

Title Page*Title* (1 pts)Dream of Saponification

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Two Hypotheses (4 pts)

The first hypothesis is that the conductivity will be higher when there is more OH^- present in solution. This is considered because NaOH is a strong base. This means that NaOH will ionize much more than the base that is produced from the reaction, CH_3COONa .

The second prediction of the lab states that increasing the temperature of the reaction system will result in an increase in the value of the rate constant. This is particularly believed because of the general definition of temperature. A higher temperature means that the molecules present in the system are moving much more rapidly. Because of the increase of motion, molecules are more likely to react with each other.

Abstract (5 pts)

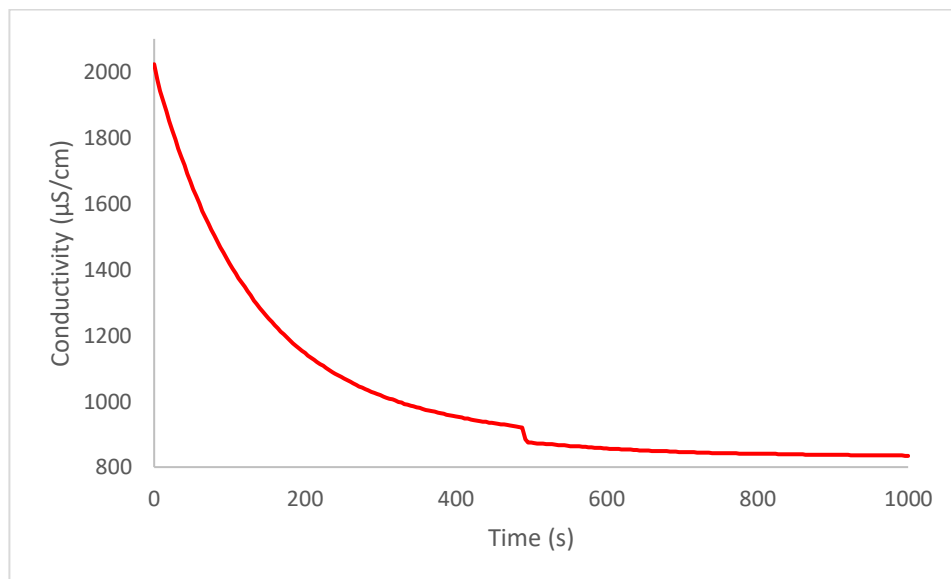
In this experiment, the conductivity of a reaction flask was measured over the reaction period to monitor the rate of the reaction. The results from the experiment give various points of insight into what makes a reaction occur and the physical and thermodynamic processes that go on at a microscopic scale. Each trial showed clear progress of a reaction at different rates. The trials also allowed for the rate of reaction to be determined experimentally, and in turn determine the rate constants of the reactions occurring. Many observations made with regards to the data mirror what is to be expected through multiple chemistry principles, and in turn can be used in multiple other reactions. For example, the data received shows that temperature has an effect on the rate constant, and in turn, affects the rate of the reaction. Overall, this experimental method over measuring the conductivity of both the reaction flask and a control flask is a good way to monitor the progress of a reaction, assuming that the conductivity increases or decreases between forming the product from the reactants.

