

Kinetics of Coconut Oil Alcoholysis Reaction at Atmospheric Pressure Using Sulphuric Acid Catalisator

By Erna Astuti

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Catalisator

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Abstract

Alcoholysis reaction of plant oil, particularly coconut oil, to glycerol and ester, have been done at various order for several type of oils. The aim of this research is to observe reaction order of coconut oil alcoholysis by establish several reaction kinetic models.

Coconut oil alcoholysis using sulphuric acid catalisator is carried out in batch mode at triple neck flask, by varying temperature at determined stirring speed. Sample was taken at every 10 minutes for glycerol content analysis.

Based on experiment result, coconut oil alcoholysis with sulphuric acid catalysator follows first order to oil, while the reaction constant equation at temperature range 60 – 80°C is $k=0,0902 e^{(-144,1220/T)}$.

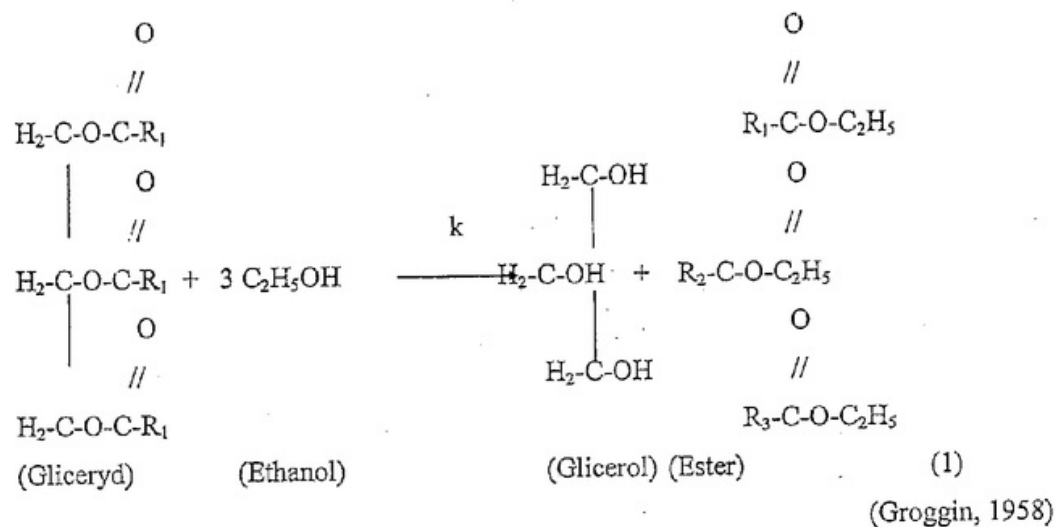
Introduction

Coconut plants is reported in 1995 to be produced at 2,6 million tons every year in Indonesia while the coconut plantation area in Indonesia is known to be the widest area in the world, i.e 3,7 hectare (Tondok, 1996). One effort to make benefit of coconut oil, which main compound is glycerin, is by converting to ester and glycerol thorough alcoholysis process. Glycerol is used in large quantity in plastic container, pharmacy, toothpaste, explosive material, cosmetics and food industries. Mean while, ester can be use as substitution to diesel fuel (Kirk and Othmer, 1979).

Alcoholysis is division reaction of any compound by alcohol, including addition reaction of double chain alcohol (Kirk and Othmer, 1979). This process can be done in batch or continuously. Batch process use three neck flask (for atmospherical pressure process) or autoclave (for higher pressure process).

There are a lot of research on alcoholysis have been done. Titik Mahargiani (2000) examined sawit coconut oil alcoholysis that use mixture of natrium hydroxide and potassium hydroxide as catalyst. It was found that the reaction is approaching first order reversible reaction to oil, ethanol, glycerol and ester. Meanwhile, the alcoholysis reaction of used fried oil whit activated natural zeolite catalyst at pressure higher than 1 atm is observed to follow pseudo-first order to glycerol (Retno Ambarwati dkk, 2001). First order reaction is obtained from alcoholysis of kapok seed oil that used NaOH as catalyst (Sofiyah, 1995). The objective of this research is to find reaction kinetics of coconut oil alcoholysis with sulphuric acid catalyst.

