

Thermodynamic analysis of synthesis of cyclopentanol from cyclopentene and comparison with experimental data

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Abstract Cyclopentanol is a very important chemical intermediate, which has been widely used in the chemical industry, and could be prepared from cyclopentene by two steps: an initial addition-esterification reaction of cyclopentene with acetic acid and the subsequent transesterification reaction with methanol. However, so far, no direct theoretical or experimental work has been reported on this process. In this work, we have carried out the thermodynamic calculation of the indirect process and also validated the thermodynamic prediction through experimental work. The liquid heat capacities of cyclopentanol and cyclopentyl acetate were estimated using the Ruzicka–Domalski group contribution method, the standard enthalpy of formation and standard entropy of gaseous cyclopentyl acetate by the Yoneda group contribution method, the standard vaporization enthalpy of cyclopentyl acetate by the Ducros group contribution method. The enthalpy changes, free energy changes, equilibrium constant and equilibrium conversion of the addition-esterification and transesterification reactions were calculated according to the principles of chemical thermodynamics in the temperature range from 273.15 to 373.15 K. The results

showed that both the addition-esterification reaction and transesterification reaction were exothermic, the free energy changes increased with a rise on temperature, which indicated that low temperature was favorable for the reactions in the temperature range from 273.15 to 373.15 K. The optimal addition-esterification reaction conditions were a temperature range from 333.15 to 353.15 K, molar ratios of acetic acid to cyclopentene in the range from 2:1 to 3:1. For the transesterification reaction, the ideal temperature ranges from 323.15 to 343.15 K, with a molar ratio of methanol to cyclopentyl acetate in the range from 3:1 to 4:1. These thermodynamic calculation results for the addition-esterification reaction of cyclopentene and acetic acid experiments results are in good agreement with the experimental results.

Keywords Cyclopentene · Acetic acid · Methanol · Cyclopentanol · Cyclopentyl acetate · Group contribution method · Thermodynamic analysis

Nomenclature

List of symbols

C_p	Heat capacity
G	Gibbs energy
H	Enthalpy
S	Entropy
K	Equilibrium constant
T	Temperature
R	Universal gas constant
x	Equilibrium conversion
r	Molar ratio
Δ	Value of change

Superscripts and subscripts

θ	Standard state
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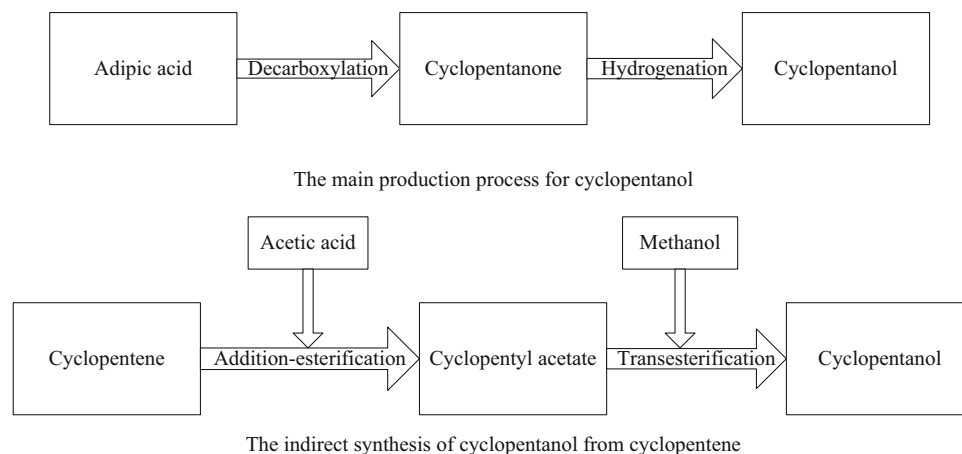
P	Production
R	Reactant
f	Formation
r	Reaction
g	Gas phase
l	Liquid phase
1	Addition-esterification reaction
2	Transesterification reaction

Introduction

Cyclopentanol is an important fine chemical intermediate, which has been used in the production of perfumes, medicines and dyes, and as a solvent for medicines and perfumes [1]. The main production process for cyclopentanol was cyclopentanone hydro-conversion, and the cyclopentanone was produced by decarboxylation of adipic acid at high temperature; however, the development of this process was limited due to the formation of a great deal of pollutant [2, 3]. Cyclopentanol can also be produced from furfural using the Noble-metal catalysts (such as Pt/C and Ru/C); however, the selectivity of cyclopentanol is quite low, and future development of high efficient, stable and economical catalysts will be highly desired [4, 5].