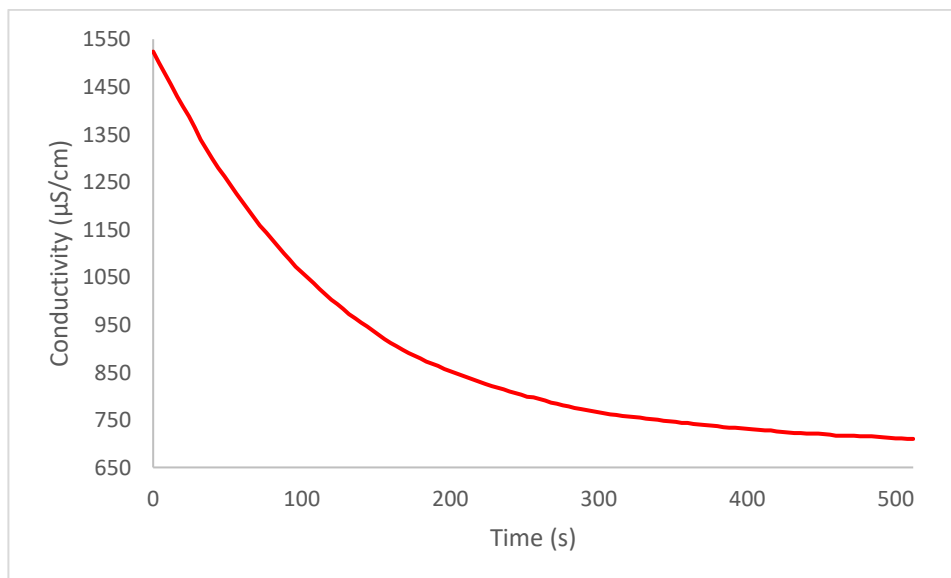
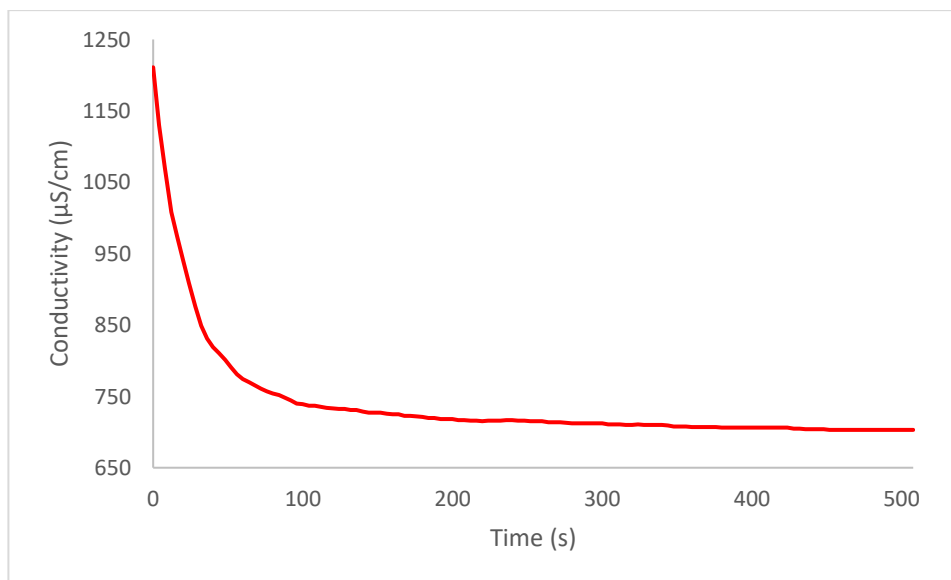
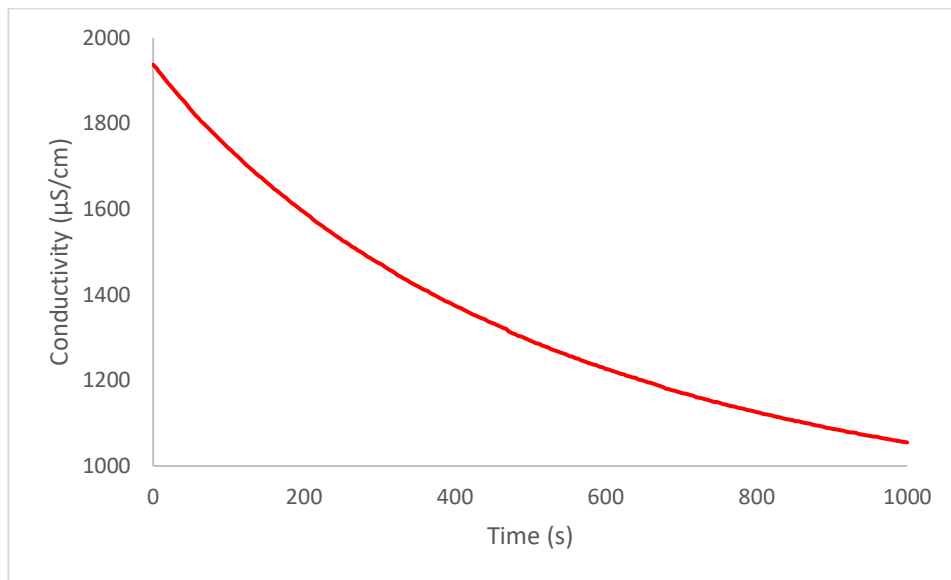
Results (35 pts)

Four trials were performed for the experiment. For these, trials 1 and 3 had excess amounts of ethyl acetate, and trials 2 and 4 had comparable amounts of ethyl acetate. Trials 3 and 4 are identical to trials 1 and 2, with the only difference being that trials 3 and 4 are performed at higher temperatures. The table below details the concentrations of the reactants used to run the reactions for each trial.

| Table 1 – Concentrations of Reactants Used for Each Trial | | |
|--|---|--|
| Trial # | Concentration of Sodium Hydroxide $[A]_0$ (M) | Concentration of Ethyl Acetate $[B]_0$ (M) |
| 1 | 0.020 | 0.20 |
| 2 | 0.020 | 0.050 |
| 3 | 0.020 | 0.20 |
| 4 | 0.020 | 0.050 |