Alcoholysis reaction to oil general is as follow (assumed only forwad reaction is occurred):



R₁, R₂, R₃ are alkyl group.

When simplified, equation (1) becomes: $A + B \xrightarrow{k} D + E$ (2)

Reaction rate equation for above equation is: $(r_A) = -\left(\frac{\partial C_A}{\partial t}\right) = kC_A^a C_B^b$ (3)

Reaction order determination is done through several order model assessment:

a. Model 1 : first order reaction to oil (a=1)

If $C_A = C_{A0}(1-X_A)$, by integrating equation (3) obtained:

$$\ln(1-X_A) = kt + C \quad (4)$$

b. model 2 : first order reaction to oil, first order to alcohol (a=1, b=2)

With $M = \frac{C_{B0}}{C_{A0}}$ Then integrated formula is obtained as follow:

$$\ln \frac{(M-X_A)}{M(1-X_A)} = (M-1)kC_{A0}t + C \quad (5)$$

c. Model 3 : second order reaction to oil (a=2)

Equation used: $\frac{X}{(1-X_A)} = KC_{A0}t + C$

Errors from those three models are calculated and the most appropriate order for the reaction is determined from order that gives the least error.

Experiment

Coconut oil at a certain volume is poured into triple neck flask, then this liquid is heated and stirred by using stirrer while the cooler is turned on. At the same time, mixture of ethanol and a certain volume of sulphuric acid are heated in separated flask. After it reached determined temperature, this mixture is poured into flask which already filled up with heated coconut oil. Reaction time started when ethanol completely poured into flask contained oil and sulphuric acid. Sample was taken at every 10 minutes for glycerol content analysis.

Experiment Result and Discussion

This experiment is carried out to investigate kinetics of coconut oil alcoholysis at various process temperatures. Temperature variation is within range 60-80 °C, reactant ratio 7:1 and stirring speed 850 rpm. Conversions of glycerol at various temperatures are shown in table 1. Reaction order is determined by take glycerol conversion data into calculation of reaction order equation assessed.

Table 1. Conversion at several reaction temperature

Time, t (minutes)	Conversion, X_A		
	60 °C	70 °C	80 °C
10	0,1638	0,2662	0,2942
20	0,2485	0,3990	0,3567
30	0,2970	0,3837	0,4099
40	0,3207	0,5007	0,5087
50	0,4158	0,5233	0,6240
60	0,4762	0,5442	0,6856

Referring to first model equation, $-\ln(1-X_A) = kt + C$, the value of reaction rate constant (k) and equation error can be determined from correlation chart between $-\ln(1-X_A)$ versus time. The result are shown in table 2 and figura 1. Average error obtained for model 1 is 6,54%.

Table 2. k value for model 1 at various temperature

Time, t (minutes)	$-\ln(1-X_A)$		
	60 °C	70 °C	80 °C
10	0,1789	0,3096	0,3485
20	0,2857	0,5091	0,4412
30	0,3524	0,4840	0,5275
40	0,3868	0,6946	0,7106
50	0,5375	0,7409	0,9782
60	0,6466	0,7857	1,1569
k	0,0089	0,0094	0,0167
C	0,0852	0,2587	0,1102
Error, %	5,0329	8,8143	5,7913

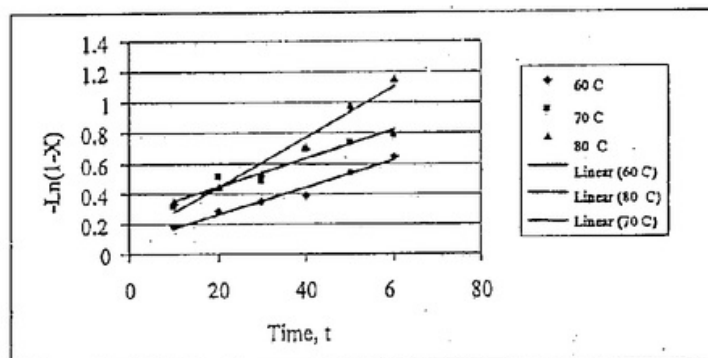


Figure 1. Correlation chart $-\ln(1-X)$ versus time

Reaction order determination for model 2 is using equation : $\ln[(M - X)/M(1 - X_A)] = (M - 1)kCA_0t + C$. The value of $\ln[(M - X)/M(1 - X)]$ at several reaction time is shown in Table 3.

