In addition, the distribution of one solute between one solvent in one phase and two "mixed" solvents in the other phase, i.e., in the double binary quaternary system can be predicted by an equation similar to Raoult's Law when ternary data only is needed for predicting the distribution in the quaternary.

NOTATION

$A, B, C \ldots$ = components $A, B, C \ldots$, respectively; X_{AB} = mole fraction of A in B rich phase
A = water
B = acetic acid
b = constant
C = n-butyl alcohol
D = n-heptane
E = n-butyl acetate
F = benzene
G = carbon tetrachloride
I = acetone
J = chloroform
K, K' = constants
L = methanol
M = methylnaphthalene
N = p-cresol
m, m' = constants
n, n' = constants
r = constant
EXP = experimental
FOR = formula

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Part II: Reaction Rate Studies and the Analysis of Batch Esterification in two phase Systems

The kinetics of the esterification of n-butyl alcohol with acetic acid has been studied experimentally in concentrated solutions at near ambient temperature in the presence of a sulphuric acid catalyst and the rate constants for the forward and reverse reaction determined.

The rate data obtained from the homogeneous system has been applied to analyse the performance of a batch-extractive reactor using n-heptane as solvent. The rate of mass transfer of the ester was found to be significant and when introduced in a model of the reaction process gave good agreement with the experimental results.

SCOPE

Butyl acetate is manufactured by the esterification of n-butyl alcohol with acetic acid in the presence of sulphuric acid at temperatures of the order of 100°C and the ester is removed from the reaction mixture by distillation using live steam. The esterification reaction has therefore been studied extensively at these elevated temperatures and rate equations and rate constants have been published that accurately describe the course of the esterification under these conditions. However, no kinetic data is available describing this reaction near ambient conditions. Therefore, since the object of the overall study was to assess the feasibility of producing n-butyl acetate in an extractive reactor, it was necessary to ascertain the kinetics of this esterification reaction under conditions that would prevail in an extraction column containing an organic solvent. In this particular study n-heptane was selected as solvent.

The esterification reaction has been performed in a single phase batch reactor and the rate of esterification determined. The effect of catalyst concentration on the specific reaction rate has been investigated and the influence of butyl sulphate on the course of the reaction at near ambient conditions ascertained. The rate data obtained from the homogeneous reaction studies have been applied to evaluate the performance of a two phase batch reactor using heptane as the immiscible hydrocarbon solvent. The effects of the rate of mass transfer on the rate of esterification and particularly on the significance of the reverse reaction have been considered in order to develop a model predicting the course of the extractive-reaction under batch operation.

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CONCLUSIONS AND SIGNIFICANCE

The kinetics of the reaction between n-butyl alcohol and acetic acid in concentrated solutions have been determined in the presence of sulphuric acid at 20°C in a homogeneous liquid system and the specific reaction rate determined as a function of sulphuric acid and water concentration. Near ambient conditions the esterification reaction rate is not catalysed by butyl sulphate.

The mechanism of two phase batch esterification reaction of n-butyl alcohol in the presence of n-heptane has been studied experimentally and the batch process has been modelled by assuming that the reaction rate constant for the solvent-free system applies to the reactive phase of an extractive batch-reactor. The equilibrium concentrations of the reactants have been computed from the distribution equations developed in Part I of this study, allowing for the rate of mass transfer of ester out of the reactive phase and introducing the instantaneous net quantity of ester remaining in the phase. This ester concentration was significant and with these modifications it was found that good agreement was obtained between the predicted and experimental results.

INTRODUCTION

n-butyl acetate is manufactured by the continuous esterification of n-butyl alcohol with acetic acid in the presence of a sulphuric acid catalyst at elevated temperatures and the product is removed continuously from the reaction mixture by steam distillation. The esterification reaction kinetics have been studied extensively for the conditions prevailing in this process, but no data are available for these kinetics near ambient temperature in a homogeneous or two phase liquid system: conditions that would prevail if n-butyl acetate was produced by a simultaneous chemical reaction-solvent extraction process. Therefore, an investigation of the rates of this esterification was undertaken as part of a feasibility study of such a process and the results obtained are presented in the following paragraphs.

The term "extractive" reaction was first used by Trambouze and his coworkers (1960) to describe reacting systems where an immiscible extractive component is deliberately added to increase the yield. Such processes encompass several unit operations and have been practiced for some time in liquid-liquid reacting systems as well as in simultaneous reaction and distillation processes. In an extractive reaction in a liquid-liquid system, the reaction is performed in the presence of a suitable solvent, and such a process was patented by Martin and Krchma (1930) for the production of butyl acetate by the transesterification reaction,

$$C_4H_9OH + CH_3COOC_2H_5 \overset{H_2SO_4}{\rightleftarrows} C_2H_5OH + CH_3COOC_4H_9 \tag{1}$$

Equilibrium was displaced in favor of the product by performing the reaction in a two phase water-hydrocarbon system. The hydrocarbon preferentially dissolved the butyl acetate, but not the other product, ethyl alcohol, which remained in the aqueous phase.

The production of butyl acetate has been utilized in this investigation with heptane the hydrocarbon solvent.

