Studies on the Kinetics of Adiabatic batch reactor at lab scale

K.S.R. Murthy[1*] and Srinivas T[1]

[1]*College of Engineering, Dept of Chemical Engineering, Al Imam Islam University,*

Kingdom of Saudi Arabia, Riyadh-11432

[1*]*Department of Chemistry, University of Petroleum and Energy Studies, Dehradun,*

Uttarakhand 248007

**Corresponding Author E-Mail: srmurthy@ddn.upes.ac.in;*

Abstract

The objective of this paper is to determine the conversion of NaOH with respect to time (steady state value) in an adiabatic batch reactor operation for saponification reaction. The obtained results demonstrate that the reaction is of zero order. The activation energy calculated using the Arrhenius rate equation and is found to be E = 759982.74 J/mole. After adding ethyl acetate to NaOH, the concentration of NaOH decreased from 2 minutes to 5 minutes, and the steady state was observed, demonstrating the declined nature of the curve. The conversion is slow from 0 to 1.8 minutes, then increases from 2 minutes to 5 minutes, reaching a steady state at 3 minutes. Similarly, the temperature vs. time gives nearly identical results. Similarly, the temperature Vs time graph is nearly straight (Adiabatic Q = 0), and T = 22.5^{o}C is maintained and increased from 4 to 5 minutes of time.

Keywords: Adiabatic operation, activation energy, Arrhenius equation, reaction order, NaOH, Conversion

1. Introduction and Theory of Batch Reactors

A batch reactor is typically used for small-scale operations, testing new processes that have not yet been fully developed, producing very expensive products, and processes that are difficult to run continuously. Batch reactors are typically used in isothermal and adiabatic modes for small amounts (quantities) in both isothermal and adiabatic modes. To produce a desired product and achieve the chemical reaction, isothermal and adiabatic operation reactors are run at exothermic and isochronic (constant volume) of the reactants. [1, 6, 8].

Accurately identifying the temperature reached and concentration of reactants left in an adiabatic batch reactor is relevant to fields pertaining to the prediction of temperatures in chemical reactions, such as chemical engineering and process engineering. Batch reactors are also used in small scale laboratory applications, for instance, the production and inducting of fermentation of beverage products. Batch reactors are greatly used in the field of waste water treatment because of their effectiveness in reducing the biological oxygen demand of waste water. [7]

For batch reactors, material balance yields the following governing equation:

$$\frac{dC_A}{dt} = (-r_A) \qquad 1.1$$

C_A is the final concentration (mol /m3) where the terms in Eq 1.1 are defined as follows

Time (min or sec)

r_A denotes the rate of reaction (mol/m^3).

In this experiment, the liquid phase reaction was carried out as follows:

$CH_3COOC_2H_5 + NaOH \rightarrow CH_3COONa + C_2H_5OH$

From stoichiometry of the above reaction, the relation between concentration of sodium hydroxide (A) as function of conversion as follows [2]

$$C_A = C_{Ao}\,(1 - X) \qquad 1.2$$

Where:

C_{Ao} is the initial concentration

X is the conversion

Assuming the reaction is pseudo first order reaction with respect to sodium hydroxide, one can easily get

ions, resulting in ethanol, while acetate will be bound with sodium, yielding sodium acetate. The presence of hydroxide ions can be determined by measuring the solution's conductivity. Thus, the following equation [3] can be used to directly relate the conversion of the reaction to the conductivity.

Furthermore, a fact that requires attention is the change in heat of the reactions. Both reactions released enough heat to increase the temperature of the adiabatic batch reactor by 25 K (Asiedu and Hildebrandt) [4].

$$-r_A = k.C_A{}^2 \qquad 1.3$$

Substitute eq. (2) to (3) and later substitute for –(r_A) in eq. (1), one can eventually get:

$$=\frac{\partial X}{\partial t} = \frac{C_{Ao} - C_A}{C_{Ao}\, C_A} \qquad 1.4$$

$$X = 1 - \left(\frac{\lambda_\infty - \lambda}{\lambda_\infty - \lambda_o}\right) \qquad 1.5$$

