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Estimation of Parameters of Arrhenius Equation for Ethyl Acetate Saponification Reaction

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Abstract

In this scientific research a Saponification Reaction between Ethyl Acetate and caustic soda is carried out in a Batch Reactor at STP Conditions. The aim of this scientific research is to estimate the parameters of Arrhenius equation which are rate constant and activation energy for ethyl acetate saponification. For this purpose the reaction is experimentally performed in a Batch Reactor and change in Concentration (in terms of Electrical Conductivity) is measured with time at different temperatures of 25°C, 30°C, 35°C, 40°C, 45°C and 50°C. at each temperature different values of rate constant are obtained at various time and concentration data. Finally to analyze our experimental data graphical method is used and a graph is plotted between ln(k) and 1/T and finally results shows that the value of rate constant is find out from the graph intercept which is 2.314×10^{10} and the activation energy is calculated from the slope of graph which is $43.094 KJmole^{-1}$.

Keywords: Saponification, arrhenius equation, activation energy, rate constant.

Introduction

Saponification reaction is the hydrolysis of a carboxylic acid ester in a basic medium. The role of alkali in the saponification reaction is that it breaks the ester bond and releases the fatty acid salt and glycerol. Esters are usually present in the form of tri-glycerides. Industrial importance of the reaction product sodium acetate demands for process improvements in terms of maximum conversion and economical and environmental friendly usage of raw materials[1].

Arrhenius Equation is now eighty years old continues to play a dominant role in classical studies of chemical kinetics it makes experimentally possible to express the dependence of temperature over rate constant in terms of only two variables. Activation energy is strictly combined with the kinetics of chemical reaction. The relationship is described by.

$$k = Ae^{\left(\frac{-E_a}{RT}\right)} \quad (1)$$

Where K is the rate constant A is the frequency factor a temperature independent term Ea is the activation energy T is the temperature and R is general gas constant. Activation energy is the amount of energy that ensures to make the reaction happen. Usually common sense is that higher temperature causes the two molecules to collide with each other more fastly. So usually the concept is that the rate of a chemical reaction is directly proportional to the temperature and the effect of the temperature on the rate of chemical reaction is calculated by the Arrhenius equation[2,3].

Previous study shows that Specific rate constant and conversion increase almost linearly with temperature. Conversion increases from 50.2 % to 58.8 % corresponding to a temperature change from 25^0C to 30^0C. But for a reaction temperature more than 30 0C, behavior of conversion change became more sluggish[4]. Further reaction rate is increased by the catalysis. Catalyst is the material that increases the rate of a chemical reaction, and for equilibrium system it increases the rate of which a chemical system approaches equilibrium without being consumed in the process[5]. If the value of activation energy is greater than $20 KJmole^{-1}$ it is possible that the process is involve in the breaking of primary chemical bond may occur[6].

Reaction Kinetics: Saponification Reaction of Ethyl Acetate and Sodium Hydroxide is an irreversible 2nd order overall, 1st order with respect to reactants furthermore reaction order decreases and become sequential rather than 2nd order when equimolecular concentrations of both reactants are used[7-10].

This reaction is non-catalytic and carried out in a constant density system. This is a homogeneous phase (liquid/liquid) reaction and mild exothermic in nature.

$$CH_3COOC_2H_5 + NaOH \rightarrow CH_3COONa + C_2H_5OH$$

The rate of a chemical reaction is usually depend upon the two terms 1st is temperature dependent and 2nd is composition dependent and the temperature dependent term is measured by using the Arrhenius Equation[11]. So we may write as.

$$r = f_1(\text{Temperature}) \times f_2(\text{Composition}) \quad (2)$$

$$r = k \times f_2(\text{Composition})$$

Where: k is rate constant and described by using the Arrhenius equation.

$$k = k_o e^{\left(\frac{-E_a}{RT}\right)}$$

Rate constant and activation energy can be calculated by solving the above equation.

$$\ln k = \ln k_o + \ln e^{\left(\frac{-E_a}{RT}\right)} \quad (3)$$

$$\ln k = \ln k_o - \left(\frac{-E_a}{RT}\right) \ln e$$

$$\ln k = \left(\frac{-E_a}{R}\right)\frac{1}{T} + \ln k$$

Now compare the above equation with the equation of straight line we get.

$$y = mx + c \quad (4)$$

Hence by plotting the graph between 1/T on x-axis and lnk on y-axis then antilog of intercept gives the value of rate constant and the slope of straight-line will give the value of $-E_a/R$.