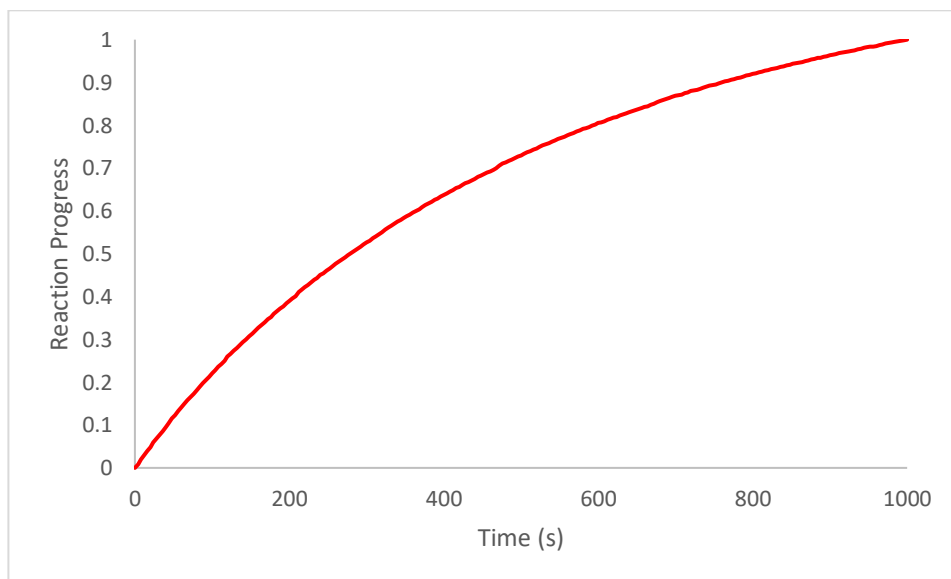
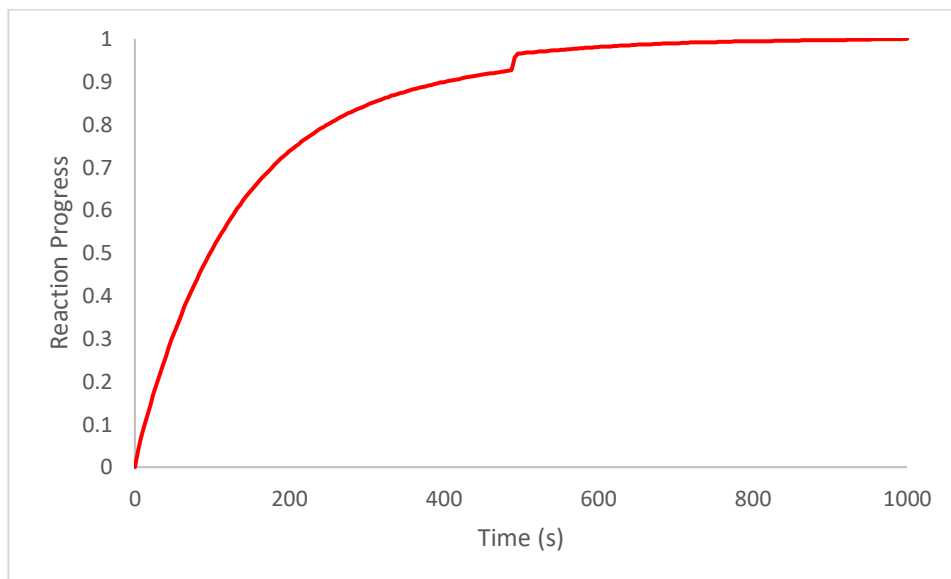
The trials were run, measuring the conductivity between the reaction medium and a control medium, which has no reaction. The conductivity difference was plotted with LoggerPro over a certain amount of time for each trial. Likewise, a temperature probe is used to measure the temperature that the reaction is in. The time-conductivity plots are used for the determination of the rate orders of the reactions, and the average values of the time-temperature plots are used for the determination of activation energies and pre-exponential factors. The four figures below are the time-conductivity plots for each of the four trials.

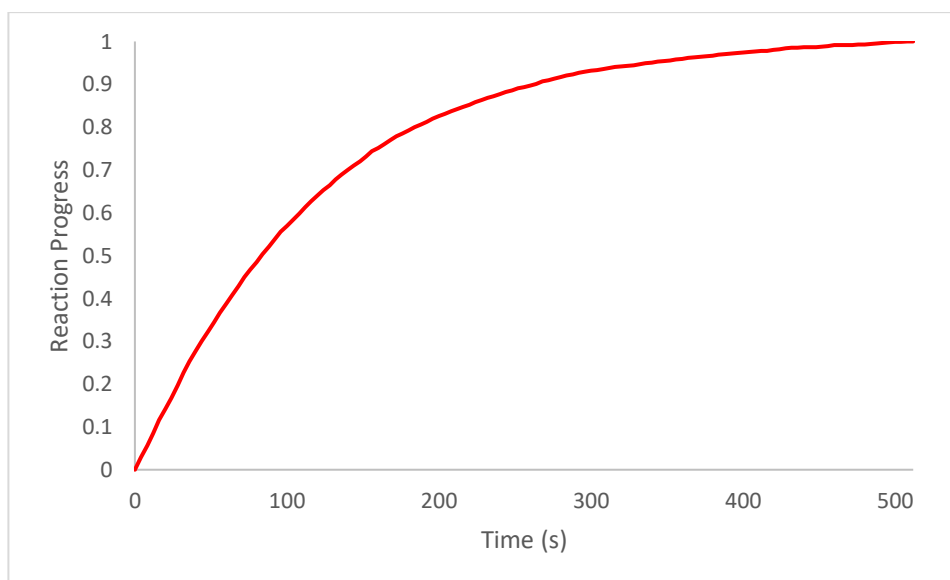
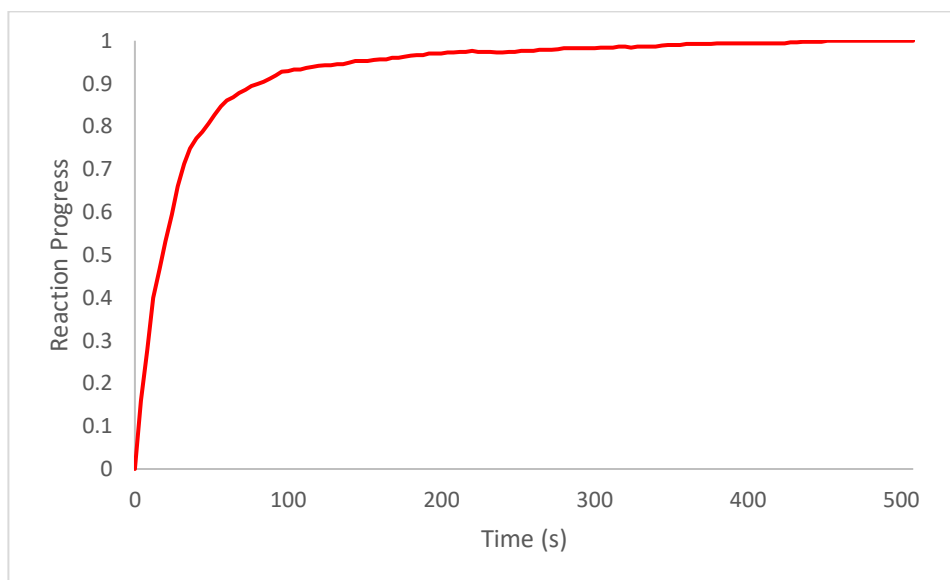




Figures 1-4 – Time-Conductivity plots for each trial run, listed in order of trial.
(Figure 1 corresponds to Trial 1, Figure 2 corresponds to Trial 2, etc.)

