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Saturday, February 17, 2007

Proceeding

Hosted by
Fakultas Matematika dan Ilmu Pengetahuan Alam
(Faculty of Mathematics and Natural Sciences)
Universitas Ahmad Dahlan
Proceeding of The International Seminar on Natural Sciences and Applied Natural Sciences

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Preface

Assalamu’alikum warohmatullahi wabarokatuh.

Today there is a fact that many qualified researches conducted by researchers from universities have a few opportunities to be communicated in the forum like international seminars and also are rarely published in periodicals or journals though it is realized that they are significantly important not only for the development of science, technology, and industry but also for the teaching-staffs of higher educations themselves to improve their professions. Therefore an effort to provide a medium accommodating that demand needs appreciating.

In relation to the problem Faculty of Mathematics and Natural Sciences Ahmad Dahlan University Yogyakarta vigorously holds an International Seminar on Mathematics, Natural Sciences, and their Applications which is divided into two sessions-panel discussion, and parallel sessions comprising papers on biology, physics, mathematics, computer science, education mathematics and natural sciences, and their applications. It is hoped that this program can serve as a medium for sharing information and publishing the results of researches on that field either conducted by higher educations, research institutes, industries or observers. To fulfill that hope the committee tries to publish the proceeding of the seminar so that the results can become new beneficial references and be widely read by various circles of people for further studies and applications.

In addition, we also wish this program could become an important moment of meeting between higher educations and industries so that they could make some win-win cooperations especially directed to the sustainable civil-society development.

Finally, we realize that the success of the seminar depends very much on all people involving in it, accordingly we express our deep gratitude and high appreciation to those who have participated in the program.

Wassalamu’alaikum warohmatullahi wabarokatuh.

Dr. Hj. M. Dwi Suhartanti, M.Si.
Chief of The Organizing Committee
Assalmu’alaikum Wr Wb
Bismillahirahmanirahim

In the name of Allah, Most gracious Most merciful. I would like to say thanks to Allah that blesses us in the meeting on International Seminar of Natural Sciences and Applied Natural Sciences.

Allah is Most gracious has given us every things on the earth as well as in the sky for human living demands in the world, to gain successfully life in the beyond of hereafter. Human Living demands are different from one generation to next generation. We aware that human demands more complex in the future, therefore it needs higher technology that is more sophisticated. We are sure, it very depends on improving Mathematics and Natural sciences as its foundations.

Based on those reasons, this forum would be very important because this forum will give experiment results and the latest issues of Mathematics and Natural sciences improvement. Furthermore Mathematics and natural sciences education will be communicated. The communications between researchers to share experience will make improving in the next experiments and expand our knowledge. It will raise new ideas for other researchers to conduct the new experiments. Therefore the beneficial of all things were created by Allah for human demands would be more useful.

As a care taker, I would like to say “Well come to Faculty of Mathematics and Natural Sciences, Ahmad Dahlan University, thank you very much for all your attention and participation” I hope this seminar will be successful, Good luck for all of us.

Wassalamu’alaikum Wr Wb

Yogyakarta, February 17, 2007

Dean of Mathematics and Natural Sciences

Drs. Aris Thobirin, M.Si
SPEECH OF THE RECTOR
AHMAD DAHLAN UNIVERSITY

First of all, I would like to express my gratitude to all participants of this seminar in having a lot of spirit to make success of the seminar. Secondly, I would like to appreciate all the speakers, both from Indonesia and from abroad. Special thanks I would like to address to Prof. Mustafa Matdris and Prof. Ismail bin Mohammad from Malaysia and Prof Sukarti who will be presenting many important issues in the keynote speeches of the seminar.

Natural science is the science that is basically needed by everyone. It is very close to all phenomena about life and all activities of human being. Moreover, everyone who would be mastery in advance technology needs natural science. How aircraft could fly, boats and ships could float, power engine could pull thousand tons of wagons, green leaves could make sugar from water and carbon dioxide could only be explained if we understand natural science. Even I would like to address attention of all participants on the some natural disaster happened in Indonesia in the last couple years. Both the reason and how to overcome the demolishing effect of tsunami in Aceh, earthquake in Yogyakarta and Central Java, flood in Jakarta are also only could be explained if we understand the natural science.

