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Study the kinetics of catalytic esterification reaction between n-butanol and acetic acid

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ABSTRACT

Study of kinetics is very important in chemical process industries. Esterification process is very common in chemical industries in the literature. There are number of industrial application of Esterification which is discussed and the advantage of studying the kinetics of any Esterification reaction is that 1) All these reactions are empirically found to be of second order. 2) All these reactions have similar mechanism.

In this research, the study of kinetics of Esterification reaction involving acetic acid and n-Butanol as reactant using sulfuric acid as a catalyst. Various experimental runs using laboratorial batch reactor have been conducted applying different combinations of temperatures, mole ratio and catalyst concentrations and finally a kinetic expression, as a function of these parameters, has been investigated.

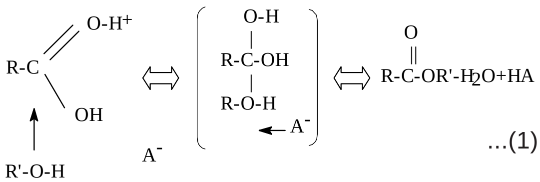
Key words: Esterification, chemical kinetics, rate of hydrolysis, thermodynamics, and activation energy.

INTRODUCTION

Esterification proceeds by attack of an alcohol molecule on the slightly positive carbonyl carbon of an acid. The larger this positive charge, more the rapid reaction will be. While the nature of R group attached to the carbonyl group will influence this charge, catalyst can be used to increase the positive charge so that given, acid will etherify more rapidly.

Esterification catalysts are compounds, which are acidic in nature. Acidic compounds in this case, are those in which the central atom has an incomplete external electron shell. A neutralization reaction of such an acid is written as the donation of an electron pair by a base to the acid.

When an acid (HA) is added to an esterification mixture present will act as bases and coordinate with the acid. A mechanism may be written in two ways, depending on which oxygen of the carbonyl group acts as the base[2].



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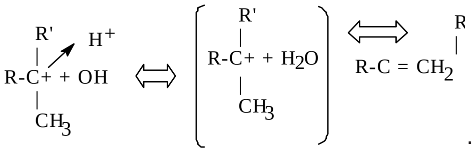

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Chemicals involved

The main chemicals required for the reaction are Acetic acid and n-Butanol. The Sulphuric acid is used as a catalyst. NaOH pellets are required to prepare dilute solution of NaOH, which is in turn used for analysis. Oxalic acid solution is prepared for cross-rectification of normality of NaOH solution. All the chemicals are of the 'Analytical Reagent (A.R.)'grade and procured from Thomas Baker.

Experimental set up

A Leibig type of condenser is used applied to condense and hence reflux back the escaped vapors that are volatile at high temperature as shown in Fig.1.

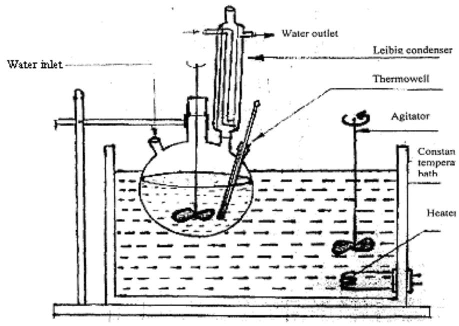

Fig. 1: Schematic representation of experimental setup

Experimental procedure

The total assembly is fixed and required temperature is taken in bath. The temperature controller is adjusted to the required set point value. By the time the temperature rises steadily, solutions of n-Butanol and Acetic acid of known mole ratio are prepared. The n- Butanol solution is weighed and transferred into the flask using a laboratorial funnel through the sampling socket. When the reactor temperature reaches the desired magnitude, i.e. the set point Acetic acid is also transferred. A known amount of catalyst (Sulphuric acid) is added. The amount of catalyst to be added is decided on the weight % basis in terms of the reaction mixture. The reaction begins from here and the measurement of time is started.

Operating Parameters

Various runs have been taken at different temperatures, mole ratio, and catalyst concentrations. Different combinations have been applied. Those conditions that gave considerable conversion of the limiting reactant have been put forth. They have been tabulated below:

Observation tables

Table 1: Operating Conditions

Temperature	:	70°C
Mole Ratio	:	3:1
Catalyst Concentration	:	0.3 weight
% NaOH	:	0.5 N

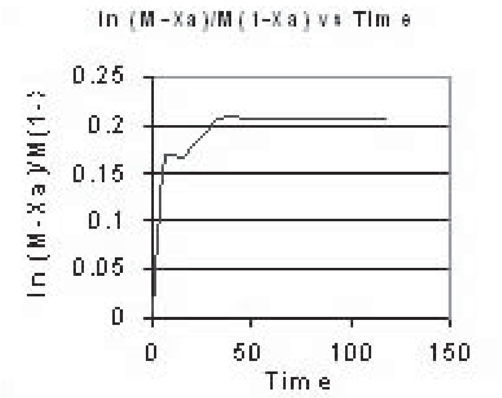

Fig. 2: Second order plot for run 1

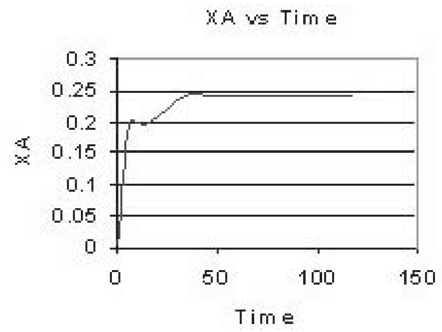

Fig. 3: Conversion - time curve for run 1

Table 2: Operating Conditions

Temperature	:	80°C
Mole Ratio	:	3:1
Catalyst Concentration	:	0.3 weight
% NaOH	:	.513 N

