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Kinetics of Esterification of Propionic Acid and Cyclohexanol

T. Koteswara Rao[1], D. Santosh Kumar[2], M. Vijay[3], K.V. Ramesh[4],
[1,2]Department of Chemical Engineering, Andhra University, Visakhaptnam-530003, India
[3]Centurion University of Technology and Management, Paralakhemundi-761211, Odisha, India.
[4]Department of Chemical Engineering, Andhra University, Visakhaptnam-530003, India.
[3]vijay.miditana@cutm.ac.in, [4]kvramesh69@yahoo.com

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Abstract
Kinetic studies of esterification of propionic acid with cyclohexanol were carried out using sulplhuric acid as catalyst. Experiments were conducted in a stirred, temperature controlled batch reactor. The reaction is homogeneous. The effects of different variables that influence the rate constant such as temperature, catalyst concentration and mole ratio or reactants were studied. The reaction rate followed second order with respect to the acid concentration. The mole ratio is varied between 0.5 and 2.0, temperature between 50 and 70oC and catalyst concentration between 1.5 and 4.5 weight percent. An equation is obtained for the prediction of rate constant.
Keywords: *Esterification, rate constant, Arrhenius, propionic acid, cyclohexanol, homogeneous.*

I. INTRODUCTION

Esters are very important ingredients for many chemical industries. Esters are useful in solvents, plasticizers, perfumes, cosmetics, soaps, medicines, pharmaceuticals, varnishes, paints, lubricants, resins and plastics etc. [1]. Although, there is some information available on esterification of alcohols with organic acids, but there is no reported literature on systematic study of the variables affecting the esterification of propionic acid with cyclohexanol. Sulphuric acid is widely preferred in industry to use as a catalyst especially due to its low cost[2-5].

The main interest of a chemical engineer is the design aspects of a chemical reactor. For optimum design kinetic data is essential. Hence, in the present investigation, focus is placed towards obtaining the kinetic data for the chosen reacting system: propionic acid and cyclohexanol using sulphuric acid as catalyst. The effect of different process variables on the rate of esterification are investigated in the present study. The present work is the application full factorial design and to develop a mathematical correlation between the reaction rate constant and the process variables such as catalyst concentration, mole ratio, and temperature.

2. MATERIALS AND METHODS

The chemicals employed in the present work are propionic acid, cyclohexanol, sulphuric acid, oxalic acid, phenolphthalein indicator and sodium hydroxide. All chemicals used were either pure grade or AR grade except sodium hydroxide which is of laboratory reagent grade. The reaction vessel consisted of a three necked flat bottom flask with a condenser. Agitation and heating is carried out with a magnetic stirrer and thermocouple controlled temperature controller of Remi make. Temperature control is maintained with an accuracy of ±0.2^{o}C.

The reaction is carried out by taking the reactants and the catalyst in required weights using single pan electric balance. They are initially heated in different flasks to the required temperature. At the beginning of the reaction, all of them are poured into the reaction vessel with stirrer speed adjusted to 500 rpm which provides complete agitation of the reaction mixture.

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At defined intervals, one milliliter of the reaction mixture is pipetted out and taken into a conical flask in which measured quantity of sodium hydroxide solution present which immediately arrests the procedure of the reaction. Then the contents of the flask are titrated against oxalic acid. After deducting the sulphuric acid equivalent, the concentration of acid at any given time is calculated.

Mole ratio (acid to alcohol) is taken as 0.5, 1.0 and 2.0. Temperature is taken as 50, 60 and 70°C. Catalyst concentration is taken as 1.5, 3.0 and 4.5 weight percent.

3. RESULTS AND DISCUSSION

In the present investigation the effect of catalyst concentration, temperature and mole ratio (acid to alcohol) on the esterification of propionic acid and cyclohexanol are studied.

3.1. Effect of catalyst concentration

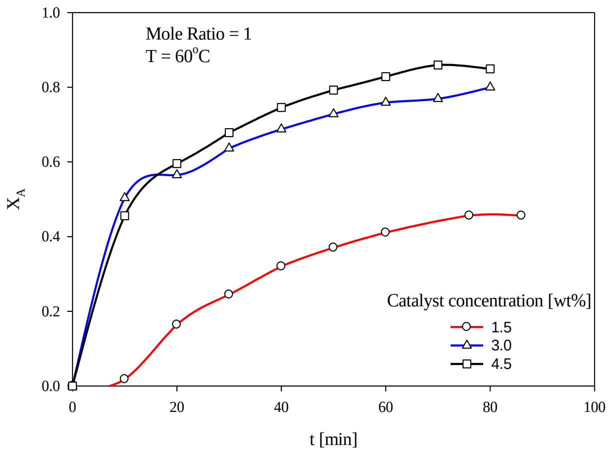

Figure1. Effect of concentration on conversion {MR =1; T = 60°C}

Fig.1 shows the conversion of propionic with time during esterification by taking mole ratio as 1 and temperature as 60°C. The catalyst concentration was varied from 1.5 to 4.5 weight percent. From inspecting the plots of this figure it is evident that the conversion increases with increase in catalyst concentration. Fig.2 shows the conversion of propionic acid with time for mole ratio being 1 and temperature being 70°C. Similarly Fig.3 gives the conversion of propionic acid with time for the same mole ratio but at a temperature of 50°C. It is evident from the three figures that the conversion increases with increase in the concentration of the catalyst.