Experimental Details: The reaction is carried out in a batch apparatus at STP conditions and the change in concentration (in terms of Electrical Conductivity) with time is measured. The experimental setup is shown in figure-1.

Apparatus: Thermostatted Bath, Volumetric Flask, Stopwatch, Conductivity Meter, reaction Vessel, Jacketed Beaker, Graduated Cylinder, Pipettes of Assorted Sizes and Burette.

Chemicals: Sodium Hydroxide (NaOH), Ethyl Acetate ($CH_3COOC_2H_5$)

Procedure: For batch experimental equal volume of both reactants is used. Concentrations of both reactants are taken to be 0.1M. Reactants should be as close to same temperature as possible before starting the experiment. Note down the conductivity meter readings (Conductivity in µs) of the reaction mixture after equal intervals of time. The procedure is continued until no change in the value of conductivity meter reading is observed. Repeat the experiment without agitation at different temperatures of 25^0C, 30^0C, 35^0C, 40^0C, 45^0C and 50^0C.

Observations and Calculations: The observations and calculation which are given below are without agitation. Because previous research shows that At STP Conditions in a Bath Reactor we got high conversion without agitation as compared to with agitation[7].

The value of rate constant at a given time-concentration data can be calculated by using this relationship[11].

$$k = \frac{1}{0.01(t)} \times \frac{C_O - C_T}{C_T - C_\infty} \quad (5)$$

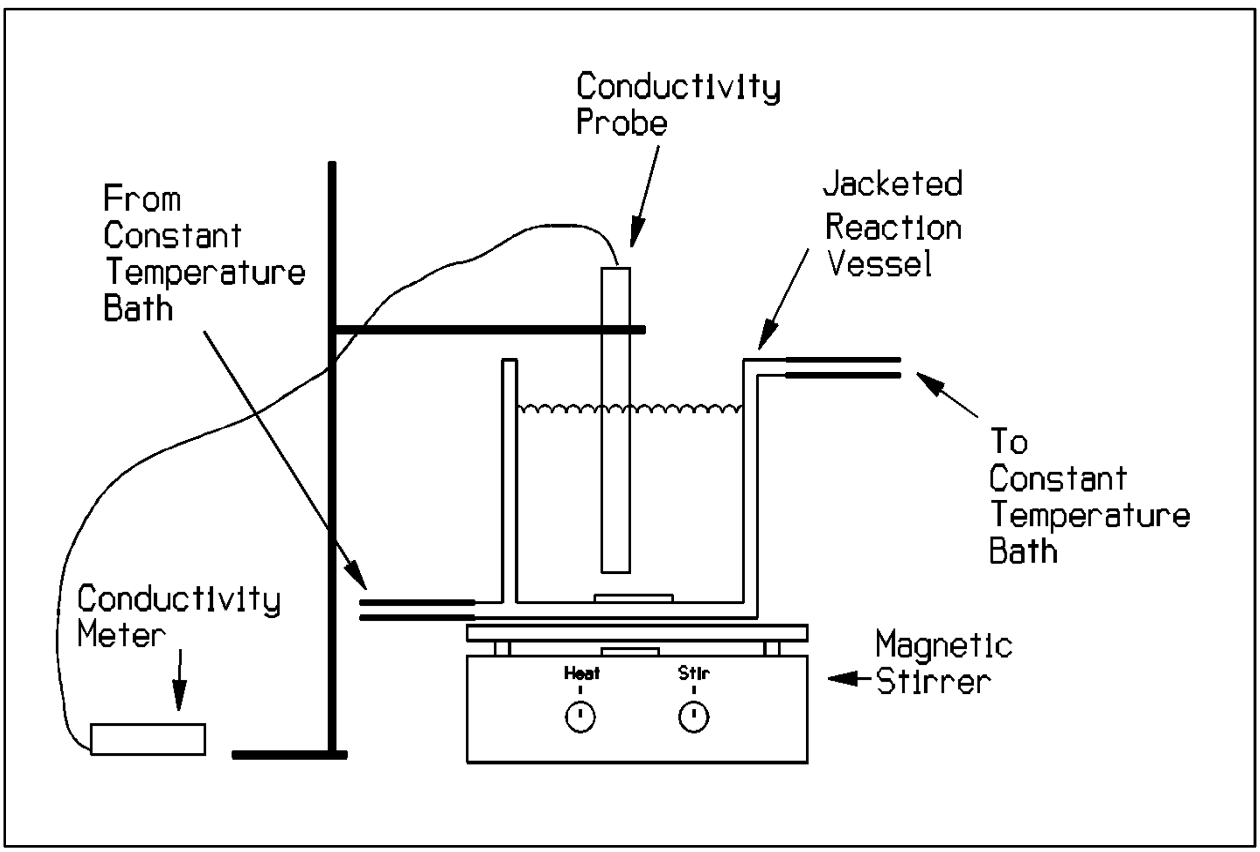