The Time-Conductivity plots show a clear representation of the progress of the reaction, as the conductivity of the reactants are much higher than the conductivity of the products. By assuming that the initial and final conductivity values on the plots are the beginning and the end of the reaction, the graph can be altered through **Calculation [1]** to make a graph monitoring the progress of each reaction, shown as $\frac{\xi}{[A]_0}$ over time. The following plots are then created.





Figures 5-8 – Plots monitoring the progress of the reaction over time. These plots were formed by taking the data points from **Figures 1-4** and plugging them into **Calculation [1]**. The reaction progress is unitless, and goes from 0 to 1, 0 being the beginning of the reaction and 1 being the end.

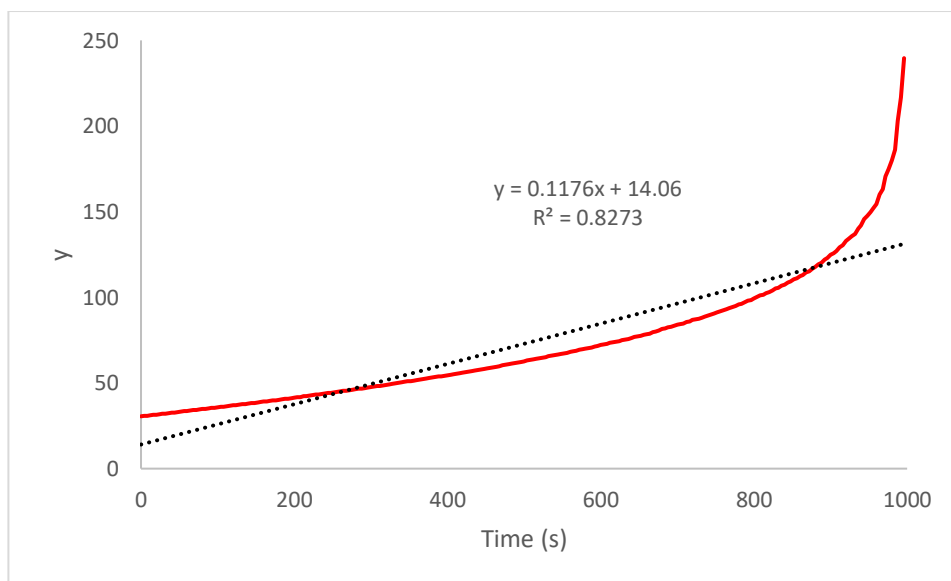
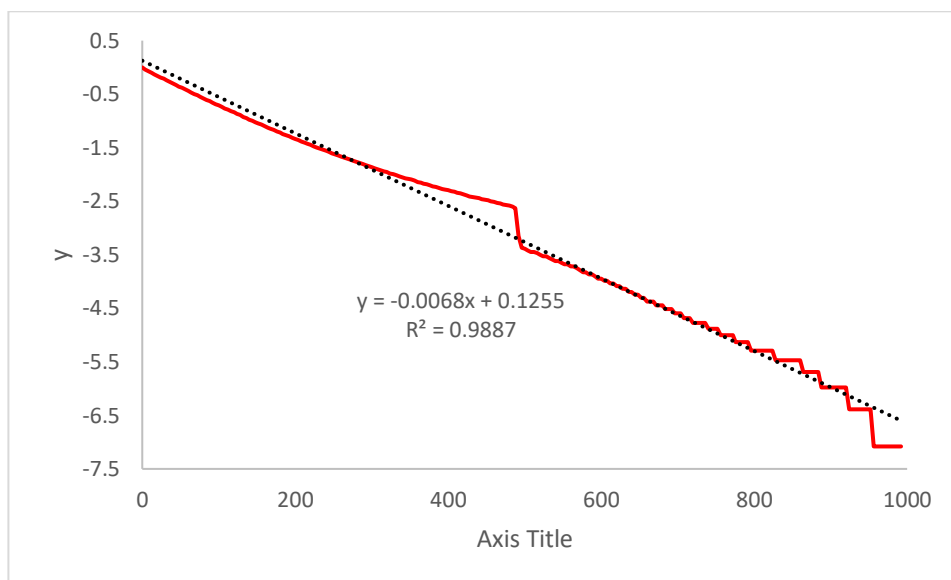
These data plots calculated can be used to create more intuitive graphs in order to determine the rate constant. Depending on the order of the reaction, the y-axis of the plots can be altered again using **Calculations [2]-[4]**. Specifically, **Calculation [2]** corresponds to a first order reaction, **Calculation [3]** to a second order reaction consisting of one second order reactant, and **Calculation [4]** to a second order reaction consisting of two first order reactants. Altogether, plugging **Figures 5-8** into these calculations should result in a linear curve with a slope of either $-k$ or k , depending on the calculation.

For this lab, the plots of all possible orders are made for each trial. For the sake of organization, only the plot that would actually correspond to the reactions will be shown in the Results Section. All other plots will be shown in the Supporting Data Section.