The term "extractive reaction" is used nowadays to describe any process involving simultaneous extraction and chemical reaction in a liquid-liquid system even when no "inert" solvent is present. Such a reaction system is the hydrolysis of animal and vegetable fats and oils which was studied by Jeffreys, Jenson and Edwards (1967) in a pilot plant batch reactor and in a spray extraction column operated continuously. The model developed by these authors to analyze the batch reactor performance has been extended here to include the effects of the rate of mass transfer of butyl acetate. In addition, the following assumptions were made:

(a) No chemical reaction takes place in the heptane rich phase.

(b) The solubility of water in the heptane rich phase, and heptane in the aqueous phase are negligible throughout the course of the reaction.

(c) No volume changes occurred on mixing during the course of the reaction.

THEORY OF THE KINETICS OF ESTERIFICATION

Stoichiometrically, the esterification of n-butyl alcohol can be written as:

$$CH_3COOH + C_4H_9OH \overset{H_2SO_4}{\rightleftarrows} CH_3COOC_4H_9 + H_2O \tag{2}$$

or

$$B + C \underset{k_2'}{\overset{k_2}{\rightleftarrows}} E + A$$

and the rate equation is,

$$\frac{d[E]}{dt} = -\frac{d[B]}{dt} = k_2[C][B] - k_2'\,[A][E] \tag{3}$$

Integration of Eq. 3 and insertion of the initial concentration of the reactants and products leads to the equation derived by Smith (1970):

$$q^{\frac{1}{2}}t = \ln\frac{\{2\gamma\,[x]/(\beta - q^{\frac{1}{2}})\} + 1}{\{2\gamma\,[x]/(\beta + q^{\frac{1}{2}})\} + 1} \tag{4}$$

where the symbols are as presented in the nomenclature.

If the initial concentration of the products are zero and the reactants are equimolar, Eq. 4 is simplified to:

$$k_2 = \frac{K^{\frac{1}{2}}}{2\,[M]_0 t}\ln\frac{1 + x[K^{-\frac{1}{2}} - 1]}{1 - x[K^{-\frac{1}{2}} + 1]} \tag{5}$$

If the specific reaction rate k_2 is known, the amount of acetic acid reacted, x, can be evaluated from a rearranged Eq. 4; that is

$$[x] = \frac{e^{q^{\frac{1}{2}}t} - 1}{\dfrac{2\gamma}{\beta - q^{\frac{1}{2}}} - \dfrac{2\gamma e^{q^{\frac{1}{2}}t} - 1}{\beta + q^{\frac{1}{2}}}} \tag{6}$$

Equations 4, 5 and 6 would be expected to apply to the esterification reaction if it were second order reversible. However, Leyes and Othmer (1945) found that the specific reaction rate "k_2" was related to various process variables by a complex empirical equation that has been attributed to the influence of the side reaction between butanol and sulphuric acid to form butyl mono sulphate (alkyl sulphuric acid). This side reaction has been verified to be particularly significant at elevated temperatures; but proceeds slowly over a period of days at 25-30°C, Suter (1934). Thus according to Dhanuka et al. (1977) both sulphuric acid and butyl monosulphate act as catalysts and the reaction rate is considerably different in the presence of these two substances. Hence, the variations in the reaction rate during the progress of the esterification reaction, starting with sulphuric acid catalyst, were attributed by these authors to be due to the change in the ratio of the two catalysts as more sulphuric acid was converted to the monosulphate.

In order to avoid this complication, Dhanuka reacted the appropriate amount of sulphuric acid and alcohol at 100°C for sufficient time for all the sulphuric acid to be converted to monosulphate before adding the carboxylic acid. Under these conditions, he claimed that the results obtained for the esterification gave the reaction rate constant in the presence of the monosulphate catalyst; and they found that their data was correlated by a second order reversible kinetic equation. If this interpretation of the esterification reaction kinetics is correct, no complication should be expected when the process is carried out at near ambient temperature since the side reaction will be so slow that there will not be any significant conversion of sulphuric acid to butyl monosulphate.

THEORETICAL ANALYSIS OF THE TWO PHASE BATCH REACTOR

The sequence of calculations required were made by computer and are summarised in the logic flow diagram presented in Figure 1. The algorithm is:

(1) From the initial reactants and solvent feed, the concentration of acid and alcohol in the aqueous phase was determined from the initial amounts of reactants and solvent charged to the reactor using the procedure developed in Part I of this study.

(2) The reaction rate was calculated from the rate equations developed above.

(3) The rate equation was to be solved numerically for E. Therefore the derivative had to be evaluated, in terms of reactants and products concentration,

$$DE = k_2[A][B] - k_2'[E][C] \tag{7}$$

$[A]$, $[B]$, and $[C]$ having been determined in step (1) above. However, according to the distribution studies described in part 1 the concentration of the ester in the aqueous phase should be zero if equilibrium exists between the phases. If this condition is satisfied, the reaction will be irreversible and the last term of Eq. 7 will be zero. However, during the computer program development it was found that the rate of mass transfer was not fast enough to maintain the aqueous phase free of the ester molecules, particularly in the early stages of the reaction when the reaction rate was relatively fast. Therefore the following procedure was developed to account for this mass transfer effect.

(4) A step was introduced into the numerical integration of the rate equation using the value of the derivative previously calculated from Eq. 7.

(5) The variables were tested for a print interval to ascertain whether the computation has reached a termination value.