The dicyclopentadiene could be separated from the cracked C₅ fraction available as a by-product of ethylene production, and the cyclopentadiene was produced by dicyclopentadiene cracking; cyclopentene was the hydrogenation product of cyclopentadiene, and the cyclopentanol could be produced from the direct hydration or indirect hydration of cyclopentene. Theoretically, cyclopentanol could be synthesized using a two-step process from cyclopentene, e.g., the addition-esterification reaction of cyclopentene with acetic acid, the transesterification of cyclopentyl acetate and methanol, the process of hydration of cyclopentene was one environment friendly technology with less pollution [6]. The flow charts of the main

Fig. 1 Flow chart of the main production process for cyclopentanol and indirect synthesis of cyclopentanol from cyclopentene

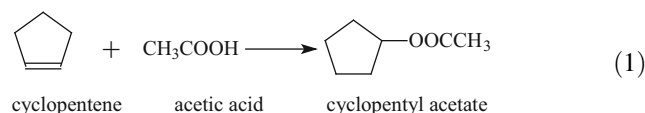


production process for cyclopentanol and indirect synthesis of cyclopentanol from cyclopentene are shown in Fig. 1. However, so far, no literatures have been published for this indirect process either from the theoretical or experimental study. In this work, the thermodynamic analysis of the two reaction steps was carried out in the paper, which could provide theoretical principle for the experimental research and industrial production, and preliminary experimental work has been carried out and the results are in good agreement with the thermodynamic calculation results.

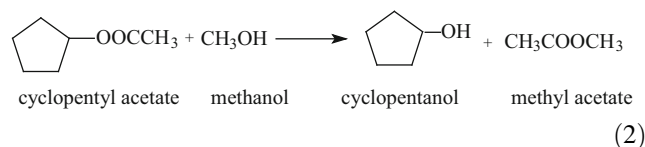
Thermodynamic calculation

Reaction equations

The two reactions have been considered in the system, the addition-esterification reaction of cyclopentene and acetic acid:



The transesterification of cyclopentyl acetate and methanol:



Physical properties data of thermodynamic analysis

The standard enthalpy of formation and standard entropy of liquid cyclopentene, acetic acid, methanol, methyl acetate

Table 1 Contribution values of group of Ruzicka–Domalski and the group numbers in the each substance

Group	a_i	b_i/K^{-1}	d_i/K^{-2}	Group number	
				Cyclopentyl acetate	Cyclopentanol
C-(H) ₃ (C)	3.8452	-0.33997	0.19489	1	-
CO-(C)(O)	29.246	3.4261	-2.8962	1	-
O-(C)(CO)	-21.434	-4.0164	3.0531	1	-
C-(H)(C) ₂ (O)(alcohol)	2.2209	-1.435	0.69508	1	1
C-(H) ₂ (C) ₂	2.7972	-0.05497	0.10679	4	4
Substituted cyclopentane	0.29183	-1.5118	0.23172	1	1
O-(C)(H)	12.952	-10.145	2.6261	-	1

Table 2 The functional correlations between $C_{p,t}$ of materials and temperature

Constituents	$C_{p,t} \sim T$
Cyclopentene	$112.71 - 0.8864 T + 6.2634 \times 10^{-3} T^2 - 1.4632 \times 10^{-5} T^3 + 1.3021 \times 10^{-8} T^4$
Acetic acid	$183.43 - 0.6817 T + 2.9953 \times 10^{-3} T^2 - 5.4815 \times 10^{-6} T^3 + 4.1430 \times 10^{-9} T^4$
Methanol	$-1373.10 + 17.5230 T - 7.9812 \times 10^{-2} T^2 + 1.6112 \times 10^{-4} T^3 - 1.1979 \times 10^{-7} T^4$
Methyl acetate	$-413.28 + 6.3422 T - 2.7999 \times 10^{-2} T^2 + 5.5006 \times 10^{-5} T^3 - 3.9106 \times 10^{-8} T^4$
Cyclopentyl acetate	$210.8325 - 0.3406 T + 1.4182 \times 10^{-3} T^2$
Cyclopentanol	$221.5974 - 1.1293 T + 3.3645 \times 10^{-3} T^2$