2. Experiment setup of the Chemical Reactor Trainer and batch reactor

2.1 Chemical reactor trainer description

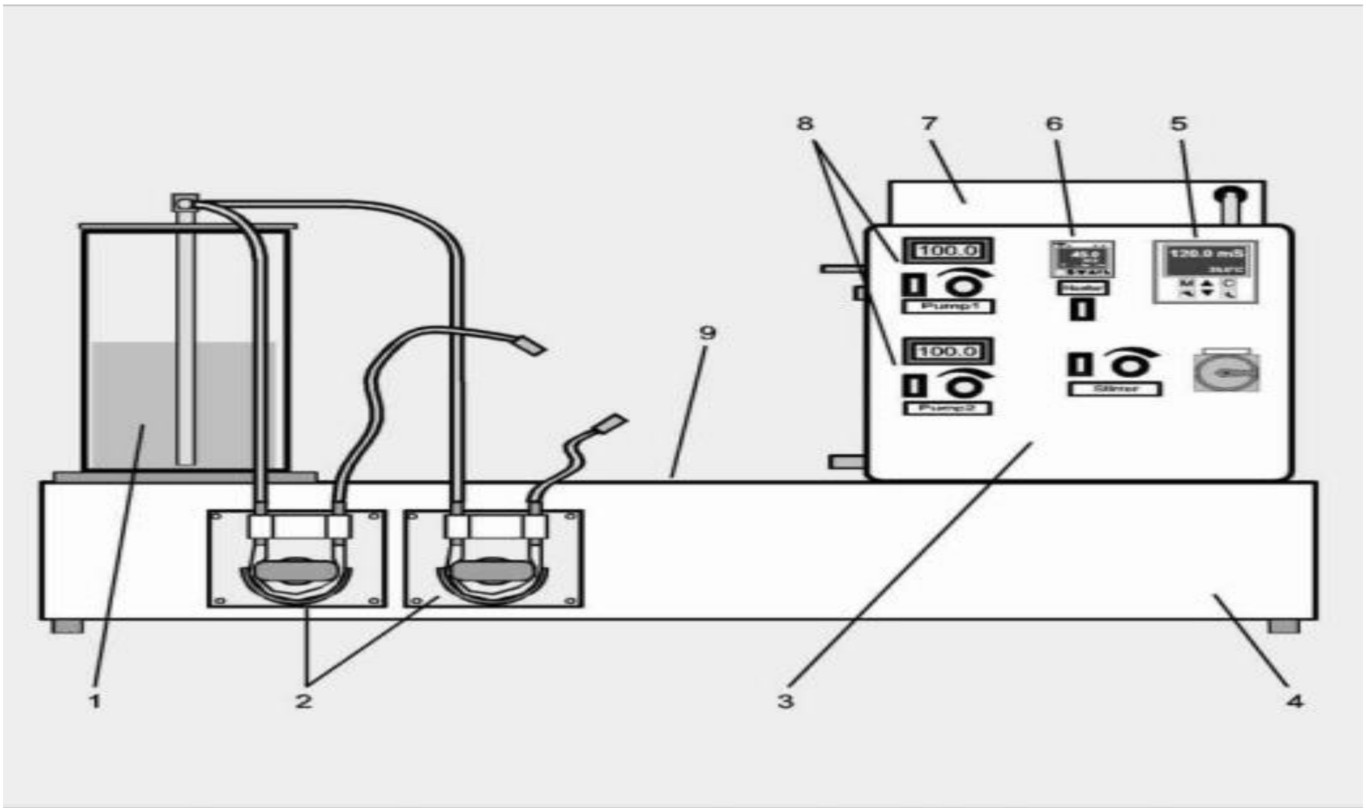

Figure 1: CHEMICAL REACTOR TRAINER (CE310) [2]

The fundamental unit is to investigate and compare various reactors using saponification as an example, and to obtain high precision, combined conductivity, and reaction temperature measurements [5]. The use of an industrial diaphragm pump results in good chemical mixing, and stirring in the reactor yields concentration values in terms of conductivity with respect to time. The chemical reactor trainer's components are as follows [6-7]

1. Benchtop unit for studying the kinetics of reaction kinetics in various types of saponification-based chemical reactors.
2. Chemicals are pumped with the help of two industrial diaphragm pumps.
3. Ethyl acetate reaction with 2.3% sodium hydroxide
4. High precision combined measuring unit for conductivity ranging from 0...200mS to 100°C.
5. Hot water circuit with centrifugal pump for reaction control
5. Hot water circuit with centrifugal pump for reaction control 2kW electrical heater
7. Two-point electronic controller
8. Self-sealing quick action hose couplings

2.2 Description of batch reactor

Using this trainer, you can investigate the properties of various chemical reactors by performing a saponification reaction. The contact time and temperature of the reaction can be adjusted. Their effect on reactant conversion is observed in the respective reactor [1]. The reactors are available as optional extras. The liquid chemicals are supplied by two supply tanks in the unit. The reactants are pumped through the reactor by two variable speed diaphragm pumps. A combined conductivity and temperature measuring unit is used to determine reactant conversion and reaction temperature. PC data acquisition is also an option. A controlled hot water circuit is used to moderate the reaction. The resulting reaction product is collected in the unit in a stainless-steel tray. [2-3]