Figure-1
Experimental Setup

The different values of rate constant at different temperatures for different time and concentration date are given below in tables for temperatures of 25^{0}C, 30^{0}C, 35^{0}C, 40^{0}C, 45^{0}C and 50^{0}C.

Table-1
At Temperature 25C^o

Sr. No.	t	C_T	k
Units →	**(min.)**	**(μs)**	**min^{-1}**
1	0	C_o= 1001	0
2	1	480	336.12
3	2	443	236.44
4	3	417	211.59
5	4	398	206.50
6	5	383	213.10
7	6	366	258.13
8	7	356	297.23
9	8	350	325.50
10	9	346	346.56
11	10	341	412.50
12	11	338	463.63
13	12	335	555.00
14	13	333	642.30
15	14	330	958.57
16	15	328	1495.56
17	16	327	2106.25
18	17	325	∞

Table-2
At Temperature 30^{0}C

Sr. No.	t	C_T	k
Units →	(min.)	(μs)	min^{-1}
1	0	C_o= 974	0
2	1	529	505.68
3	2	486	542.22
4	3	473	521.87
5	4	463	580.68
6	5	455	741.42
7	6	450	970.37
8	7	445	1889.28
9	8	442	6650.00
10	9	441	∞

Table-3
At Temperature 35^{0}C

Sr. No.	t	C_T	k
Units →	(min.)	(μs)	min^{-1}
1	0	C_o= 971	0
2	1	590	253.33
3	2	518	289.74
4	3	474	487.25
5	4	462	578.40
6	5	453	795.38
7	6	450	868.33
8	7	446	1250.00
9	8	445	1315.00
10	9	443	1955.55
11	10	442	2645.00
12	11	441	4818.18
13	12	440	∞

Table-4
At Temperature 40^{0}C

Sr. No.	t	C_T	k
Units →	(min.)	(μs)	min^{-1}
1	0	C_o= 905	0
2	1	661	117.308
3	2	579	129.36
4	3	538	143.29
5	4	491	272.36
6	5	463	884.00
7	6	456	2494.44
8	7	453	∞

Table-5
At Temperature 45^{0}C

Sr. No.	t	C_T	k
Units →	(min.)	(μs)	min^{-1}
1	0	C_o= 982	0
2	1	623	208.721
3	2	498	514.894
4	3	479	598.80
5	4	172	607.14
6	5	462	945.45
7	6	457	1458.33
8	7	453	3778.57
9	8	451	∞