and cyclopentanol were adopted from the data handbooks [7, 8], the results are shown in the Table 4. The liquid heat capacities of cyclopentene, acetic acid, methanol and methyl acetate at the temperature range from 273.15 to 373.15 K were taken from the data handbook [9, 10], and the expression of liquid heat capacities was fitted as multinomial; the results are shown in Table 2.

However, not all the physical properties of the chemicals could be obtained from handbook, the group contribution methods were investigated to estimate the physico-chemical properties of organic compounds, such as Joback method [11], Constantinou–Gani method [12], Benson method [13] and so on [14, 15]. In this paper, the liquid heat capacities of cyclopentanol and cyclopentyl acetate, the standard enthalpy of formation and standard entropy of gaseous cyclopentyl acetate at the temperature of 298.15 K, and the standard vaporization enthalpy of cyclopentyl acetate were estimated by Ruzicka–Domalski method [16], Yoneda method (ABWY) [17] and Ducros method [18, 19], respectively [20].

The liquid heat capacities of cyclopentanol and cyclopentyl acetate were estimated by Ruzicka–Domalski group contribution method [16, 20], the calculation formula was:

Table 3 Contribution values of group of Ducros

Constituents	Group	Number	$\Delta H/$ (KJ mol ⁻¹)
Cyclopentyl acetate	C-(H) ₃ (C)	1	5.65
	CO-(C)(O)	1	9.83
	O-(C)(CO)	1	8.37
	C-(H)(C) ₂ (O)(alcohol)	1	1.97
	C-(H) ₂ (C) ₂	4	4.98
	Cyclopentane adjustment	1	2.76

$$C_{p,t} = R \left[A + B \frac{T}{100} + D \left(\frac{T}{100} \right)^2 \right] \quad (3)$$

In the Eq. 3 $A = \sum n_i a_i$, $B = \sum n_i b_i$, $D = \sum n_i d_i$, the contribution values of group are shown in Table 1 and the calculation results in Table 2. The standard enthalpy of formation and standard entropy of gaseous cyclopentyl acetate at the temperature of 298.15 K were estimated using Yoneda method (ABWY) [17, 20], and the effect of substitutions was covered with data from Ref. [20], and the calculation formula being

$$\Delta_f H_{g,298.15}^\theta = \sum n_i \Delta H_i \quad (4)$$

$$S_{m,g}^\theta = \sum n_i \Delta S_i \quad (5)$$

The standard enthalpy of formation and standard entropy of liquid cyclopentyl acetate at the temperature of 298.15 K were estimated by Eqs. 6 and 7:

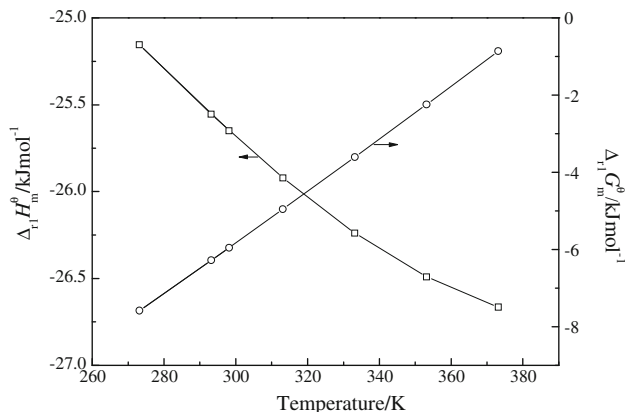
$$\Delta_f H_{l,298.15}^\theta = \Delta_f H_{g,298.15}^\theta - \Delta_v H_{298.15}^\theta \quad (6)$$

$$S_{m,l}^\theta = S_{m,g}^\theta - \frac{\Delta_v H_{298.15}^\theta}{298.15} \quad (7)$$