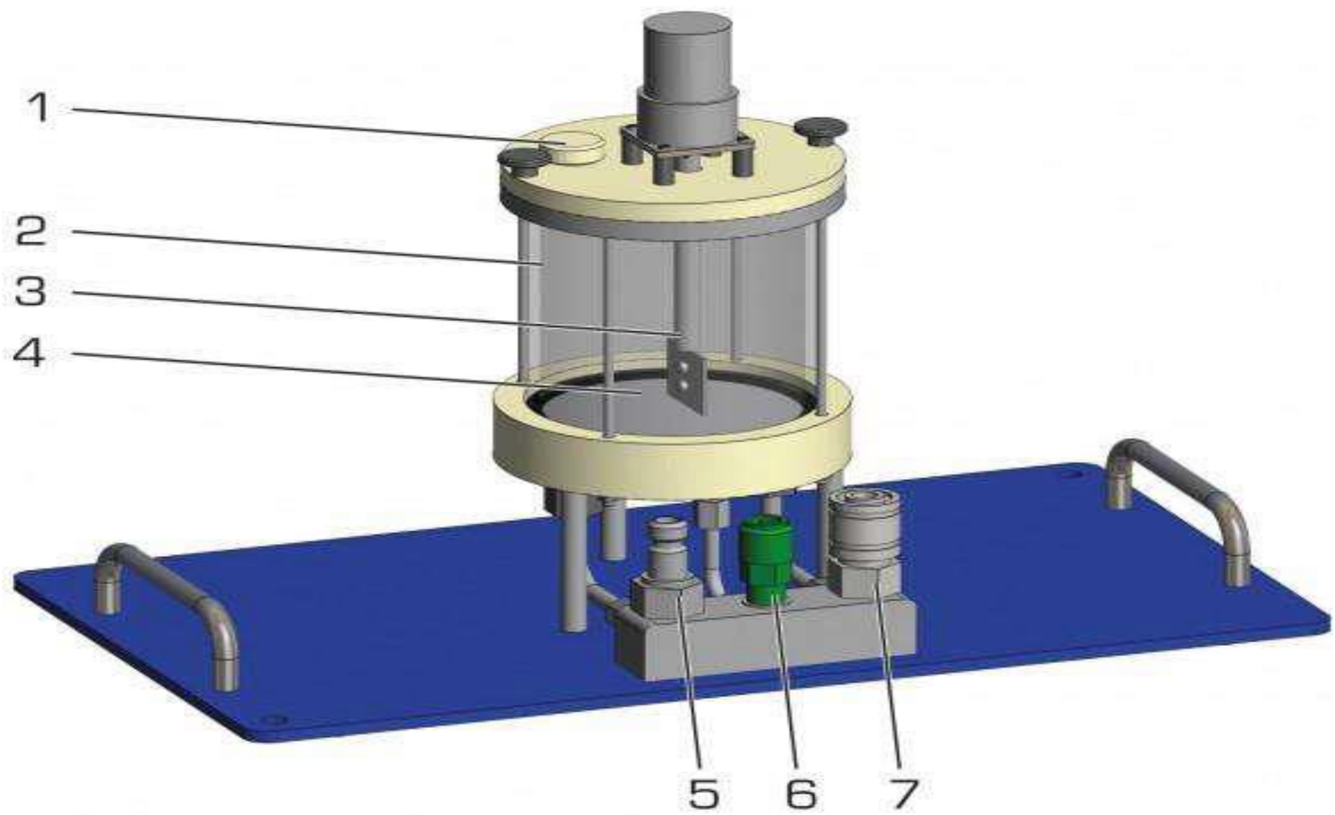

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Figure 2: Components of batch reactor

The batch reactor's components are as follows:

1. Conductivity and temperature sensor hole (included in CE 310).
2. Reactor with a stirred tank.
3. A stirrer.
4. Heat exchanger with a chambered bottom.
5. Availability of water.
6. Product waste.
7. The water drain

3. Chemical preparation, experimental procedure, and batch reactor operation

3.1 Distilled ethyl acetate and sodium hydroxide

• Prepare 1000 mL of ethyl acetate 0.1 M with 9.79 mL of ethyl acetate (= 0.9 g/cm^3 ; Mw = 88.11 g/mol).

• Dilute it in a 1 L-volumetric flask until the total volume reaches 1000 mL.

• Tightly close the flask and vigorously shake it until the ethyl acetate and water are completely mixed.

Sodium hydroxide dilution:

• Prepare 1000 mL of sodium hydroxide 0.1 M from 4 g of sodium hydroxide (M_w = 40 g/mol).

• In a 1L-volumetric flask, dilute it until the total volume reaches 1000 mL.

• Tightly close the flask and vigorously shake it until the sodium hydroxide and water are completely mixed.

3.2 Batch reactor operation:

• Carefully pour 900 mL of 0.1 M NaOH solution into the batch reactor (CE 310.04).

• Set the stirrer to medium speed but don't turn it on yet.

• Carefully pour 90 mL of 0.1 M ethyl acetate into the reactor.

• Start the stirrer and keep track of the time.