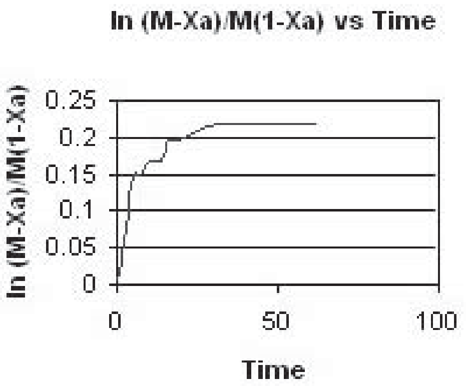

Fig. 4: Second order plot for run 1

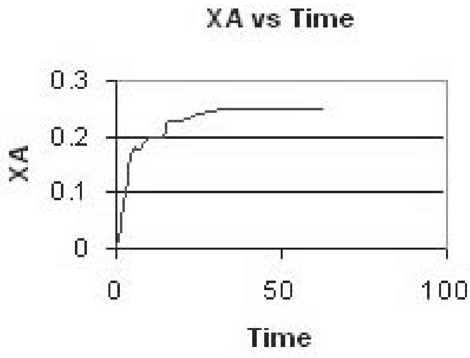

Fig. 5: Conversion - time curve for run 1

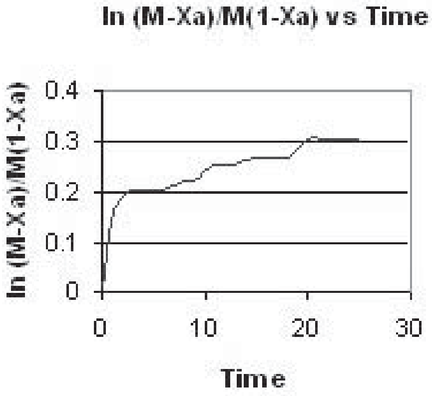

Fig. 6: Second order plot for run 1

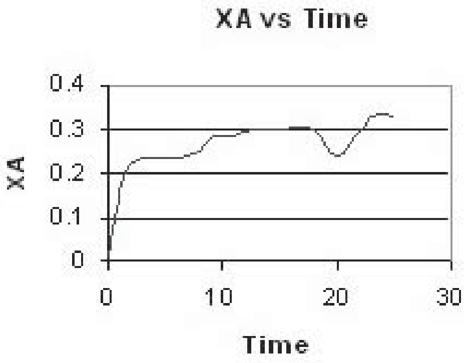

Fig. 7: Conversion - time curve for run 1

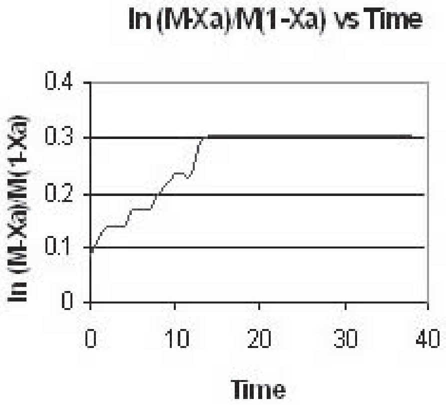

Fig. 8: Second order plot for run 1

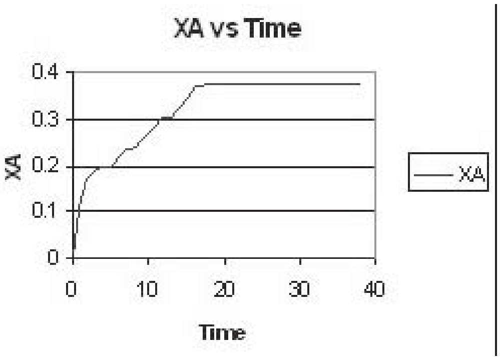

Fig. 9: Conversion - time curve for run 1

Table 3: Operating Conditions

Temperature	:	70°C
Mole Ratio	:	3:1
Catalyst Concentration	:	0.6 weight
% NaOH	:	0.39 N

Table 4: Operating Conditions

Temperature	:	70°C
Mole Ratio	:	2:1
Catalyst Concentration	:	0.6 weight
% NaOH	:	0.39 N

CONCLUSION

The following conclusions can be drawn from the experimental study of kinetics of catalytic Esterification Reaction between n-Butanol and Acetic acid using sulfuric acid as catalyst:

The esterification reaction is exothermic.

The reaction is reversible and second order.

Presence of catalyst is a must for the reaction involving n-Butanol and Acetic acid.

Optimum temperature, higher mole ratio and catalyst concentration favor the rate of reaction.

The favorable operating parameters for esterification involving n-Butanol and Acetic acid are,

Temperature in the range 100^0c

Catalyst concentration of about 0.6 % by weight.

Mole ratio of 2:1 or more

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