The standard vaporization enthalpy of cyclopentyl acetate was estimated by the Ducros method [18–20], and the contribution values of group are shown in Table 3. The

Table 4 The $\Delta_f H_{l,298.15}^\theta$ and $S_{m,l}^\theta$ of each substance at 298.15 K

Constituents	$\Delta_f H_{l,298.15}^\theta / (\text{KJ mol}^{-1})$	$S_{m,l}^\theta / (\text{J mol}^{-1} \text{K}^{-1})$
Cyclopentene	4.27	201.25
Acetic acid	-484.5	159.8
Methanol	-239.1	126.8
Methyl acetate	-445.8	210.7
Cyclopentyl acetate	-505.88	294.99
Cyclopentanol	-300.1	206.3

**Fig. 2** The $\Delta_{r_1} H_m^\theta$ and $\Delta_{r_1} G_m^\theta$ for the addition-esterification reaction as functions of temperature

standard enthalpy of formation and standard entropy of liquid cyclopentyl acetate appear in Table 4.

Calculation results and discussion

The enthalpy changes, free energy changes of each reaction were calculated by Eqs. 8–12 [21]:

$$\Delta_r H_{298.15}^\theta = \sum (\Delta_f H_{l,298.15}^\theta)_p - \sum (\Delta_f H_{l,298.15}^\theta)_R \quad (8)$$

$$\Delta_r H_m^\theta = \Delta_r H_{298.15}^\theta + \int_{298.15}^T (\sum (C_p)_P - \sum (C_p)_R) dT \quad (9)$$

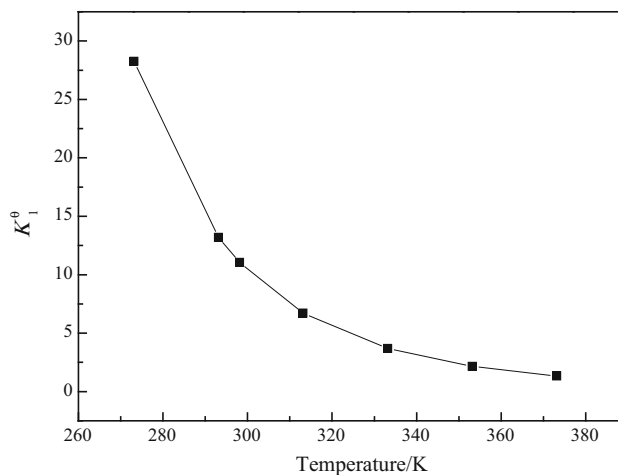
$$\Delta_r S_{m,298.15}^\theta = \sum (S_m^\theta)_p - \sum (S_m^\theta)_R \quad (10)$$

$$\Delta_r S_m^\theta = \Delta_r S_{m,298.15}^\theta + \int_{298.15}^T \left(\frac{C_p}{T} \right) dT \quad (11)$$

$$\Delta_r G_m^\theta = \Delta_r H_m^\theta - T \Delta_r S_m^\theta \quad (12)$$

The equilibrium constant of each reactions was calculated by Eq. 13 [21, 22]:

$$K^\theta = \exp(-\Delta_r G_m^\theta / RT) \quad (13)$$

**Fig. 3** Changes of the addition-esterification reaction equilibrium constant (K_1^θ) with temperature

Addition-esterification reaction of cyclopentene and acetic acid

The enthalpy changes and free energy changes of the addition-esterification reaction

The enthalpy changes ($\Delta_{r_1} H_m^\theta$) and free energy changes ($\Delta_{r_1} G_m^\theta$) of addition-esterification reaction were calculated at different temperature, the results are shown in Fig. 2.

As seen from Fig. 2, the $\Delta_{r_1} H_m^\theta$ was less than 0 in the temperature range from 273.15 to 373.15 K, the addition-esterification reaction was exothermic, and the $\Delta_{r_1} H_m^\theta$ decreased with increasing temperature in the range 273.15 to 373.15 K.

