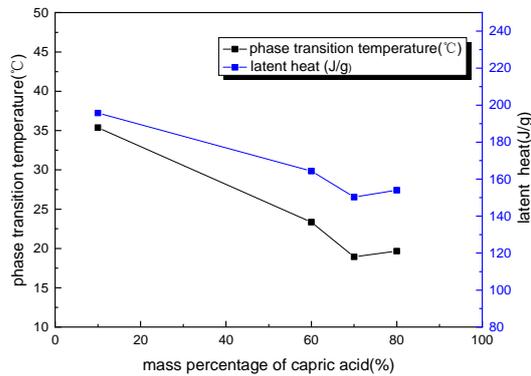


Figure 3. Experimental values of phase transition temperature and latent heat of capric acid and lauric acid in different ratios

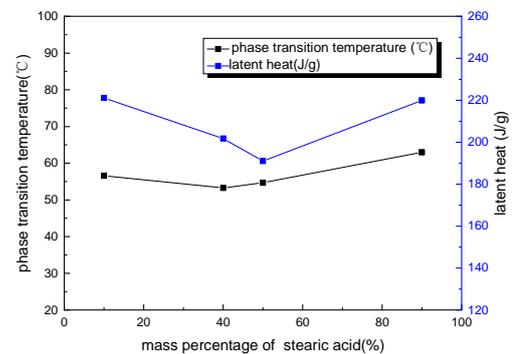


Figure 4. Experimental values of phase transition temperature and latent heat of Stearic acid and palmitic acid in different ratios

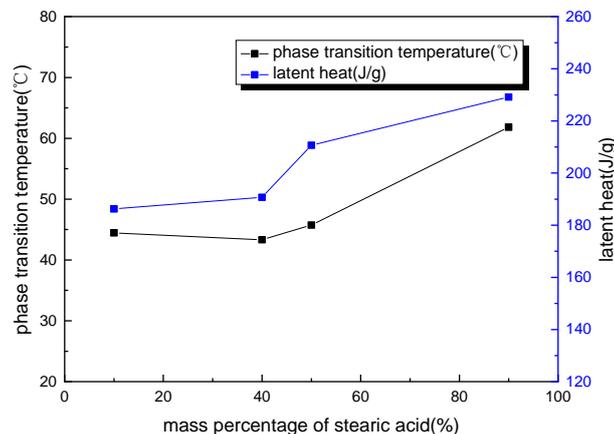


Figure 5. Experimental values of phase transition temperature and latent heat of stearic acid and myristic acid at different ratios

3. Selection and Calculation of Theoretical Prediction Formula

3.1 Theoretical Prediction Formula Selection

Professor Zhang Yiping [1] introduced the theoretical prediction formula of phase transition temperature and latent heat of N-ary mixed eutectic system based on the theory that entropy is state quantity and entropy change is independent of path. The theoretical prediction formula of phase transition temperature is shown in formula (1).

$$T_m = \left(\frac{1}{T_i} - \frac{R \ln X_i}{H_i} \right)^{-1} \quad (1)$$

In the formula:

T_m - phase transition temperature of the mixture, K;

T_i —the phase transition temperature of component i, K;

X_i - the mole percent of component i in the mixture;

H_i - latent heat of phase change of component i, J/mole.

The prediction formula of the latent heat theory of phase change is shown in formula (2).

$$H_m = T_m \sum_{i=1}^n \left[\frac{X_i H_i}{T_i} + X_i (C_{pli} - C_{psi}) \ln \frac{T_m}{T_i} \right] \quad (2)$$

In the formula:

H_m - latent heat of phase change of the mixture, J / mole;

C_{pli} —the specific pressure specific heat capacity of component i in the molten state, J/(Kg·K);

C_{psi} —the specific pressure specific heat capacity of component i in a solid state, J/(Kg·K);

Since the range of temperature change is small before and after the phase change process, $C_{pli} = C_{psi}$ can be approximated.

Then equation (2) can be simplified to equation (3).

$$H_m = T_m \sum_{i=1}^n \frac{X_i H_i}{T_i} \quad (3)$$

3.2 Theoretical Calculation of Phase Transition Temperature and Latent Heat of Fatty Acid Binary Mixture

According to the above theoretical prediction formula, the phase transition temperature and latent heat of phase change of a binary mixture of capric acid, stearic acid, myristic acid and palmitic acid mixed in different ratios were theoretically calculated. The four fatty acids selected were identical to those selected for the experiment. The theoretical calculation results are shown in Tables 3-7.