The orders of the reactions can be determined simply by examining the initial concentrations of each reactant. The concentrations are listed in **Table 1**, and the orders are listed immediately below.

| Table 2 – Reaction Order Pertaining to Trial | |
|--|-------------------------------|
| Trial # | Reaction Order |
| 1 | 1 |
| 2 | 2 (Two First Order Reactants) |
| 3 | 1 |
| 4 | 2 (Two First Order Reactants) |

The plots for the trials corresponding to their reaction orders are shown directly below.



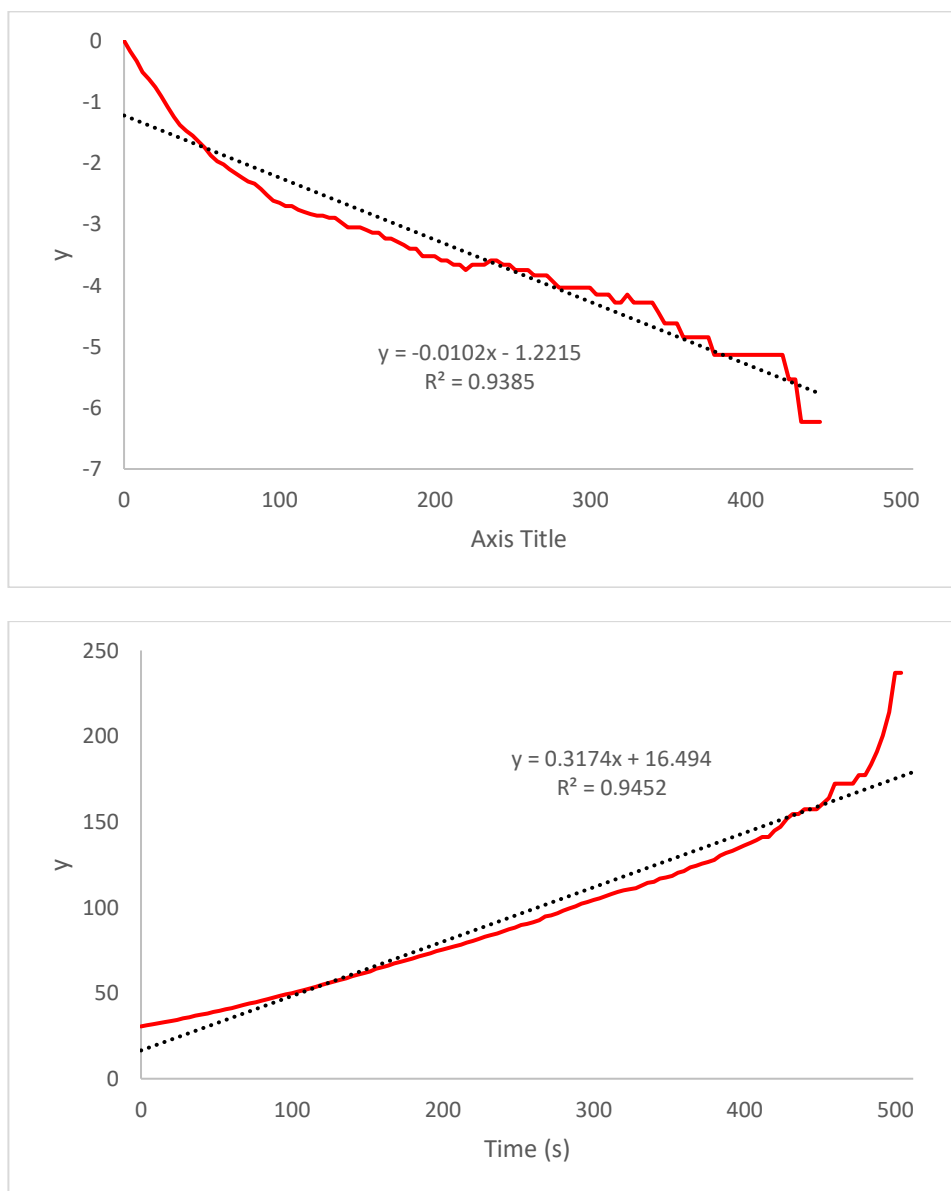


Figure 9-12 – Linear Fit Plots for each trial of the reaction. A trendline is included to receive the slope of the curve, which in turn leads to the rate constant of the reaction. The LINEST function in excel is also used to receive the standard deviation of the slope value. **Table 3** shows these values in tabular form.

| Table 3 – Determination of Rate Constant through Linear Regression | | | |
|---|----------|----------------|---|
| Trial # | Slope | δ Slope | k |
| 1 | -0.00678 | 0.00005 | $0.00678 \pm 0.00005 \text{ s}^{-1}$ |
| 2 | 0.118 | 0.003 | $0.118 \pm 0.003 \text{ M}^{-1} \text{ s}^{-1}$ |
| 3 | -0.0102 | 0.0002 | $0.0102 \pm 0.0002 \text{ s}^{-1}$ |
| 4 | 0.317 | 0.007 | $0.317 \pm 0.007 \text{ M}^{-1} \text{ s}^{-1}$ |

The final values that are calculated are the values for activation energy (E_a) and pre-exponential factor (A). First, the activation energy value can be calculated by comparing both trials 1 and 3, and 2 and 4. This is done through **Calculation [6]**, and will yield two values, one for the reaction with excess ethyl acetate, and one for the reactions with one for the reactions with NaOH as the limiting reagent. Once the values for the activation energies are found, they can be used in **Calculation [7]** to determine the pre-exponential factor values for each trial.