The $\Delta_{r_1} G_m^\theta$ value was less than 0 in the 273.15 to 373.15 K, which showed that the addition-esterification reaction could occur spontaneously. $\Delta_{r_1} G_m^\theta$ increased with the temperature rise, which indicated that lower temperatures were more favorable for the reactions in the temperature range from 273.15 to 373.15 K.

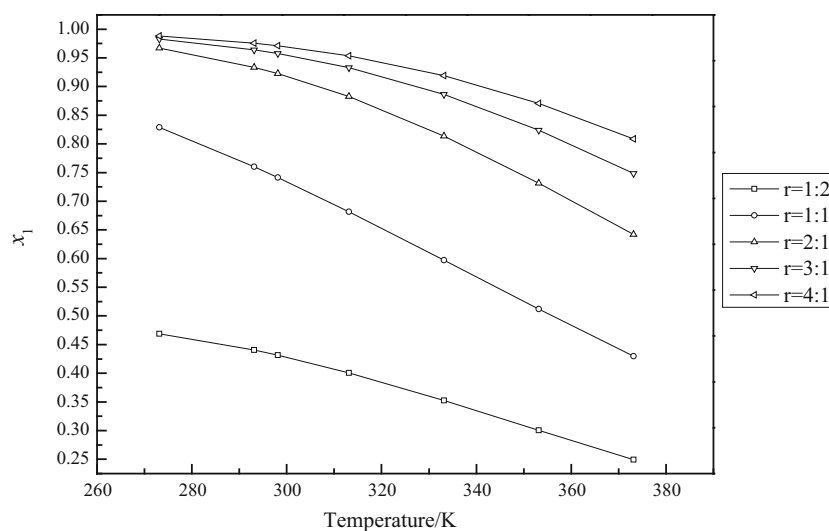
Equilibrium constant and equilibrium conversion of the addition-esterification reaction

The molar ratio of acetic acid to cyclopentene was set as r_1 , the conversion of cyclopentene was set as x_1 , so:

$$K_1^\theta = \frac{x_1}{(1-x_1)(r_1-x_1)} \quad (14)$$

The equilibrium constant (K_1^θ) of the addition-esterification reaction at different temperature was calculated from Eq. 13, and the conversion of cyclopentene as x_1 at different temperature with different r_1 was calculated from Eq. 14 and the results appear in Figs. 3 and 4.

Fig. 4 Changes of the cyclopentene equilibrium conversion (x_1) with temperature



Figures 3 and 4 show that K_1^θ and x_1 decreased at higher temperature and that the x_1 increased at higher values, r_1 , at the same temperature. The conversion of cyclopentene was higher at lower temperature and a greater molar ratio of acetic acid to cyclopentene. However, very low temperatures reduced the reaction rate, and the acetic acid spent increased with increasing of r_1 , and the cost of separation of acetic acid and cyclopentyl acetate increased. The most suitable reaction conditions were temperature in the range from 333.15 to 353.15 K with an r_1 value between 2:1 and 3:1.

Transesterification reaction of cyclopentyl acetate and methanol

The enthalpy changes and free energy changes of transesterification reaction

The enthalpy changes ($\Delta_{r_1}H_m^\theta$) and free energy changes ($\Delta_{r_1}G_m^\theta$) of transesterification reaction were calculated at different temperature and the results are plotted in Fig. 5.

Figure 5 shows that $\Delta_{r_2}H_m^\theta$ was negative in the temperature range from 273.15 to 373.15 K, the addition-esterification reaction was exothermic, and the $\Delta_{r_2}H_m^\theta$ decreased at higher temperatures from 273.15 to 373.15 K.

The $\Delta_{r_2}G_m^\theta$ was greater than 0 in the temperature range from 273.15 to 373.15 K, which showed that the addition-esterification reaction couldn't carry through spontaneously. And the $\Delta_{r_2}G_m^\theta$ increased with the raising of the temperature, which indicated that temperature increased was unfavorable for the reactions at the temperature range from 273.15 to 373.15 K.