Table-6
At Temperature 50^0C

Sr. No.	t	C_T	k
Units →	(min.)	(µs)	min^{-1}
1	0	C_o= 962	0
2	1	532	741.37
3	2	479	9660
4	3	474	∞

Table-7
At each temperature the average value of rate constant is given

Sr. No.	T	k
Units →	(^{0}C)	min^{-1}
1	25	566.56
2	30	1550.19
3	35	1386.92
4	40	673.56
5	45	1157.5
6	50	5200.68

Table-8
Values of 1/T and lnk

Sr. No.	T	T	1/T	$K_{avg.}$	ln(K)
Units →	(C^o)	(K)	T (K^{-1})	min^{-1}	
1	25	298.15	0.003	566.56	6.33
2	30	303.15	0.0033	1550.19	7.34
3	35	308.15	0.0032	1386.92	7.23
4	40	313.15	0.0032	673.56	6.51
5	45	318.15	0.0031	1157.5	7.05
6	50	323.15	0.0031	5200.68	8.55

Results and Discussion

Hence by plotting the graph between 1/T on x-axis and lnk on y-axis by using above data then antilog of intercept gives the value of rate constant and the slope of straight-line will give the value of $-E_a/R$.

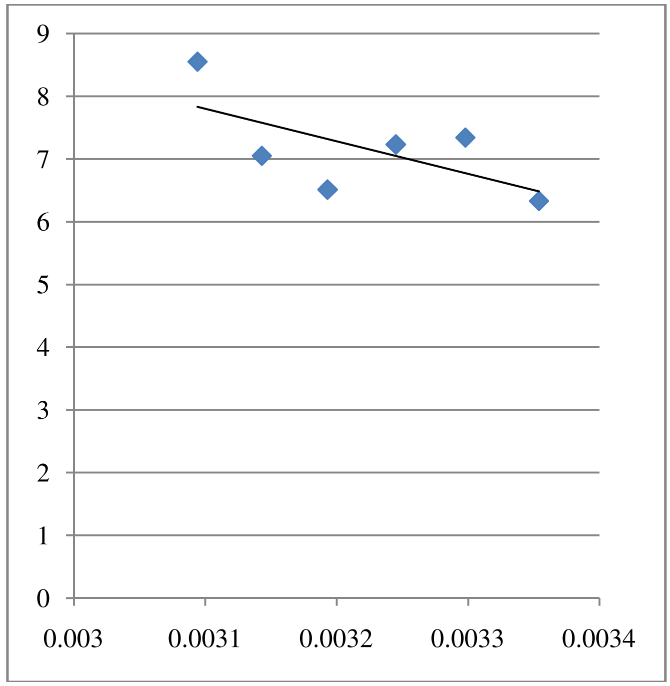

Figure-1
At Temperature 50^0C

The result shows that.
$y = -5183.4x + 23.865$

Compare above equation with the equation of straight line we get.
$y = mx + c$
$$m = -\frac{E_a}{R} = -5183.4$$
$$E_a = -5183.4 \times 8.314 = 43.094 KJmole^{-1}$$
And
$lnk = 23.865$
$$k = e^{23.865} = 2.314 \times 10^{10} min^{-1}$$

Conclusion

In this research paper a saponification reaction of ethyl acetate and sodium hydroxide is carried out in a Batch Reactor and change in Concentration (in terms of Electrical Conductivity) is measured with time at different temperatures of 25^0C, 30^0C, 35^0C, 40^0C, 45^0C and 50^0C. at each temperature different values of rate constant are obtained at various time and concentration data in order to estimate the parameters of Arrhenius equation which are rate constant and activation energy. The results show that the value of rate constant is 2.314×10^{10} and the value of activation energy is 43.094KJmole^{-1}.

Nomenclature

C_o : A Frequency Factor
C_t : Initial Concentration
C_∞ : Concentration at any Time t
E_a : Final Concentration
k_o : Activation Energy
k : Pre Exponential Term in Arrhenius Equation
R : Constant
t : Rate General Gas Constant
T : Time
: Temperature

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