| Table 4 – Activation Energy and Pre-Exponential Value Values | | | | |
|---|--------------------------|-----------------------------|--------------------------------|--------------|
| Trial # | Average Temperature (°C) | Average Temperature (K) [5] | E _a (J/mol) [6] {1} | A [7] {2} |
| 1 | 21.3 | 294.5 | 9010 ± 600 | 0.269 ± 0.06 |
| 3 | 57.6 | 330.8 | | 2420 ± 900 |
| 2 | 21.3 | 294.5 | 24300 ± 900 | 0.269 ± 0.06 |
| 4 | 54 | 327.2 | | 2420 ± 800 |

Sample Calculations (15 pts)

[1]

$$\frac{\xi}{[A]_0} = \frac{\kappa_0 - \kappa}{\kappa_0 - \kappa_\infty}$$

$$\left\{ \frac{\xi}{[A]_0} \right\}_{12} = \frac{2023 \frac{\mu S}{cm^{-1}} - 1975 \frac{\mu S}{cm^{-1}}}{2023 \frac{\mu S}{cm^{-1}} - 834 \frac{\mu S}{cm^{-1}}} = 0.0404$$

[2]

$$-kt = \ln \left(1 - \frac{\xi}{[A]_0} \right)$$

$$\{-kt\}_{12} = \ln(1 - 0.0404) = -0.0412$$

[3]

$$-kt + \frac{1}{[A]_0} = \frac{\left(\frac{1}{1 - \frac{\xi}{[A]_0}} \right)}{[A]_0}$$

$$\left\{ -kt + \frac{1}{[A]_0} \right\}_{12} = \frac{\left(\frac{1}{(1 - 0.0404)} \right)}{0.020 \text{ M}} = 52.1$$

[4]

$$kt + \frac{1}{[B]_0 - [A]_0} \ln \left(\frac{[B]_0}{[A]_0} \right) = \frac{1}{[B]_0 - [A]_0} \ln \left(\frac{\frac{[B]_0}{[A]_0} - \frac{\xi}{[A]_0}}{1 - \frac{\xi}{[A]_0}} \right)$$

$$\left\{ kt + \frac{1}{[B]_0 - [A]_0} \ln \left(\frac{[B]_0}{[A]_0} \right) \right\}_{12} = \frac{1}{0.20 \text{ M} - 0.020 \text{ M}} \ln \left(\frac{\frac{0.20 \text{ M}}{0.020 \text{ M}} - 0.0404}{1 - 0.0404} \right) = 13.0$$

[5]

$$T_K = T_{°C} + 273.15$$

$$T_{K1} = 21.3 \text{ °C} + 273.15 = 294.5 \text{ K}$$

[6]

$$E_a = -R \cdot \frac{\ln \left(\frac{k_{T_2}}{k_{T_1}} \right)}{\left(\frac{1}{T_2} - \frac{1}{T_1} \right)}$$

$$E_a = -8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}} \cdot \frac{\ln \left(\frac{0.00678 \text{ s}^{-1}}{0.0102 \text{ s}^{-1}} \right)}{\left(\frac{1}{330.8 \text{ K}} - \frac{1}{294.5 \text{ K}} \right)} = 9.01 \cdot 10^3 \frac{\text{J}}{\text{mol}}$$

[7]

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

$$A = \frac{0.00678 \text{ s}^{-1}}{e^{\left[\frac{-9.01 \cdot 10^3 \frac{\text{J}}{\text{mol}}}{\left(8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}}\right)(294.5 \text{ K})}\right]}} = 0.289 \text{ s}^{-1}$$

{1}

$$\delta E_a = E_a \sqrt{\left(\frac{\sqrt{\left(\frac{\delta T_2}{T_2}\right)^2 + \left(\frac{\delta T_1}{T_1}\right)^2}}{\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}\right)^2 + \left(\frac{\sqrt{\left(\frac{\delta k_2}{k_2}\right)^2 + \left(\frac{\delta k_1}{k_1}\right)^2}}{\ln\left(\frac{k_2}{k_1}\right)}\right)^2}$$

$$\delta E_a = 9010 \frac{\text{J}}{\text{mol}} \sqrt{\left(\frac{\sqrt{\left(\frac{0.05 \text{ K}}{(330.8 \text{ K})^2}\right)^2 + \left(\frac{0.05 \text{ K}}{(294.5 \text{ K})^2}\right)^2}}{\left(\frac{1}{330.8 \text{ K}} - \frac{1}{294.5 \text{ K}}\right)}\right)^2 + \left(\frac{\sqrt{\left(\frac{0.0002 \text{ s}^{-1}}{0.0102 \text{ s}^{-1}}\right)^2 + \left(\frac{0.0005 \text{ s}^{-1}}{0.00678 \text{ s}^{-1}}\right)^2}}{\ln\left(\frac{0.0102 \text{ s}^{-1}}{0.00678 \text{ s}^{-1}}\right)}\right)^2}$$

$$= 600 \frac{\text{J}}{\text{mol}}$$

{2}

$$\delta A = A \sqrt{\left(\frac{\delta k}{k}\right)^2 + \left(\frac{-E_a}{RT} \sqrt{\left(\frac{\delta E_a}{E_a}\right)^2 + \left(\frac{\delta T}{T}\right)^2}\right)^2}$$

$$\delta A_1 = 0.269 \sqrt{\left(\frac{0.0005 \text{ s}^{-1}}{0.00678 \text{ s}^{-1}}\right)^2 + \left(\frac{-9010 \frac{\text{J}}{\text{mol}}}{\left(8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}}\right)(294.5 \text{ K})} \sqrt{\left(\frac{600 \frac{\text{J}}{\text{mol}}}{9010 \frac{\text{J}}{\text{mol}}}\right)^2 + \left(\frac{0.05 \text{ K}}{294.5 \text{ K}}\right)^2}\right)^2}$$

$$= 0.06$$

Discussion, 1 (min) – 2 (max) pages, single spaced (35 pts)