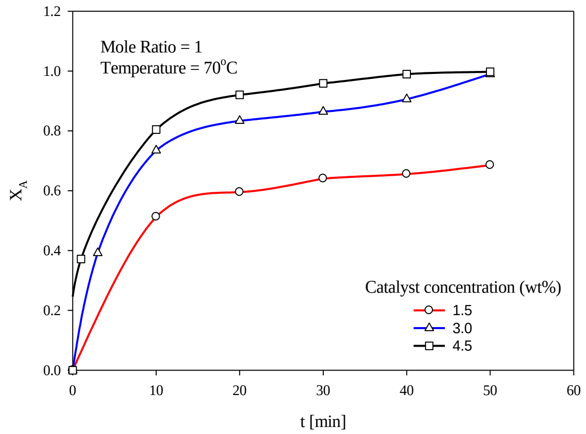

Figure 2. Effect of concentration on conversion {MR =1; T = 70°C}

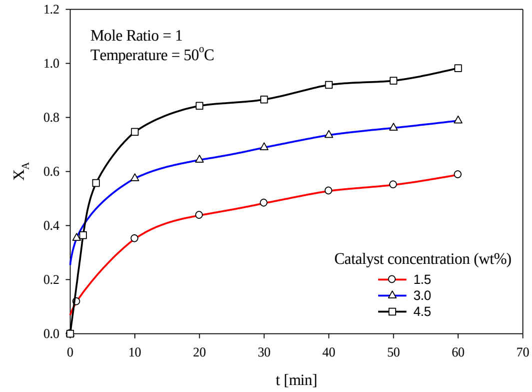

Figure 3. Effect of concentration on conversion {MR =1; T = 50°C}

3.2. Effect of temperature

Fig.4 shows the conversion of propionic with time during esterification by taking mole ratio as 1 and catalyst concentration as 3 weight percent. The temperature was varied from 50 to 70°C. From examining the plots of this figure it is evident that the effect of temperature on conversion followed a mixed trend. Fig.5 and Fig.6 are also the graphs drawn to elicit the information on conversion for different mole ratio and catalyst concentration. A keen look at the

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plots of these figures also reveals that the effect of temperature on conversion is not discernible.