(6) All the variables were updated according to the stoichiometry of the reaction and new values of $[A]$, $[B]$, $[C]$ and $[E]$ evaluated according to the distribution model, i.e., the computation was recycled to the beginning.

Initially the program was tested on the assumption that all the ester was transferred instantaneously to the solvent phase as it was formed. That is, it was assumed that the reaction was completely irreversible since it had been previously established in Part I that practically all the ester distributes to the heptane phase. However, when the program was run on the assumption of reaction irreversibility, the computed values were exceptionally high, indicating the existence of a mass transfer effect.

The equation for the overall mass transfer coefficient for the transfer of the ester is:

$$\frac{1}{K_G} = \frac{1}{k_c} + \frac{1}{mk_d} \tag{8}$$

but, the value of "m" was found to be very large; therefore, from Eq. 8 it would appear that:

$$K_G \simeq k_c$$

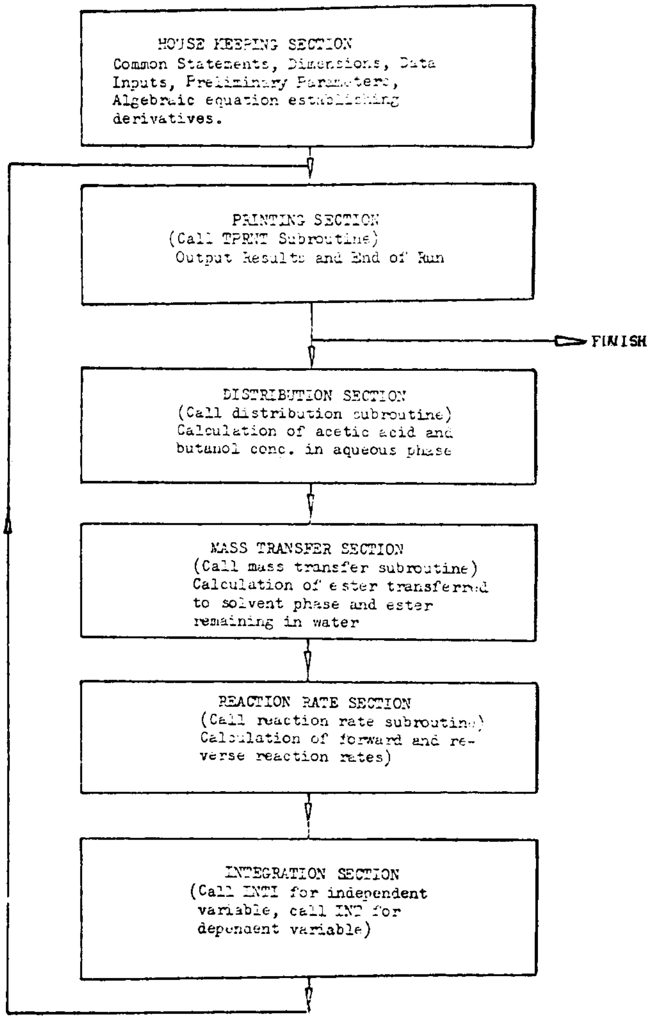

Figure 1. General arrangement of program for calculating conversion in esterification reaction in the presence of solvent.

However, when k_c was evaluated theoretically using established correlations it was found to be consistently larger than $(K_G)_{EXP}$ indicating the existence of an additional resistance. This could be attributed to the effects of the reverse reaction causing hydrolysis of the ester as it was transferred to the organic phase. Murdoch and Pratt (1953) and Lewis (1958) have reported similar findings. They proposed that the total resistance to mass transfer in such a case is given by:

$$\frac{1}{K_G} = \frac{1}{k_c} + \frac{1}{mk_d} + r_i \tag{9}$$

where the value of r_i is $1/\bar{k}_1$ and $\bar{k}_1$ is the reverse specific reaction rate evaluated on the basis of a pseudo first order reaction. $\bar{k}_1$ was calculated from the equation for the forward reaction rate and the equilibrium constant. Combination of the continuous phase mass transfer coefficient k_c and a reaction resistance effect, given by the reciprocal of $\bar{k}_1$ gave a revised value of K_G which was introduced into the overall batch-extraction-reaction model. K_Ga was calculated from the K_G value obtained from Eq. 9 and the area "a" from the mean drop size by application of Kolmogoroff's law (1949).

EXPERIMENTAL

The equipment for the evaluation of the esterification consisted of a 1.0 L round bottom flask containing three openings. The central opening was provided with a glass gland through which passed the stirrer shaft and a thermometer was inserted into one of the side openings. The third opening was stoppered and was used for withdrawing samples to follow the reaction. The flask was immersed in a constant temperature

Table 1. Esterification of Butanol at 20°C

Run No. 1. Feed Composition
Acetic Acid 40.67%, Butanol 49.53%, H_2SO_4 9.8%.

Time min	%Free Acetic Acid	% Conversion	k_2 L/(gmol) (min)	Mean Water Conc. g·mol/L
1	36.65	9.88	0.0170	0.319
3	32.5	20.01	0.0129	0.646
6	28.7	29.43	0.0108	0.950
10	24.65	39.39	0.0101	1.272
15	21.85	46.27	0.0090	1.494
20	19.8	51.30	0.0083	1.656
30	17.05	58.08	0.0076	1.875
24 hours	6.4	84.26	—	—

Run No. 2 Feed Composition
Acetic Acid 43.1%, Butanol 52.35%, H_2SO_4 4.55%.