Different amounts of error can be observed in the plots received and the calculations done in the experiment. A majority of error from the calculations come from either the lack of precision that the instrumentation provides and the lack of an ideal system to perform the experiments in. Trials 3 and 4 had a significant amount of error in comparison to Trials 1 and 2, and this is likely because of the temperature changing over time (**Figure 13**). If the temperatures were kept constant rather than allowed to decrease over time, it can be believed that the linear regression data would be much less noisy and yield more favorable and precise results. Also, the Time-Conductivity plot seems to show a major decrease in conductivity only at one data value (**Figure 1**). This is likely caused by one of the conductivity probes being bumped, but as shown in **Figure 9**, the trendline still remains fairly accurate to what is to be expected.

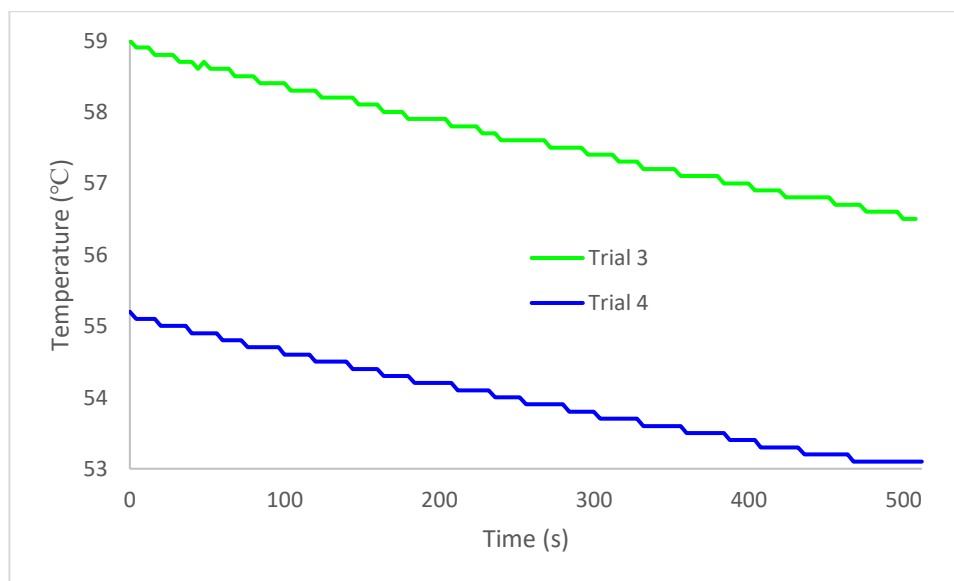


Figure 13 – Time-Temperature plots of Trials 3 and 4. If the temperatures were to be constant, the results from the calculations would likely be more favorable.

The first hypothesis proposed prior to the experiment believes that the conductivity of the solution would be greater with the presence of more OH^- ions present in solution. **Figures 1-4** prove this hypothesis to be true, as all graphs show decreasing conductivity as the reaction is performed. When NaOH is introduced to water, all of the NaOH molecules ionize, forming free Na^+ and OH^- ions in solution. The presence of free ions increases the conductivity altogether. When the reaction is performed, the OH^- are removed from the solution and instead used to form $\text{C}_2\text{H}_5\text{OH}$. Not having the OH^- free in solution would decrease the conductivity.

The other hypothesis to be considered was in relations to the temperatures of the system and how they affect the rate constant values. The values of k (as shown in **Table 3**) mimic the hypothesis, for both reaction cases. For Trials 1 and 3, where ethyl acetate is in excess, the increase in temperature led to an increase in the rate constant. For Trials 2 and 4, where NaOH was the limiting reagent, the same is true. The hypothesis can also be proven just by looking at **Calculation [7]**. If temperature increases, rate constant also increases.