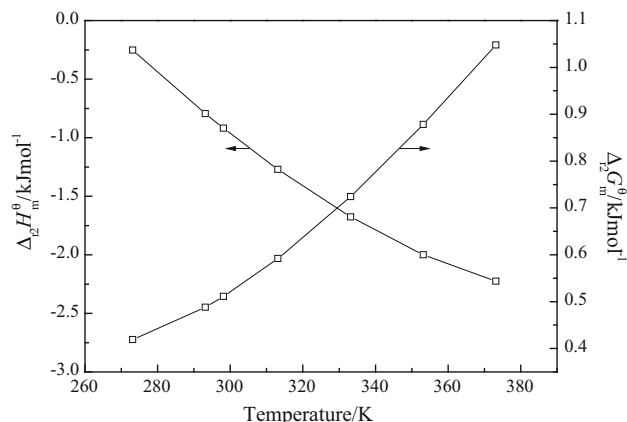


Fig. 5 The $\Delta_{r_2}H_m^\theta$ and $\Delta_{r_2}G_m^\theta$ of transesterification reaction as functions of the temperature

Equilibrium constant and equilibrium conversion of the transesterification reaction

The molar ratio of methanol to cyclopentyl acetate was set as r_2 , the conversion of cyclopentyl acetate was set as x_2 , so:

$$K_2^\theta = \frac{x_2^2}{(1-x_2)(r_2-x_2)} \quad (15)$$

In the same way, the equilibrium constant (K_2^θ) of the transesterification reaction at different temperature was calculated from Eq. 13, and the conversion of cyclopentene as x_1 at different temperature with different r_1 was calculated from Eq. 15, and the results are shown in Figs. 6 and 7.

Similarly, as seen from Figs. 6 and 7, the K_2^θ and x_2 decreased with the raising of the temperature, the x_2 increased with the raising of the r_2 at the same temperature. The conversion of cyclopentyl acetate was higher with

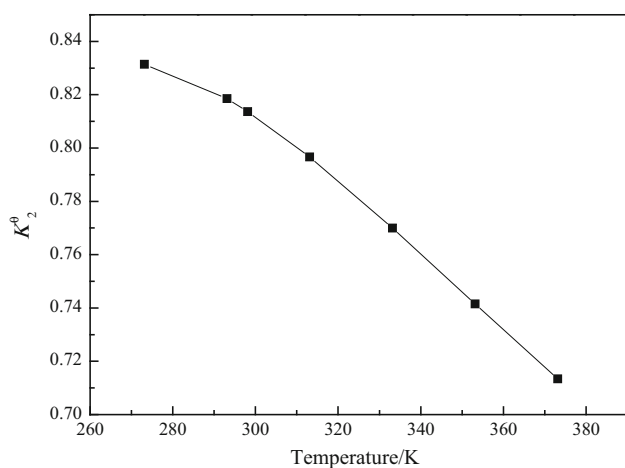


Fig. 6 Changes of the transesterification reaction equilibrium constant (K_2^0) with temperature

lower temperature and greater molar ratio of methanol to cyclopentyl acetate. However, the extremely lower temperature reduced the reaction rate which was unfavorable for the transesterification reaction, and the methanol spent increased with increasing of r_2 , and the cost of separation increased. The suitable reaction conditions were temperature of range from 323.15 to 343.15 K, r_2 of range from 3:1 to 4:1.

Experimental validation, results and discussion

Chemical and catalysts

Cyclopentene [AR > 98.0 % (wt)] was purchased from Changzhou Sinly Pharmchem Co., Ltd. Acetic acid [AR > 99.5 % (wt)] was purchased from Reagent No. 1 Factory of Shanghai Chemical Reagent Co., Ltd. Methanol [CP > 99.9 % (wt)] was purchased from Shanghai Coking Co., Ltd. Amberlyst-35 strong acidic cation-exchange resin catalysts were obtained from Rohm and Haas Shanghai Chemical Industry Co., Ltd. QRE-01 strong acidic cation-exchange resin catalysts were obtained from Research Institute of Qilu Petrochemical Co., SINOPEC.