Time min	%Free Acetic Acid	% Conversion	k_2 L/(gmol) (min)	Mean Water Conc. g·mol/L
1	41.3	4.18	0.0073	0.136
3	39.0	9.51	0.0058	0.309
6	36.15	16.13	0.0053	0.524
10	33.3	22.74	0.0049	0.739
15	30.8	28.54	0.0045	0.928
20	28.85	33.06	0.0041	1.074
30	25.92	39.86	0.0037	1.295
24 hours	8.5	80.28	—	—

bath that was capable of maintaining the reaction temperature to within ±0.1*K* of that desired for the reaction experiment.

Experimental Procedure

The following operating procedure was adhered to:—The water bath was set to the desired temperature for the experiment and the reactants and catalyst were weighed separately. The acetic acid, water and sulphuric acid were charged into the reactor and well mixed while the butanol was placed in a separate flask which was also immersed in the water bath until its temperature was constant. When all the liquids had reached the required temperature, the alcohol was poured into the reactor and the stirrer started. This was considered to be the commencement of the reaction and a stop watch was started. After one minute, a sample of the reaction mixture was withdrawn and put immediately into a preweighed flask containing 25 cc of chilled water to quench the reaction. The flask was weighed again to determine the exact weight of the sample and the contents were then titrated with 0.1N NaOH solution. As the reaction proceeded, further samples were taken in the same way at definite time intervals. The duration of an experiment was usually 30 minutes and the sampling frequency varied between one sample per minute at the beginning and one sample every 10 minutes at the end.

Finally for the kinetic study the mixture was kept overnight and stirred again for several hours the next day and a sample taken as before and titrated to determine the equilibrium concentration. The extent to which the side reaction between n-butanol and sulfuric acid occurred at the temperature of the esterification reaction was ascertained by reacting n-butanol with solutions of sulphuric acid of the same acid concentrations as those utilized in the esterification studies. In all experiments performed in the neighbourhood of 20°C it was confirmed that the amount of butyl sulphate produced was undetectable, and it may be concluded that this side reaction is insignificant under the esterification conditions prevailing in this study.

In all the experiments involving two phases the butanol was mixed with the heptane and this solution was added to the reactor containing a known amount of acid and catalyst. The reaction was timed from the

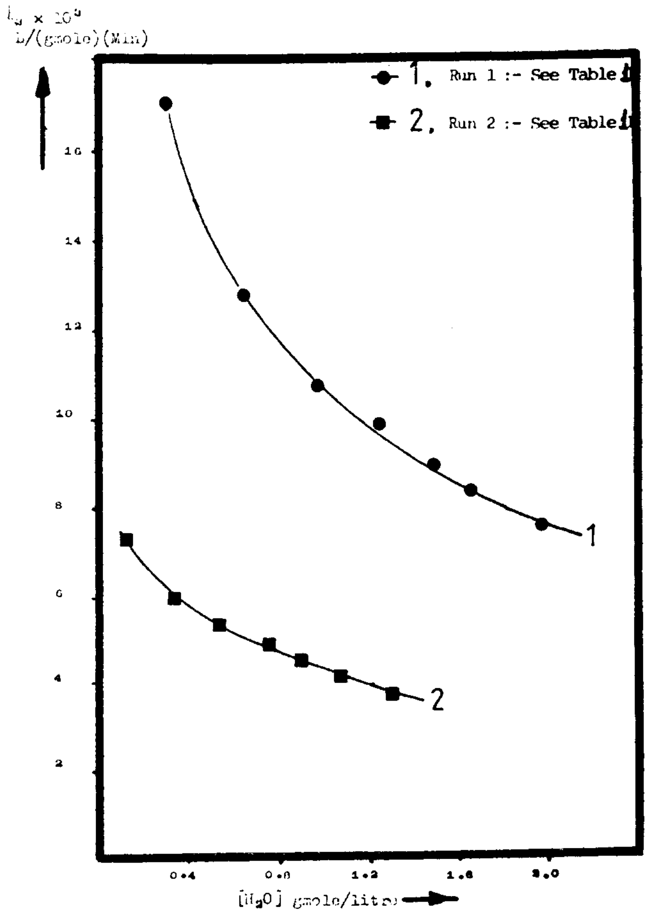

Figure 2. Esterification of butanol k_a vs. $[H_2O]$.