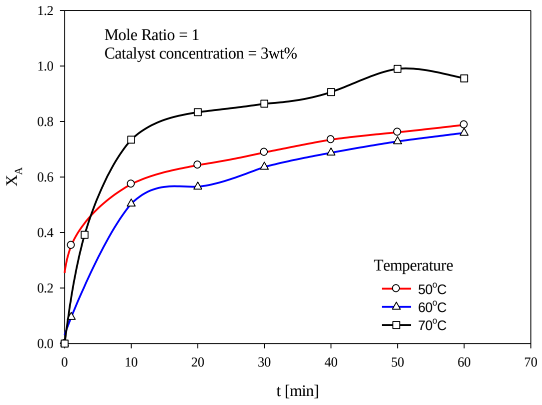

Figure 4. Effect of temperature on conversion {MR =1; CC = 3 wt%}

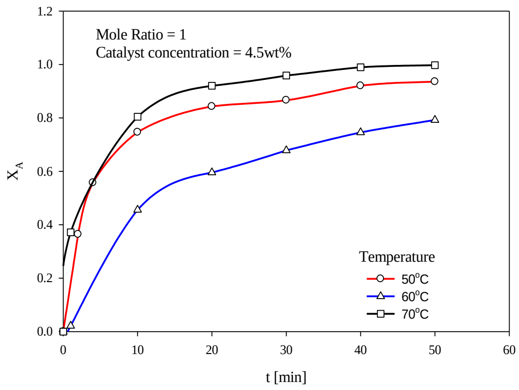

Figure 5. Effect of temperature on conversion {MR =1; CC = 4.5 wt%}

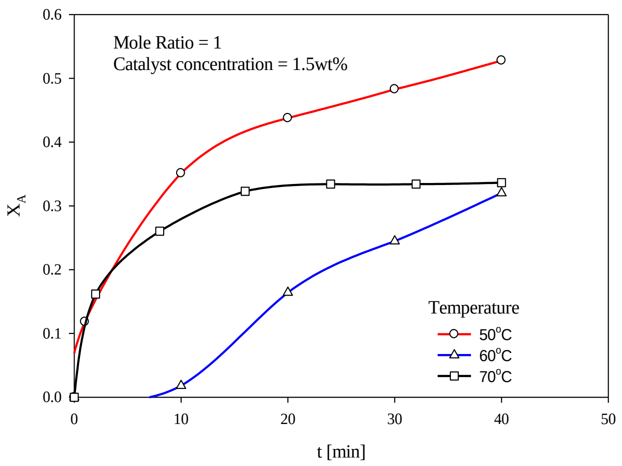

Figure 6. Effect of temperature on conversion {MR =1; CC = 1.5 wt%}

3.3. Effect of mole ratio

Fig.7 shows the conversion of propionic with time during esterification by taking catalyst concentration as 1.5 weight percent and temperature as 60°C. The mole ratio was varied from 0.5 to 2.0. From inspecting the plots of this figure it is evident that the conversion decreases with increase in mole ratio. Fig.8 shows the conversion of propionic acid with time for catalyst concentration being 4.5 weight percent and temperature being 50°C. Similarly Fig.9 gives the conversion of propionic acid with time for a catalyst concentration of 3 weight percent and at a temperature of 70°C. It is evident from these three figures that the conversion decreases with increase in the mole ratio.

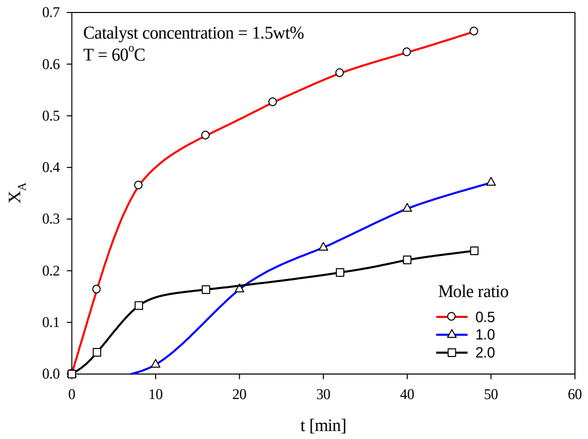

Figure 7. Effect of mole ratio on conversion {T = 60°C; CC = 1.5 wt%}

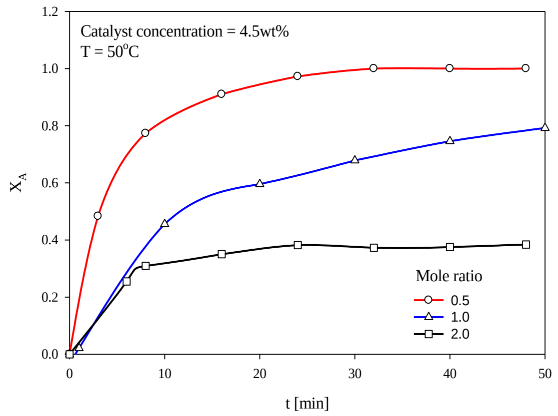

Figure 8. Effect of mole ratio on conversion {T = 50°C; CC = 4.5 wt%}

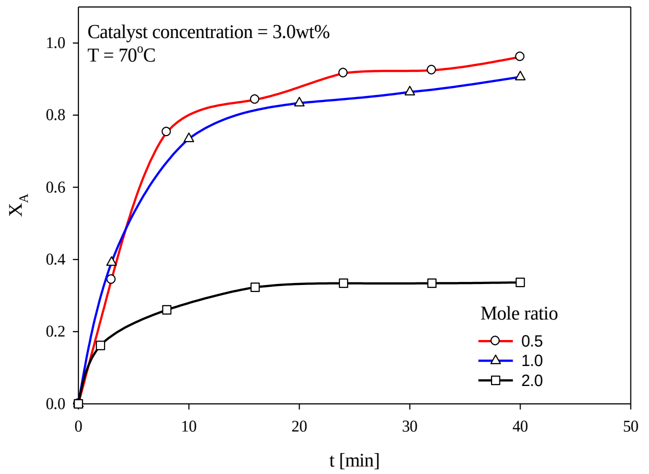

Figure 9. Effect of mole ratio on conversion {T = 70°C; CC = 3.0 wt%}

3.4. Equation for rate constant

Entire data obtained in the present study on kinetics of esterification is subjected to least squares regression analysis and the following equation for rate constant is obtained.

$$k = 10.24\times10^{6}(MR)^{-2.2}(CC)^{1.87}e^{-5815/T} \quad \ldots(1)$$

Average deviation = 6.50 percent

Standard deviation = 8.72 percent

4. CONCLUSIONS

The following observations were made from a study of esterification of propionic acid with cyclohexanol.

i. The reaction rate of the esterification can be increased by increasing catalyst concentration and decreasing mole ratio.
ii. The effect of temperature on reaction rate did not follow specific trend.
iii. The reaction rate constant follows Arrhenius law as far as the temperature effect is concerned.

Nomenclature

CC catalyst concentration

k rate constant, $[m^3/kmol.s]$

MR mole ratio

t time

T temperature

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