Analysis and calculations

Chemical composition of products was analyzed using a gas chromatography (Agilent GC-6890) with a HP-FFAP silica capillary column (30 m × 0.32 mm × 0.25 μm). Nitrogen was used as the carrier gas at a flow rate of 0.7 mL/min. The temperature of column oven was programmed from 60 °C increased at 5 °C/min to 80 °C, and held with an isothermal for 4 min, then increased at 10 °C/min to 220 °C, and held with an isothermal for 15 min. The temperature of injector

and detector was set at 220 and 250 °C, respectively. The split ratio was 1:100; the sample injection volume was 0.4 μL. Calibration normalization method was performed on the GC to ensure accuracy of the measurements.

The conversions of cyclopentene and cyclopentyl acetate, the selectivity of cyclopentyl acetate and cyclopentanol can be determined with the Eqs. (16–20).

$$\begin{aligned} & \text{Conversion of cyclopentene (\%)} \\ &= \text{Con}_{\text{Cyclopentene}} \\ &= \frac{m_{\text{Cyclopentene, raw materials}} - m_{\text{Cyclopentene, products}}}{m_{\text{Cyclopentene, raw materials}}} \times 100 \end{aligned} \quad (16)$$

$$\begin{aligned} & \text{Selectivity of cyclopentyl acetate (\%)} \\ &= \text{Sel}_{\text{Cyclopentyl acetate}} \\ &= \frac{m_{\text{Cyclopentyl acetate}}}{m_{\text{Cyclopentene, raw materials}} - m_{\text{Cyclopentene, products}}} \times 100 \end{aligned} \quad (17)$$

$$\begin{aligned} & \text{Conversion of cyclopentyl acetate (\%)} \\ &= \text{Con}_{\text{cyclopentyl acetate}} \\ &= \frac{m_{\text{cyclopentyl acetate, raw materials}} - m_{\text{cyclopentyl acetate, products}}}{m_{\text{cyclopentyl acetate, raw materials}}} \times 100 \end{aligned} \quad (18)$$

$$\begin{aligned} & \text{Selectivity of cyclopentanol (\%)} \\ &= \text{Sel}_{\text{cyclopentanol}} \\ &= \frac{m_{\text{cyclopentanol}}}{m_{\text{cyclopentyl acetate, raw materials}} - m_{\text{cyclopentyl acetate, products}}} \times 100 \end{aligned} \quad (19)$$

$$\begin{aligned} & \text{Yield of cyclopentanol (\%)} \\ &= \text{Yie}_{\text{Cyclopentene}} \\ &= \frac{\text{Con}_{\text{cyclopentyl acetate}} \times \text{Sel}_{\text{cyclopentanol}}}{100} \end{aligned} \quad (20)$$

Experiment

The addition-esterification reaction of cyclopentene with acetic acid was operated in a glass tube fixed bed reactor (φ25 mm × 500 mm) over Amberlyst-35 strong acidic cation-exchange resin catalysts, the reaction temperature was adjusted by the temperature control system, the reactants mass flow rate was controlled by the feeding pump. The addition-esterification reaction of cyclopentene and acetic acid with different reaction conditions was carried out under normal pressure, the mass space velocity of 2.0 h⁻¹. The analysis results showed that the selectivity of cyclopentyl acetate was around 98 %. The cyclopentyl acetate product (mass fraction of 99 %) was obtained by distillation, the unreacted cyclopentene and superfluous acetic acid could be reused by distillation recovery. The conversion of cyclopentene from experimental results and the equilibrium conversion of cyclopentene from

Fig. 7 Change of the cyclopentyl acetate equilibrium conversion (x_2) with temperature