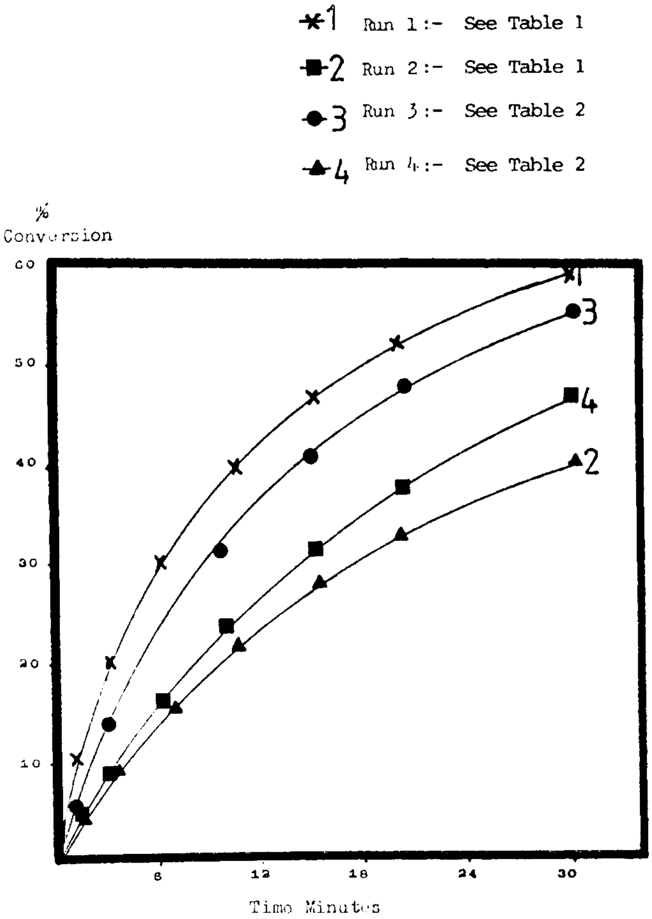

Figure 3. Esterification of butanol conversion vs. time.

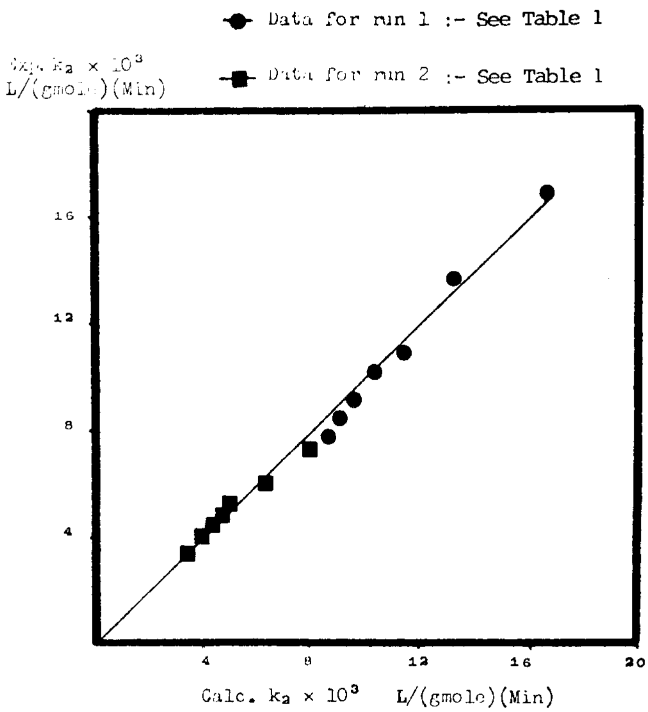

Figure 4. Batch esterification experimental vs. calculated k_2.

TABLE 2. ESTERIFICATION OF BUTANOL AT 20°C

Run No. 3 Feed Composition:	Run No. 4 Feed Composition:
Acetic Acid 38.2%	Acetic Acid 36.0%
Butanol 46.95%	Butanol 44.3%
H_2SO_4 9.89%	H_2SO_4 9.66%
H_2O 4.96%	H_2O 10.04%

Time (min)	Exp. Conv. %	Computed Conv. %	Expt. Conv.	Computed Conv. %
1	4.92	4.74	3.61	3.17
3	12.95	12.87	8.72	8.90
6	21.05	22.56	15.96	16.26
10	29.64	32.33	23.87	24.30
15	38.73	41.31	30.51	32.29
20	47.25	47.98	36.90	38.64
30	55.01	57.16	46.17	48.06
24 hours	76.04	—	75.1	—

moment all the reactants had been introduced into the reactor. Samples were withdrawn at selected intervals as described above and the results obtained are presented in Figures 2 to 9.

Materials Used

The following reagents were used in the reaction studies:

(i) Glacial Acetic Acid; G.P.R. "A" grade of density 1.048-1.051 gm/cc

(ii) n-Butyl Alcohol; G.P.R. grade of density 0.809-0.811 gm/cc

(iii) Sulphuric Acid; G.P.R. grade of density 1.84 gm/cc

(iv) n heptane conforming to I.P. specification of density 0.682-0.684 gm/cc

TABLE 3. ESTERIFICATION REACTION EQUILIBRIUM CONSTANT

Run No.	H_2SO_4 wt. %	H_2O wt. %	K
1	9.8	0.0	28.7
2	4.55	0.0	16.0
3	9.89	4.96	22.4
4	9.60	10.04	18.2