Table 3. Theoretical calculations of phase transition temperature and latent heat of capric acid and myristic acid at different ratios

Mass percentage	Phase transition temperature (°C)	Phase change latent heat (J/g)
1: 9	49.28	210.48
6: 4	20.56	165.24
7: 3	22.47	162.19
8: 2	22.98	157.43

Table 4. Theoretical calculations of phase transition temperature and latent heat of capric acid and palmitic acid at different ratios

Mass percentage	Phase transition temperature (°C)	Phase change latent heat (J/g)
1: 9	58.72	231.93
6: 4	19.98	172.09
7: 3	23.27	167.36
8: 2	34.21	162.24

Table 5 . Theoretical calculations of phase transition temperature and latent heat of capric acid and lauric acid at different ratios

Mass percentage	Phase transition temperature (°C)	Phase change latent heat (J/g)
1: 9	40.83	215.17
6: 4	27.12	176.12
7: 3	22.72	167.23
8: 2	16.81	157.53

Table 6. Theoretical calculations of phase transition temperature and latent heat of stearic acid and palmitic acid at different ratios

Mass percentage	Phase transition temperature (°C)	Phase change latent heat (J/g)
1: 9	59.26	239.08
4: 6	52.88	232.68
5: 5	50.15	230.18
9: 1	66.06	239.43

Table 7. Theoretical calculations of phase transition temperature and latent heat of stearic acid and myristic acid at different ratios.

Mass percentage	Phase transition temperature (°C)	Phase change latent heat (J/g)
1: 9	48.41	215.82
4: 6	42.31	201.24
5: 5	40.93	205.46
9: 1	66.19	236.28

4. Results Comparison and Analysis

4.1 Comparison of Theoretical and Experimental Values

The theoretical calculation results of the binary mixture prepared by the four fatty acids according to different ratios are compared with the experimental test results as shown in Figs.

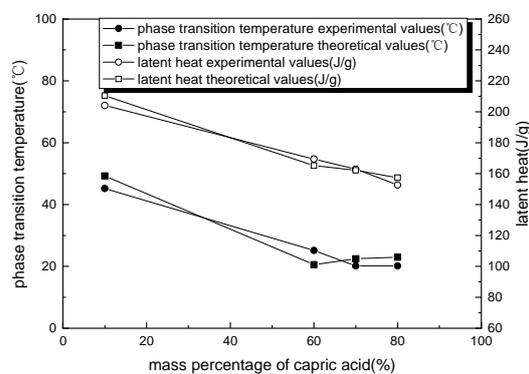


Figure 6. Phase transition temperature and latent heat of capric acid and myristic acid mixture comparison between experimental and theoretical values

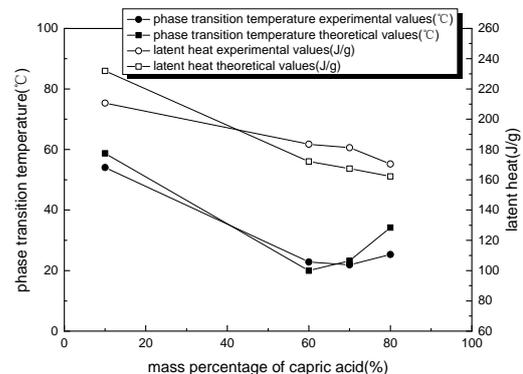


Figure 7. Phase transition temperature and latent heat of capric acid and palmitic acid mixture comparison between experimental and theoretical values

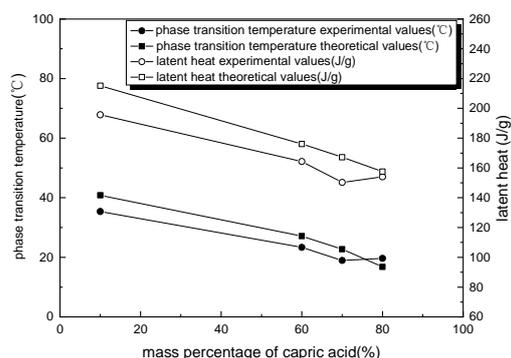


Figure 8. Phase transition temperature and latent heat of capric acid and lauric acid mixture comparison between experimental and theoretical values