• Measure conductivity and temperature for 30 minutes.

• Repeat the experiment three times to obtain the concurrent values [8]

4.1 Data and observations

Table 1 shows the data and results obtained for the adiabatic batch reactor, and figures 3 to 10 show the analytical and graphical analysis of the batch reactor in adiabatic operation.

Table 1: Data of conductivity, time, temperature, rate constant and Conversion

Time Min: sec	Conductivity Λ (S/cm)	Temperature T (°C)	Conversion X	Concentration C_A (mol/m^3)	$(C_{AO}-C_A)/(C_{AO}*C_A)$	k (rate constant)
0:00	28	22.7	0	0.125	0	
0:20	24.7	22.5	0.75	0.03125	24	6.932
0:40	24.5	22.5	0.8	0.02557	31.11	1.0034
1:00	24.3	22.5	0.84	0.02	42.30	0.4189
1:20	24.2	22.5	0.86	0.0171	50.7	0.771
1:40	24	22.5	0.91	0.0114	80	2.027
2:00	23.9	22.5	0.93	0.0085	109.33	0.4795
2:30	23.8	22.5	0.95	0.0057	168	1.352
3:00	23.8	22.5	0.95	0.0057	168	0
3:30	23.7	22.5	0.98	0.00284	344	2.3105
4:00	23.7	22.5	0.98	0.002841	344	0
4:30	23.6	22.5	1	0		
5:00	23.6	23.6	1	0		

4.3 Discussion & Analysis

The temperature will be equal to 24°C, which is the set point temperature for this experiment, and a reading will be taken every 20 seconds as shown in Table 1. The experiment will end when the conductivity is stabilized (constant values with respect to time) for steady state.

In **Figure 3**, the concentration increased and then abruptly decreased between the values of 0 sec and 0.2 sec, and the concentration continued to decrease until it was completely consumed after 4.3 minutes.

Similarly, in **Figure 5**, the temperature decreased and then increased abruptly to a final value of 23.6 °C.

Figure 7 shows the relationship between ln(k) and (1/T). The slope in this plot from the Arrhenius equation is = (-E)/R, where E is activation energy and R is ideal gas constant, [10] so the slope is 91.41= (-E)/R

E= -91.41*8314 = 759982.74 J/mole

The slope value is the rate of reaction, and the higher the value of the correlation factor or regression coefficient (closer to 1), the higher the order of the reaction, whether it is zero order, first order, or second order.