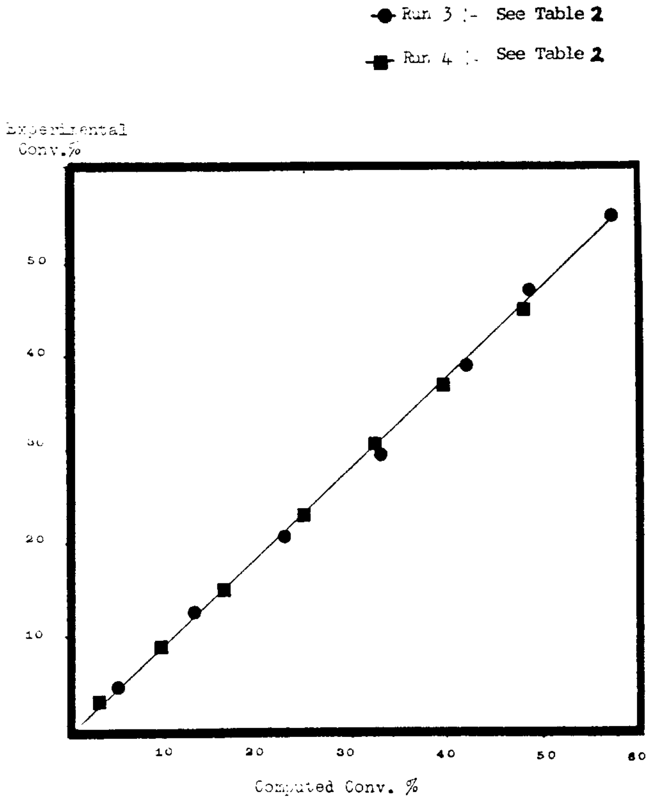

Figure 5. Batch esterification experimental vs. computed conversion.

DISCUSSION

Table 1 gives the results of kinetic studies of the esterification for two experiments initiated with 9.8% and 4.55% sulphuric acid and stoichiometric quantities of acetic acid and butanol.

The equilibrium constant K was calculated from the concentrations of products and reactants at 24 hours, and k_2 was calculated from Eq. 5. The instantaneous concentration of water generated was also evaluated. The initial reaction rate was rapid but this decreased as the water formed diluted the catalyst. The results are further illustrated in Figure 2 and the results for all four experiments are summarized in Figure 3.

Regression analysis was undertaken on the data of Table 1 and the following correlation for k_2 was obtained

$$k_2 = (0.0112)\,[H_2SO_4]^{1.18}[H_2O]^{-0.324} \qquad (10)$$

where k_2 is in L/(g mol)(Min).

The experimental values of specific reaction rate of the forward reaction are plotted against k_2 evaluated from Eq. 10 in Figure 4, and it will be seen that good agreement has been obtained; the maximum deviation being about 13%, and the average deviation 5%.

Equations 6 and 10 were used to estimate the conversion of different mixtures of A, B, C, E and catalyst charged into the reactor. However, since in Eq. 6 $[x]$ is implicit, because $\propto$, β and γ are functions of x, a computer program was written to evaluate $[x]$ by iteration.

Results of the computer calculations for two runs together with the actual experimental values are shown in Figure 5 and Table 2 where it will be seen that good agreement was achieved between the experimental and computed values, the maximum deviation was about 8%.

The values of the equilibrium constant K are presented in Table 3 which indicates that K increases as the catalyst concentration is increased, or the initial concentration of water is decreased. These values are considerably larger than the average of 2.35 reported by Leyes and Othmer (1945). The variation is thought to be due to the very much higher catalyst concentration employed in this study.

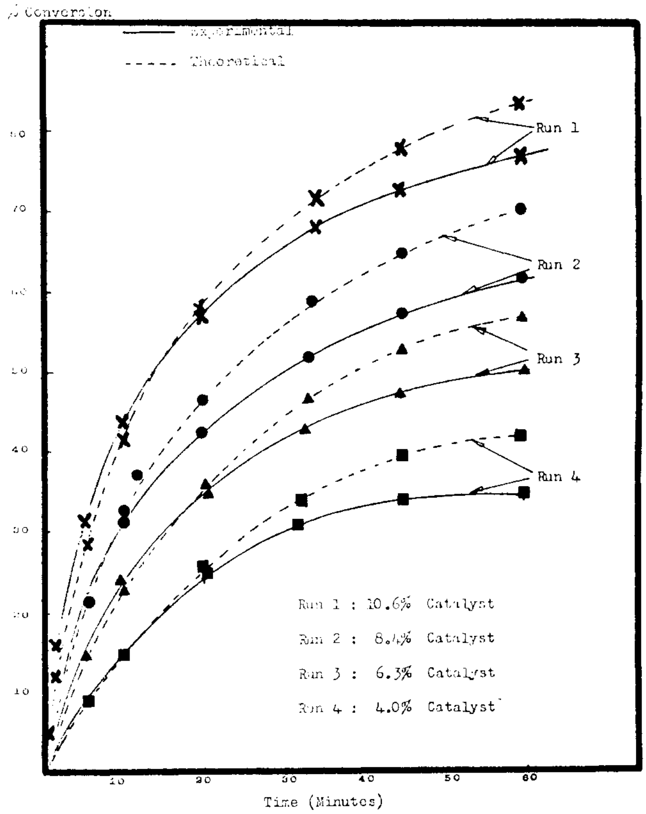

Figure 6. Batch extraction reaction. Theoretical and experimental conversion at various catalyst concentrations.