In the other hand, a lot of people do not realize that they need the natural science. Special case in Indonesia, many study programs offering the natural sciences do not significantly attract new students to join. Even in secondary schools, physics, biology and mathematics, three fields representing the natural sciences are the most unfavorable subject among the pupils. Therefore, this seminar in the natural science takes the significance in opening new horizon saying that we need the natural science because of its role in so many disciplines of scientific world.

At last, I hope that the seminar would benefit to all the participants.

Yogyakarta, February 17, 2007
Rector of Ahmad Dahlan University,

Prof. Dr. Sugiyanto, Pharmacist
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**Chemistry 6**
Kinetics of Coconut Oil Alcoholysis Reaction at Atmospheric Pressure Using Sulphuric Acid Catalisator

Erna Astuti

Chemical Engineering Department, Ahmad Dahlan University Yogyakarta

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 results, coconut oil alcoholysis with sulphuric acid catalisator follows first order to oil, while the reaction constant equation at temperature range 60 - 80°C is \( k = 0.0902 \cdot e^{-0.4},0007 \).

Introduction

Coconut plants is reported in 195 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 through alcoholysis process. Glycerol is used in large quantity in plastic container, pharmacy, toothpaste, explosive material, cosmetics and food industries. Meanwhile, 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 atmospheric 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 with 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 in general is as follow (assumed only forward reaction is occurred):

\[
\begin{align*}
\text{(Glicerol)} & \quad \text{(Ester)} \\
\text{H}_2\text{C}-\text{O}-\text{C-R}_1 & \quad \text{R}_1\text{-C}-\text{O-}2\text{H}_3 \\
\text{H}_2\text{C}-\text{O}-\text{C-R}_1 + 3 \text{C}_2\text{H}_5\text{OH} & \quad \text{R}_3\text{-C}-\text{O-}2\text{H}_3 \\
\text{H}_2\text{C}-\text{OH} & \quad \text{R}_2\text{-C}-\text{O-}2\text{H}_3
\end{align*}
\] (1)

\[R_1, R_2, R_3 \text{ are alkyl groups.}\]

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

Reaction rate equation for above equation is: \[r_A = \frac{\partial C_A}{\partial t} = kC_A^a C_B^b\] (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:

\[\ln(1-X_A) = kt + C\] (4)

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

with \(M = \frac{C_{A0}}{C_{A0}}\), then integrated formula is obtained as follow:

\[\ln \left( \frac{M - X_A}{M(1-X_A)} \right) = (M-1)kC_{A0}t + C\] (5)

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

Equation used: \[\frac{X}{(1-X_A)} = kC_{A0}t + C\] (6)

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 is 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>
<thead>
<tr>
<th>Time, t (minutes)</th>
<th>Conversion, X_A</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>60 °C</td>
</tr>
<tr>
<td>10</td>
<td>0,1638</td>
</tr>
<tr>
<td>20</td>
<td>0,2485</td>
</tr>
<tr>
<td>30</td>
<td>0,2970</td>
</tr>
<tr>
<td>40</td>
<td>0,3207</td>
</tr>
<tr>
<td>50</td>
<td>0,4158</td>
</tr>
<tr>
<td>60</td>
<td>0,4762</td>
</tr>
</tbody>
</table>

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 results are shown in Table 2 and Figure 1. Average error obtained for model 1 is 6,54%.

<table>
<thead>
<tr>
<th>Time, t (minutes)</th>
<th>-Ln (1-X_A)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>60 °C</td>
</tr>
<tr>
<td>10</td>
<td>0,1789</td>
</tr>
<tr>
<td>20</td>
<td>0,2857</td>
</tr>
<tr>
<td>30</td>
<td>0,3524</td>
</tr>
<tr>
<td>40</td>
<td>0,3868</td>
</tr>
<tr>
<td>50</td>
<td>0,5375</td>
</tr>
<tr>
<td>60</td>
<td>0,6466</td>
</tr>
<tr>
<td>k</td>
<td>0,0089</td>
</tr>
<tr>
<td>C</td>
<td>0,0852</td>
</tr>
<tr>
<td>Error, %</td>
<td>5,0329</td>
</tr>
</tbody>
</table>

**Figure 1:** Correlation chart \(-\ln(1-X)\) versus time
Reaction order determination for model 2 is using equation: \[ \ln \left[ \frac{[M-X_A]}{[M(1-X_A)]} \right] = (M-1)k \cdot C_{AO} \cdot t + C. \] The value of \( \ln \left[ \frac{[M-X]}{[M(1-X)]} \right] \) at several reaction time is shown in Table 3.