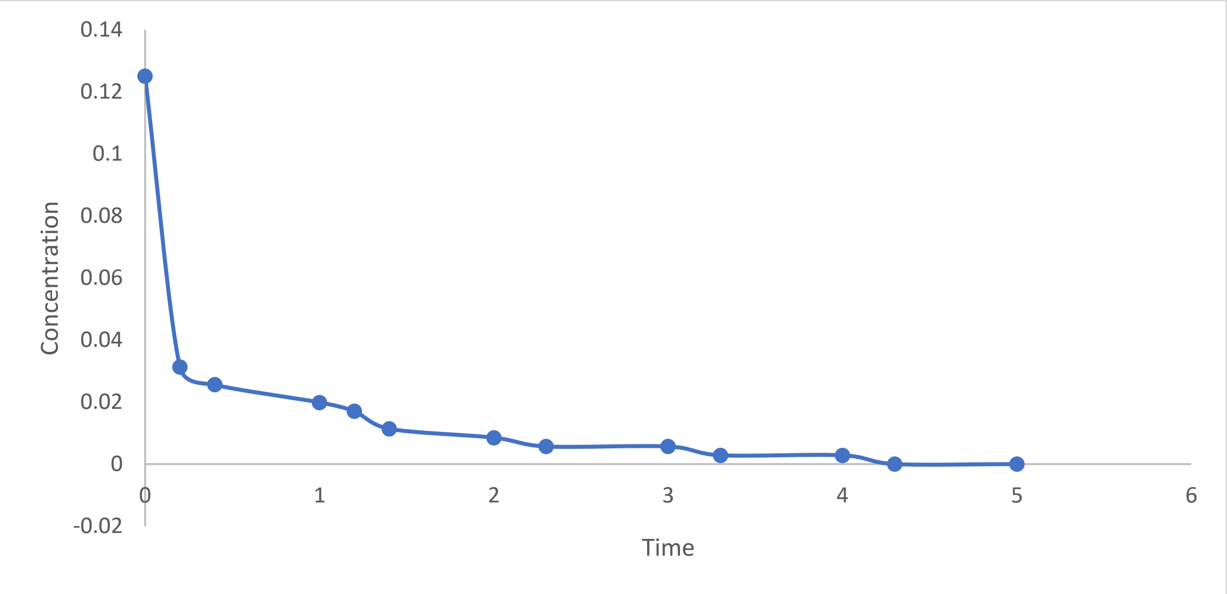

Figure 3: Concentration (C_A) vs (t) at T = 24°C

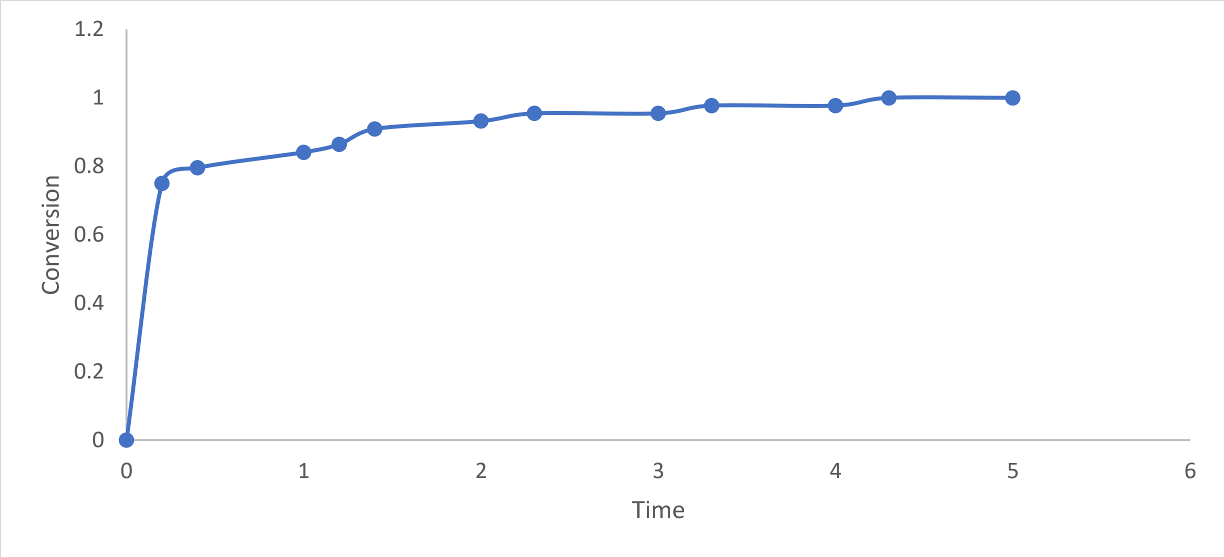

Figure 4: Conversion (X) vs (t) at T = 24°C

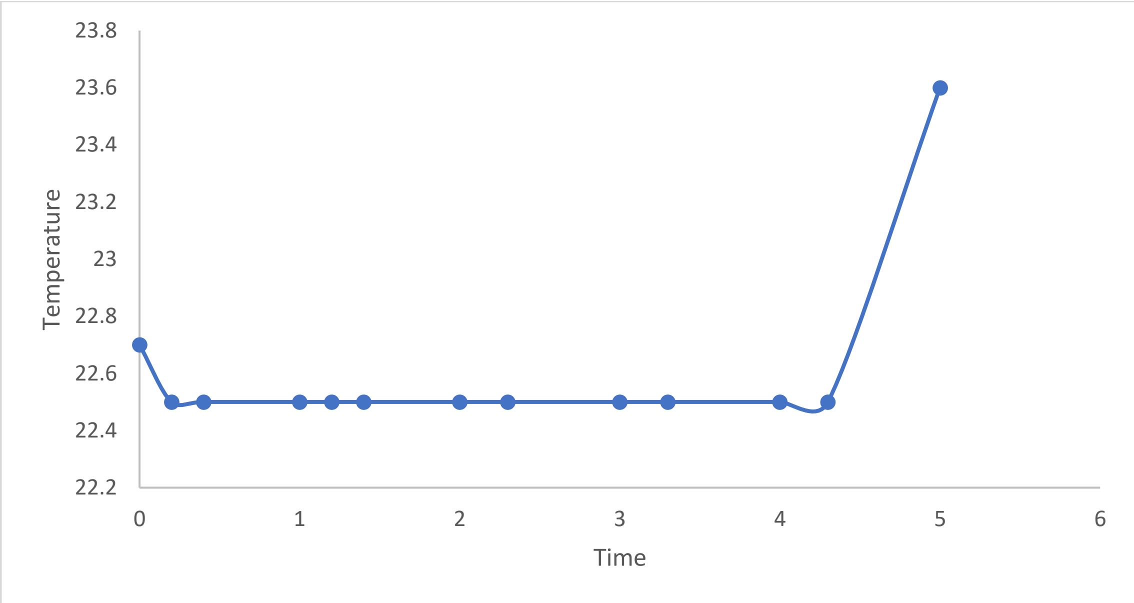

Figure 5: Temperature (T) vs (time) at T = 24°C

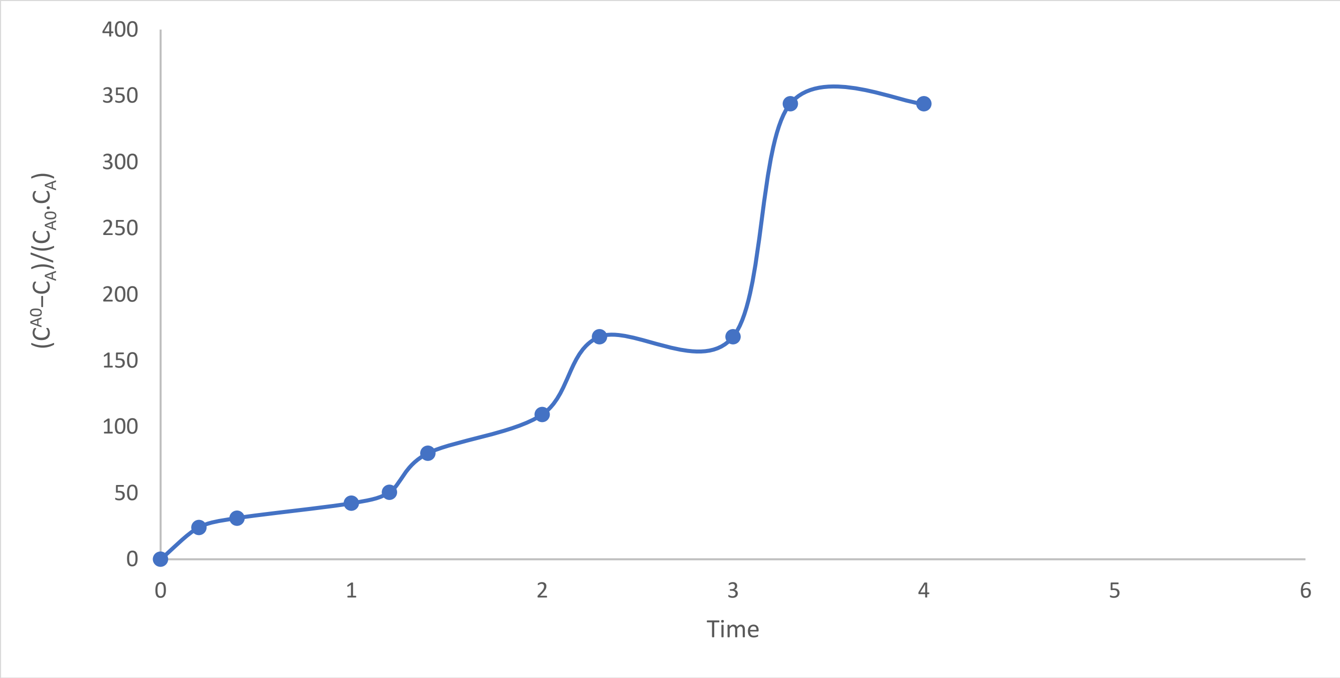

Figure 6: $\frac{CA0-CA}{CA0.CA}$ vs (t) at T = 24°C

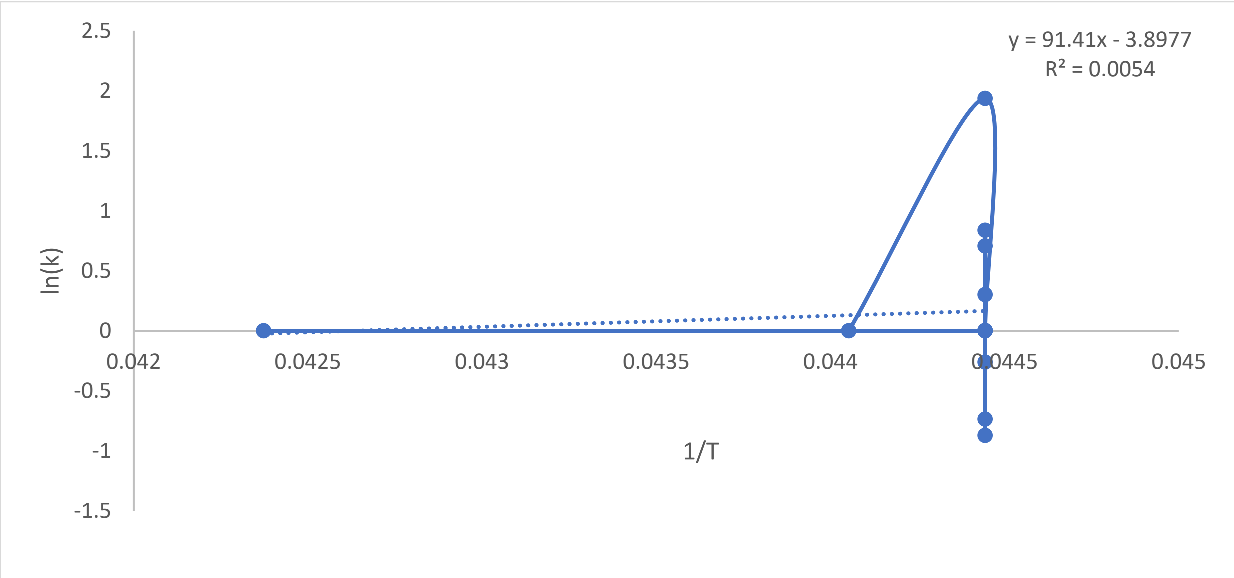

Figure 7: $\ln(k)$ vs $(\frac{1}{T})$