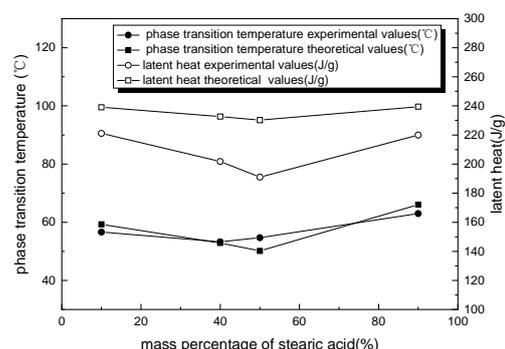


Figure 9. Phase transition temperature and latent heat of stearic acid and palmitic acid mixture comparison between experimental and theoretical values

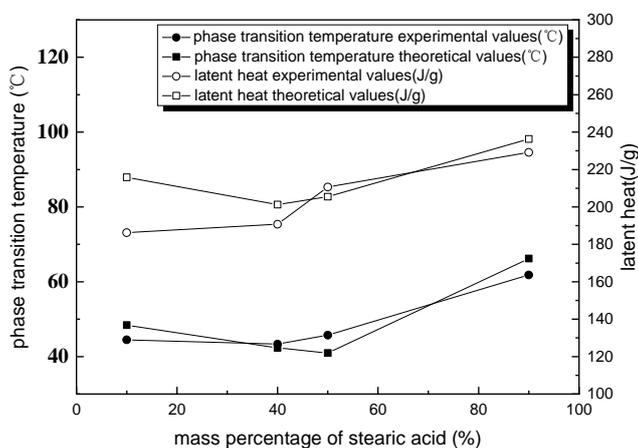


Figure 10. Phase transition temperature and latent heat of stearic acid and myristic acid mixture comparison between experimental and theoretical values

4.2 Analysis of Results

6 to 10, the phase transition temperature of a mixture of capric acid and myristic acid, a mixture of capric acid and palmitic acid, a mixture of capric acid and lauric acid, a mixture of stearic acid and palmitic acid, and a mixture of stearic acid and myristic acid. The deviation between the experimental value and the theoretical value is less than 5°C, wherein the minimum deviation value is less than 1°C, and the average relative deviation is 10.81%; in general, the experimental value and theoretical value of the phase transition temperature of the selected binary fatty acid mixture the deviation is small.

The experimental value of the latent heat of phase change of capric acid and myristic acid is less than 7J/g, the average relative deviation is 2.27%; the mixture of capric acid and lauric acid, capric acid and palmitic acid and stearic acid and nutmeg The experimental value of the latent heat of phase change of the acid mixture deviates from the theoretical value by less than 30 J/g, and the average relative deviation is 7.28%. The experimental value of the phase change latent heat of the stearic acid and palmitic acid mixture is slightly larger than the theoretical value. Less than 40 J/g, the average relative deviation is 11.49%. Taken together, the experimental values of the phase change latent heat of the selected dibasic fatty acid mixture are less than the theoretical values.

5. Conclusion

In this paper, the theoretical prediction formulas of phase transition temperature and latent heat of the mixture were selected. The phase transition temperature and latent heat of the mixture prepared by different ratios of capric acid, stearic acid, myristic acid and palmitic acid were theoretically calculated and experiments were carried out. Test, through the comparative analysis of theoretical and experimental values, can draw the following conclusions:

(1) The experimental values of the phase transition temperature of the dibasic fatty acid mixture selected in this paper are less than the theoretical value, the overall deviation is less than 5 °C, the individual point deviation is less than 1 °C, and the average relative deviation is less than 11%. In good agreement with the theoretical values. The latent heat of phase change and the experimental value have little deviation from the theoretical value. The basic deviation is less than 30 J/g. The experimental values of some points are basically coincident with the theoretical values. The deviation of individual points is slightly larger, but the deviation is less than 40 J/g. The average relative deviation is less than 11.50%.

(2) The theoretical calculation formula is feasible for the theoretical prediction of the phase transition temperature and latent heat of phase change of the binary fatty acid mixture.

(3) Due to the diversity of fatty acid species, it is more convenient and faster to use the theoretical formula calculation than the cumbersome experimental test. It provides a reference for the determination of the heat storage performance of the dibasic fatty acid organic phase change materials studied in this paper. in accordance with.

6. References

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