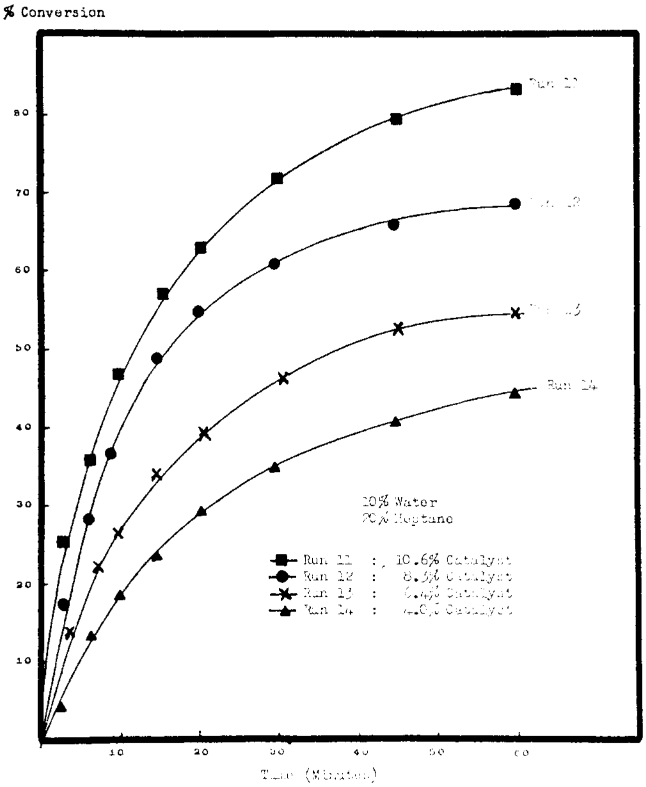

Figure 7. Batch extraction reaction experimental conversion at various catalyst concentrations.

Fourteen batch reactor experiments were undertaken with the two phase system, with the amounts of reactants, catalyst and solvent stated in Figures 6 to 10. Figures 6, 7 and 8 indicate the influence of the catalyst concentration on the reaction mixtures of the same compositions. In addition, Figure 6 includes the results of the computer calculations. These figures show that increased catalyst concentration enhance the reaction rate.

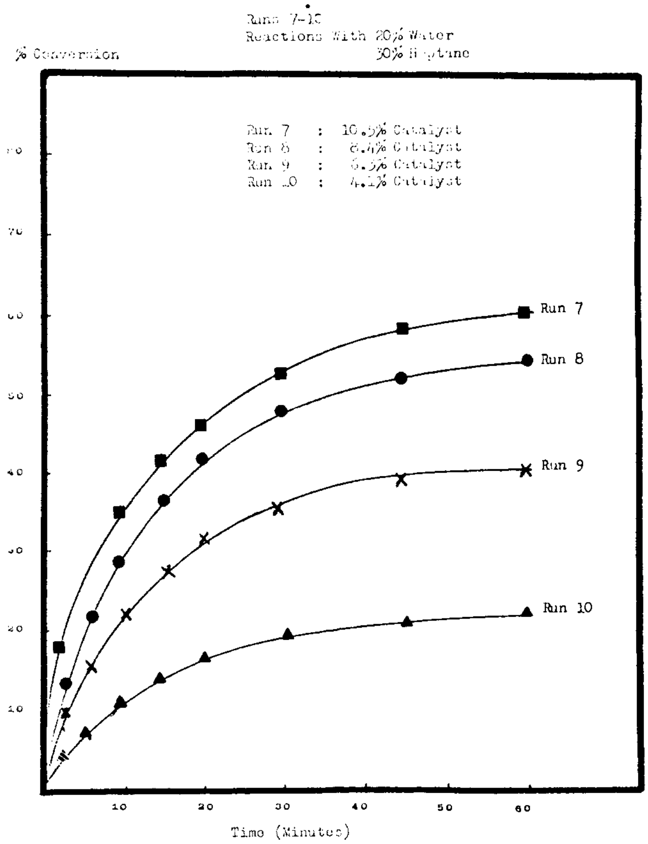

Figure 8. Batch extraction reaction experimental conversion at various catalyst concentrations.

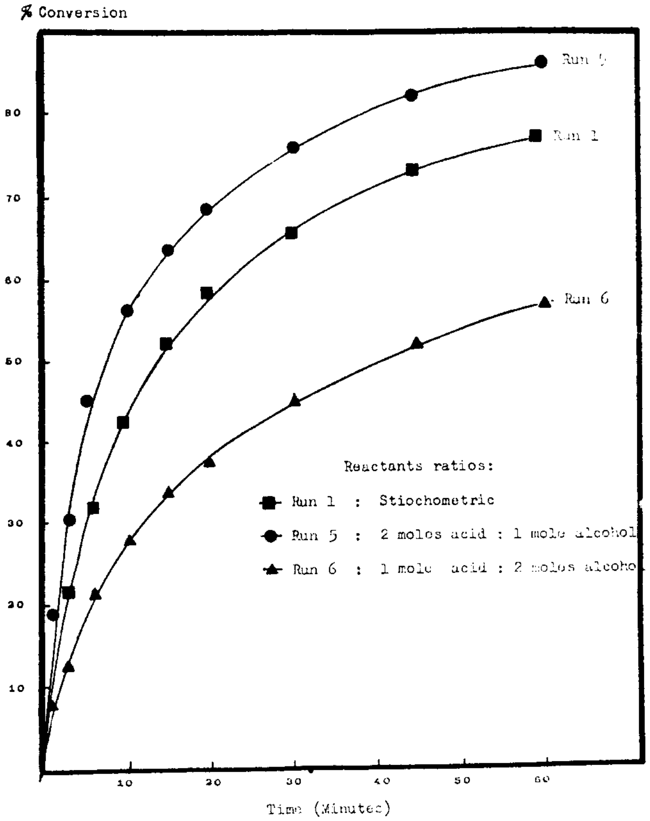

Figure 9. Batch extraction reaction influence of reactants ratio on conversion.