Table 3. k value for model 2 at various temperature

<table>
<thead>
<tr>
<th>Time, t (minutes)</th>
<th>60°C</th>
<th>70°C</th>
<th>80°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.1552</td>
<td>0.2708</td>
<td>0.3055</td>
</tr>
<tr>
<td>20</td>
<td>0.2496</td>
<td>0.4505</td>
<td>0.3889</td>
</tr>
<tr>
<td>30</td>
<td>0.3090</td>
<td>0.4276</td>
<td>0.4671</td>
</tr>
<tr>
<td>40</td>
<td>0.3399</td>
<td>0.6204</td>
<td>0.6352</td>
</tr>
<tr>
<td>50</td>
<td>0.4763</td>
<td>0.6632</td>
<td>0.8849</td>
</tr>
<tr>
<td>60</td>
<td>0.5761</td>
<td>0.7047</td>
<td>1.0539</td>
</tr>
<tr>
<td>k</td>
<td>0.0080</td>
<td>0.0086</td>
<td>0.0154</td>
</tr>
<tr>
<td>C</td>
<td>0.0695</td>
<td>0.2228</td>
<td>0.0828</td>
</tr>
<tr>
<td>Error, %</td>
<td>5.4209</td>
<td>8.9808</td>
<td>9.1283</td>
</tr>
</tbody>
</table>

Correlation chart between \( \ln \left[ \frac{[M-X_A]}{[M(1-X_A)]} \right] \) 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%.

![Correlation chart](image)

Figure 2. Correlation chart \( \ln \left[ \frac{[M-X_A]}{[M(1-X_A)]} \right] \) versus time.

Reaction order for model 3 is calculated by using equation \( X_A/(1-X_A) = kC_{AO}t + C \) and the value is shown in Table 4. Average error obtained for model 3 is 12.96%. And Figure 3 shows correlation chart between \( X_A/(1-X_A) \) versus time.

Table 4. Order 2 conversion at various reaction temperature

<table>
<thead>
<tr>
<th>Time, t (minutes)</th>
<th>60°C</th>
<th>70°C</th>
<th>80°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.1959</td>
<td>0.3629</td>
<td>0.4169</td>
</tr>
<tr>
<td>20</td>
<td>0.3307</td>
<td>0.6639</td>
<td>0.5546</td>
</tr>
<tr>
<td>30</td>
<td>0.4224</td>
<td>0.6225</td>
<td>0.6946</td>
</tr>
<tr>
<td>40</td>
<td>0.4722</td>
<td>1.0029</td>
<td>1.0353</td>
</tr>
<tr>
<td>50</td>
<td>0.7117</td>
<td>1.0978</td>
<td>1.6598</td>
</tr>
<tr>
<td>60</td>
<td>0.9090</td>
<td>1.1939</td>
<td>2.1802</td>
</tr>
<tr>
<td>k</td>
<td>0.0136</td>
<td>0.0167</td>
<td>0.0356</td>
</tr>
<tr>
<td>C</td>
<td>-0.0312</td>
<td>-0.2403</td>
<td>0.1571</td>
</tr>
<tr>
<td>Error, %</td>
<td>9.2685</td>
<td>10.0538</td>
<td>19.5534</td>
</tr>
</tbody>
</table>

Chemistry 6
Figure 3. Correlation chart $X_d/(1-X_d)$ versus time

The most appropriate reaction order for this alcoholsysis process is determined by choosing the smallest error value obtained from assessment of those three models. Model 1 has the smallest average error value, i.e.: 6.54 % and it can then be concluded that alcoholsysis 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 $k = 0.0902 \, e^{(14412390T)}$ with error ....%.

Conclusion

1. Alcoholsysis of coconut oil with sulphuric acid catalyst follows 1 order reaction to oil.
2. Correlation between $k$ and $T$ is according to equation $k = 0.0902 \, e^{(14412390T)}$ that apply for temperature range 60 - 80°C

Acknowledgement

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References