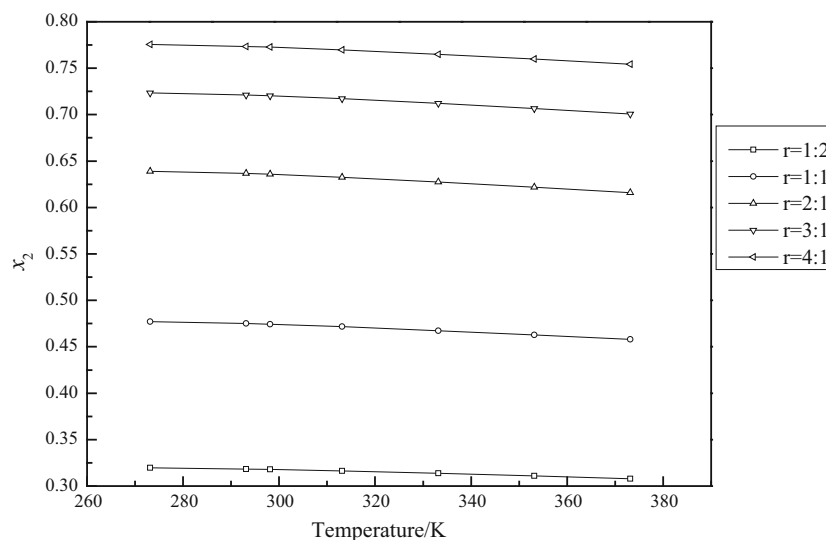


Table 5 Comparisons between experiments results and calculation data of the addition-esterification reaction

Experiment no.	Reaction temperature (°C)	r_1	Conversion of cyclopentene (%)		Absolute errors (%)	Relative errors (%)
			Experiments results	Calculation data		
1	65	1.5	75.43	71.51	-0.0392	-5.49
2	65	2	77.00	79.41	0.0241	3.03
3	65	2.5	81.46	84.13	0.0267	3.18
4	65	3	84.38	87.19	0.0281	3.22
5	65	3.5	85.63	89.29	0.0366	4.10
6	50	3	75.94	91.14	0.1520	16.68
7	55	3	79.82	89.93	0.1011	11.24
8	60	3	82.81	88.61	0.0580	6.54
9	65	3	84.38	87.19	0.0281	3.22
10	70	3	80.52	85.67	0.0515	6.01

r_1 molar ratio of acetic acid to cyclopentene

thermodynamics calculation in the addition-esterification reaction are compared in Table 5.

From Table 5, we can see that, the cyclopentene conversion relative errors of experiment nos. 6 and 7 were more than 10 %. Since the reaction rate I was slower in the lower temperature, it was difficult to achieve equilibrium at a lower reaction temperature during a short reaction time, the relative errors in the lower reaction temperature were larger than that in higher reaction temperature. The relative error of other experiments was lower than 7.0 %, and the average relative error was 2.98 % (experiment nos. 6 and 7 are not included); the thermodynamic calculation was in good agreement with the experiment results.

The transesterification of cyclopentyl acetate and methanol was operated in a glass tube fixed bed reactor ($\phi 25 \text{ mm} \times 500 \text{ mm}$) over QRE-01 strong acidic cation-exchange resin catalysts, the reaction temperature was adjusted by the temperature control system, the reactants'

mass flow rate was controlled by the feeding pump. The transesterification of cyclopentyl acetate and methanol was carried out under normal pressure, the reaction temperature of 50 °C, the molar ratio of methanol to cyclopentyl acetate of 3:1, the mass space velocity of 2.0 h^{-1} , the conversion of cyclopentyl acetate was 55.3 %, the selectivity of cyclopentanol was 99.5 %, the yield of cyclopentanol was 55.0 %. The cyclopentanol product was obtained by distillation, the unreacted cyclopentyl acetate and superfluous methanol could be reused by distillation recovery.

Conclusions

Thermodynamic analysis for reactions of indirect synthesis of cyclopentanol from cyclopentene has been carried out based on partial physical properties data of cyclopentyl acetate and cyclopentanol estimated by group contribution

methods. The enthalpy changes, free energy changes, equilibrium constant and equilibrium conversion of the addition-esterification reaction and transesterification reaction were calculated.

The addition-esterification reaction of cyclopentene and acetic acid was exothermic reaction at the temperature range from 273.15 to 373.15 K, the optimal reaction condition was temperature of range from 333.15 to 353.15 K, molar ratio of acetic acid to cyclopentene of 2:1–3:1.

The transesterification reaction of cyclopentyl acetate and methanol is exothermic reaction at the temperature range from 273.15 to 373.15 K, the optimal reaction condition was temperature of range from 323.15 to 343.15 K, molar ratio of methanol to cyclopentyl acetate of 3:1 to 4:1.

The addition-esterification of cyclopentene and acetic acid experiments were carried out in a glass tube fixed bed reactor, and the experiments results showed that the thermodynamic calculation was in good agreement with the experiment results.

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