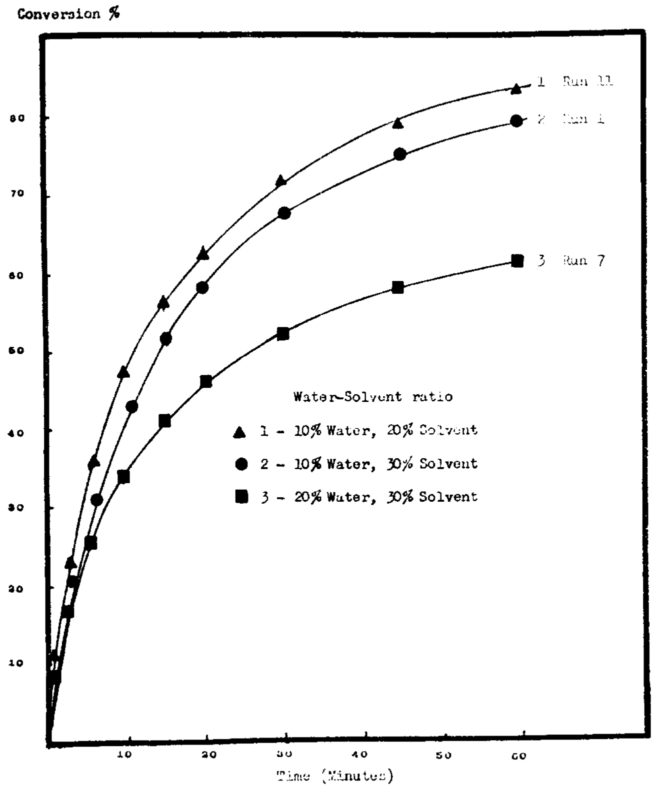

Figure 10. Batch extraction reaction influence of water solvent ratio on conversion.

Figure 9 presents the conversions for the same amounts of catalyst, water and heptane concentration, but different ratios of acetic acid to butanol. Conversion is improved as the acid:alcohol ratio is increased. This is in accordance with the distribution studies reported in Part I. Excess acetic acid salts the butanol into the aqueous phase where the reaction can proceed, whereas excess butanol salts the acid out into the organic phase thus depleting the aqueous (reactive) phase of both reactants.

Figure 10 gives the conversion for the same catalyst and reactants concentration but differing heptane and water ratios. This figure suggests that a water: heptane ratio of 2:3 gives the lowest conversion while a ratio of 1:2 gives the highest. A water:heptane ratio of 1:3 is intermediate between these extremes and these results are confirmed by the computer model. Qualitatively there appears to be two contradicting phenomenon occurring when the water:heptane ratio is changed. When this ratio is increased the overall quantity of reactants in the aqueous phase increase and this improves the ultimate conversion, but the greater the amount of water present, the lower the concentration of the reactants and particularly the catalyst concentration and therefore the rate of esterification is much slower. As will be seen by inspection of the curves in Figure 10 equilibrium is never achieved, and possibly there is an optimum water:heptane ratio for the batch reactor although this is outside the scope of this paper.

Figure 6 presents a comparison between the experimental and predicted results for four experiments with catalyst concentration ranging from 4.0-10.6%. In all the four examples the computed values were higher at the completion of the reaction. This deviation becomes progressively larger for slower reaction rates, the maximum deviation being 24% for the run with 4.0% catalyst, which indicates that the resistance to mass transfer is greater than accounted for by Eq. 9. This resistance is particularly effective at low values of the driving force, but is believed to be counteracted at high values of the driving force. The increase in mass transfer rate, at high values of the driving force, has been confirmed by Edwards and Himmelblau (1961) and Orlander and Benedict (1963) when the effect is mainly attributed to increasing interfacial turbulence as the solute concentration is increased.

NOTATION

a = interfacial area
A = product of reaction (water)
A = concentration of reaction product A
B = species of reactant
B = concentration of reactant B
C = species of reactant
C = concentration of reactant C
E = product of reaction (Ester)
E = concentration of reaction product E
k_2 = specific Reaction Rate of ester formation
k_2' = specific Reaction Rate of reverse reaction
k_c = continuous Phase Mass Transfer Coefficient
k_d = dispersed Phase Mass Transfer Coefficient
K = equilibrium Constant
K_G = overall mass transfer coefficient
m = distribution ratio
M_o = initial concentration of reactants
q = constant in kinetic Equation: $q = \beta^2 - 4\alpha\gamma$
r_i = reaction rate resistance
t = time
x = fraction of B reacted

Greek Letters

$\alpha = k_2\{[B]_o[C]_o - 1/K[E]_o[A]_o\}$
$\beta = -k_2\{[B]_o + [C]_o + 1/K([E]_o + [A]_o)\}$
$\gamma = k_2 - k_2/K$

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