Table 3. k value for model 2 at various temperature

Time, t (minutes)	$\ln[(M - X_A)/(M(1 - X_A))]$		
	60 °C	70 °C	80 °C
10	0,1552	0,2708	0,3055
20	0,2496	0,4505	0,3889
30	0,3090	0,4276	0,4671
40	0,3399	0,6204	0,6352
50	0,4763	0,6632	0,8849
60	0,5761	0,7047	1,0539
k	0,0080	0,0086	0,0154
C	0,0695	0,2228	0,0828
Error, %	5,4209	8,9808	9,1283

Correlation chart between $\ln[(M - X_A)/(M(1 - X_A))]$ versus time is set up from Table 3 to obtain reaction rate constant value (k) and equation error value. Average error obtained for this model is 7,84%.

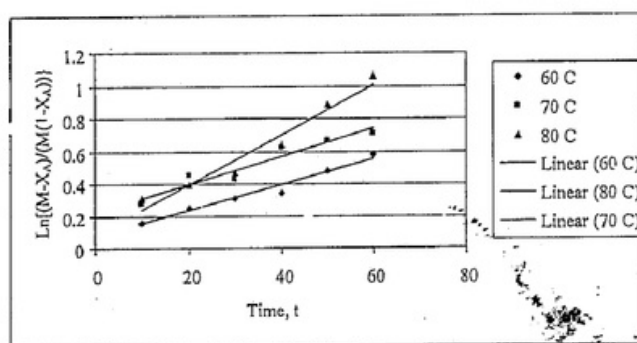


Figure 2. Correlation chart $\ln[(M - X_A)/(M(1 - X_A))]$ versus time

Reaction order for model 3 is calculated by using equation $X_A/(1 - X_A) = kC_{A0}t + C$ and the value is shown in Table 4. Average error obtained for model 3 is 12,96 %. And figure 3 shown correlation chart between $X_A/(1 - X_A)$ versus time

Table 4. Order 2 conversion at various reaction temperature

Time, t (minutes)	$X_A/(1 - X_A)$		
	60 °C	70 °C	80 °C
10	0,1959	0,3629	0,4169
20	0,3307	0,6639	0,5546
30	0,4224	0,6225	0,6946
40	0,4722	1,0029	1,0353
50	0,7117	1,0978	1,6598
60	0,9090	1,1939	2,1802
k	0,0136	0,0167	0,0356
C	-0,0312	-0,2403	0,1571
Error, %	9,2685	10,0538	19,5534

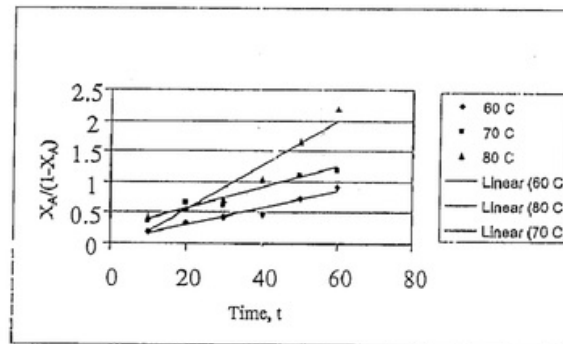


Figure 3. Correlation chart $X_A/(1-X_A)$ versus time

The most appropriate reaction order for this alcoholysis process is determined by choosing the smallest error value obtained from assessment of those three models. Model 1 has smallest average error value, I.e: 6,45 % and it can then be concluded that alcoholysis reaction of coconut oil is following first order to oil .

To determine reaction rate constant, Arrhenius equation is applied by using k data from table 2. Equation obtained is $k = 0,0902 e^{(-144,1220/T)}$ with error 12.96%

Conclusion

1. Alcoholysis of coconut oil with sulphuric acid catalyst follow 1 order reaction to oil.
2. Correlation between k and T is according to equation $k = 0,0902 e^{(-144,1220/T)}$ that apply for temperature range 60-80 °C

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