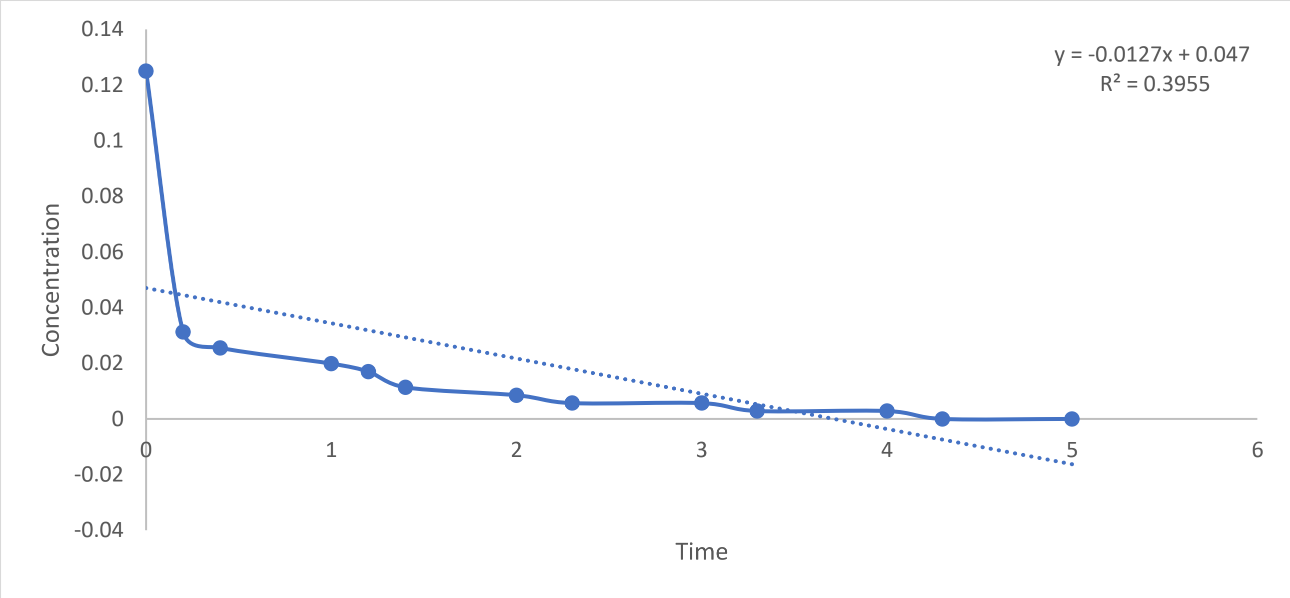

Figure 8: Concentration vs t at T = 24°C

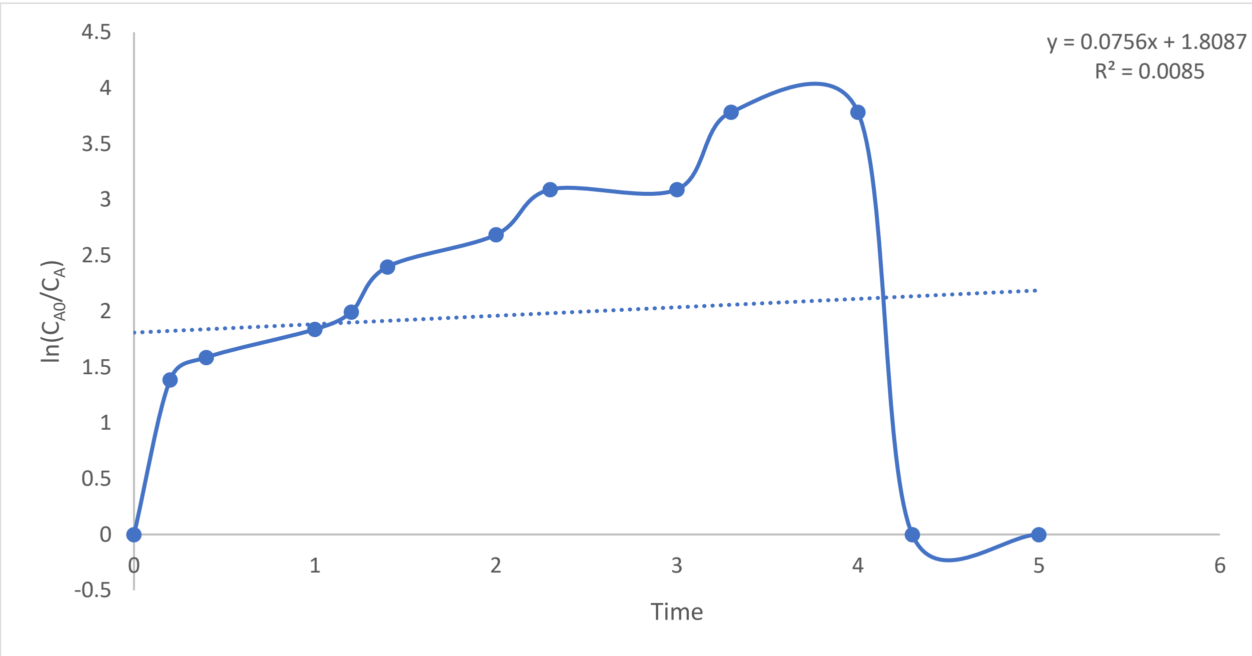

Figure 9: $\ln(\frac{C_{AO}}{C_A})$ vs t at T = 24°C

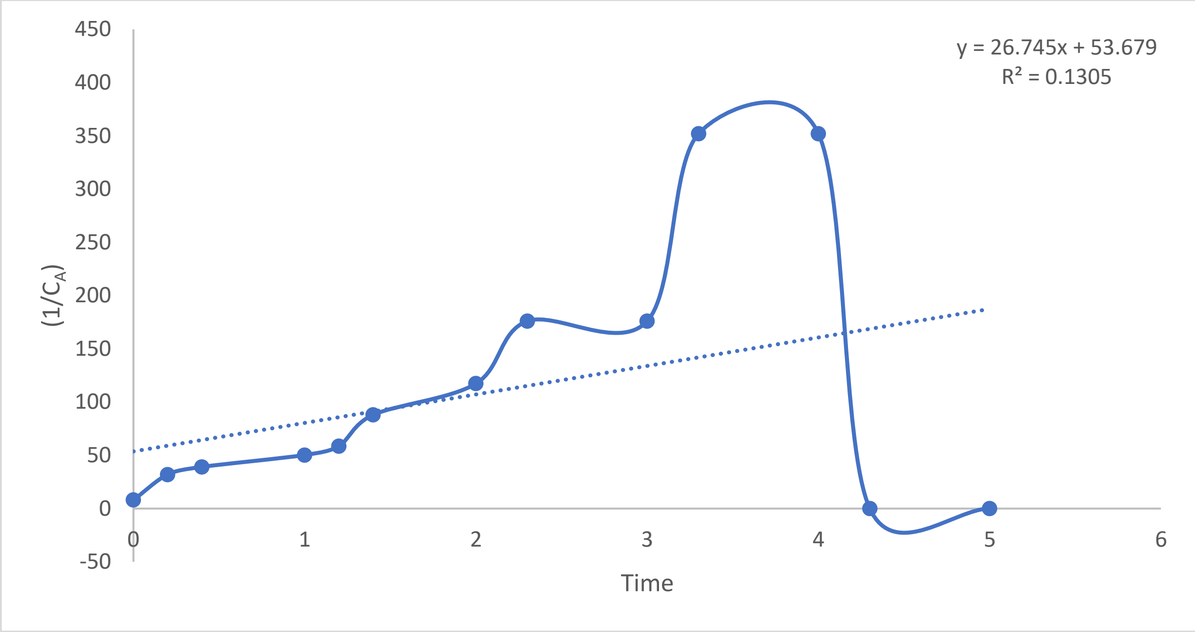

Figure 10: $(\frac{1}{C_A})$ vs t at T = 24°C

Conclusion

Finally, this experiment demonstrates many concepts, the most important of which is how the adiabatic reaction occurs, as well as how to calculate concentration using conductivity. Also, the method of calculating the chemical reaction constant, the order of the reaction from the concentration, and how much time is required to get steady state concentration (conversion) were explained graphically, as was the relationship of convergence and time at constant temperature, and the relationship of concentration with time at constant temperature, and the relationship of $(CA_o-C_A)/(C_{Ao}\ C_A)$ over time at temperatures ranging from T = 23 to 24°C. These experiments taught us how to calculate activation energy using the Arrhenius equation and how to determine the order of reaction. It can be zero, first, or second order, and zero order reactions describe chemical kinetics.

Notation

C: Concentration (in kmol/m^3)
Siemens/cm conductivity
K: Constant of reaction rate (s^{-1})
Reaction time, in seconds or minutes
T: Temperature, K: Kinetic energy

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