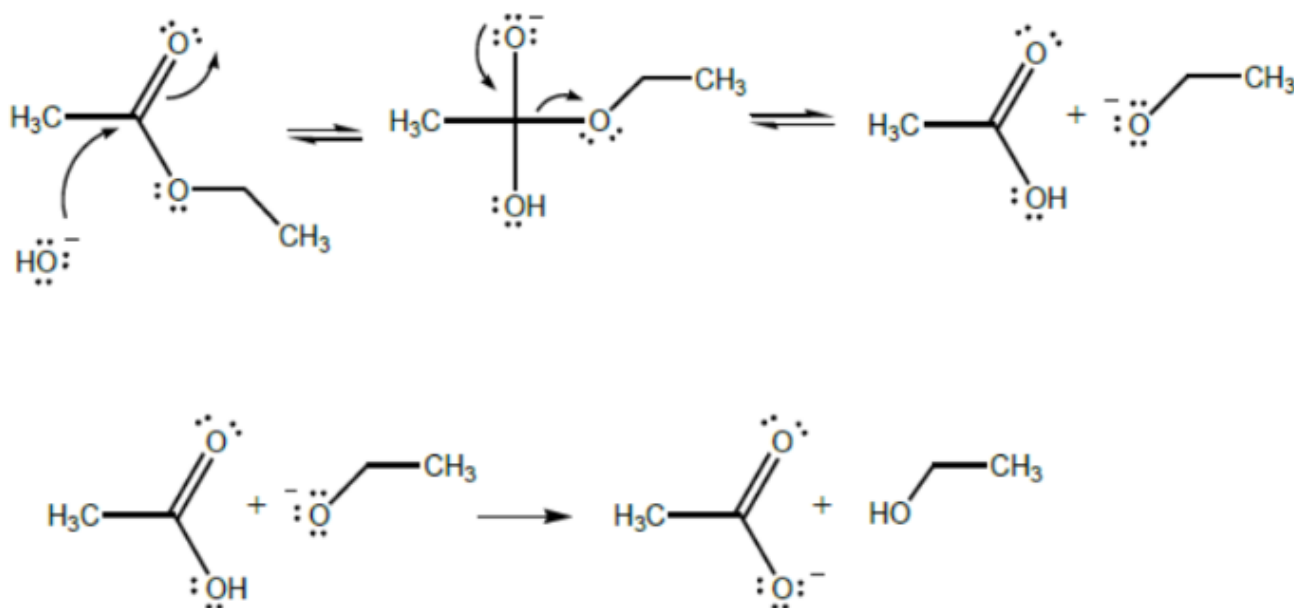


Figure 14 – Reaction Mechanism of ethyl acetate reacting with hydroxide ion. This mechanism details what is occurring in the reaction flask during the experiment.

Overall, the mechanism proposed for the reaction matches up to the reaction orders for both reaction cases. In the case of Trial 1 and 3, where ethyl acetate is in excess, the reaction is first order. This makes sense with the mechanism, as the concentration of ethyl acetate is not significant to the reaction progress, as it is in excess, thus always available. For Trials 2 and 4, the reaction order is second order with two first order reactants. The mechanism also shows this to be true, as two reactants are needed for the reaction to occur. The concentrations of both reactants need to be considered as well, in contrast to Trials 1 and 3, because ethyl acetate is not in excess in this case.

A key point to performing this experiment is to gain a greater insight into how reactions proceed, particularly to their kinetics and physical attributes. The calculations done can be used to find out other physical properties that the reaction has and shows how the two are related. In specific, this experiment shows how temperature and concentrations of reactants can relate to the progress of the reaction, and show the activation energy and rate constants of the reactions. Outside of this experiment, these calculated values can be used to determine the thermodynamic properties that the reaction exhibits. For example, the following equations show how to calculate the enthalpy and entropy of each reaction.

[8]

$$\Delta H^{\circ\ddagger} = E_a - RT$$

$$\Delta H^{\circ\ddagger}_1 = 9010 \frac{\text{J}}{\text{mol}} - \left(8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}} \right) (294.5 \text{ K}) = 6560 \frac{\text{J}}{\text{mol}}$$

[9]

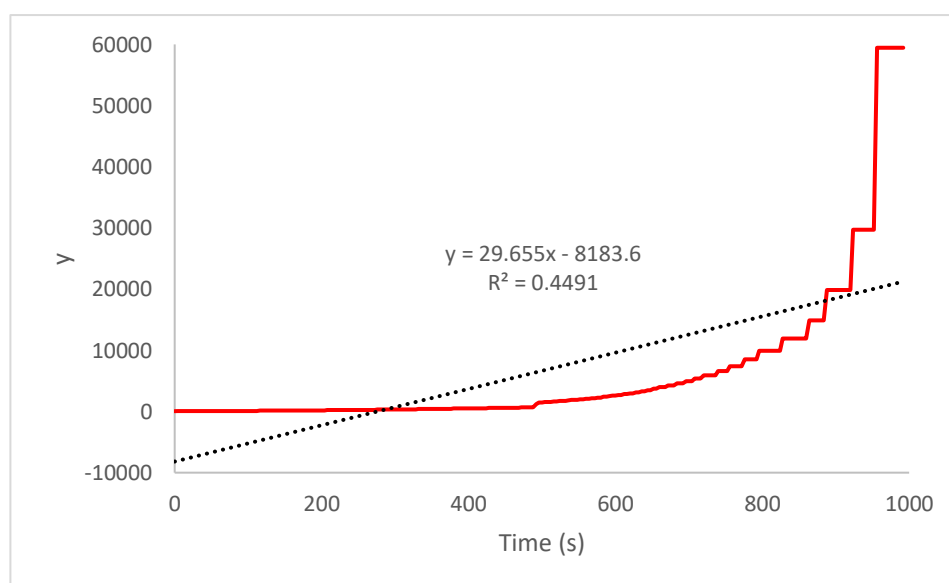
$$\Delta S^{\circ\ddagger} = R \ln \left[\frac{\left(\frac{k_{\text{rate}} h}{k_b T} \right)}{e^{\frac{-\Delta H^{\circ\ddagger}}{RT}}} \right]$$

$$\Delta S^{\circ\dagger}_1 = \left(8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}}\right) \ln \left[\frac{\left(\frac{(0.00678 \text{ s}^{-1})(6.626 \cdot 10^{-34} \text{ J} \cdot \text{s})}{(1.38 \cdot 10^{-23} \frac{\text{J}}{\text{K}})(294.5 \text{ K})} \right)}{e^{\left(\frac{-6560 \frac{\text{J}}{\text{mol}}}{(8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}})(294.5 \text{ K})} \right)}} \right] = -264 \frac{\text{J}}{\text{K}}$$

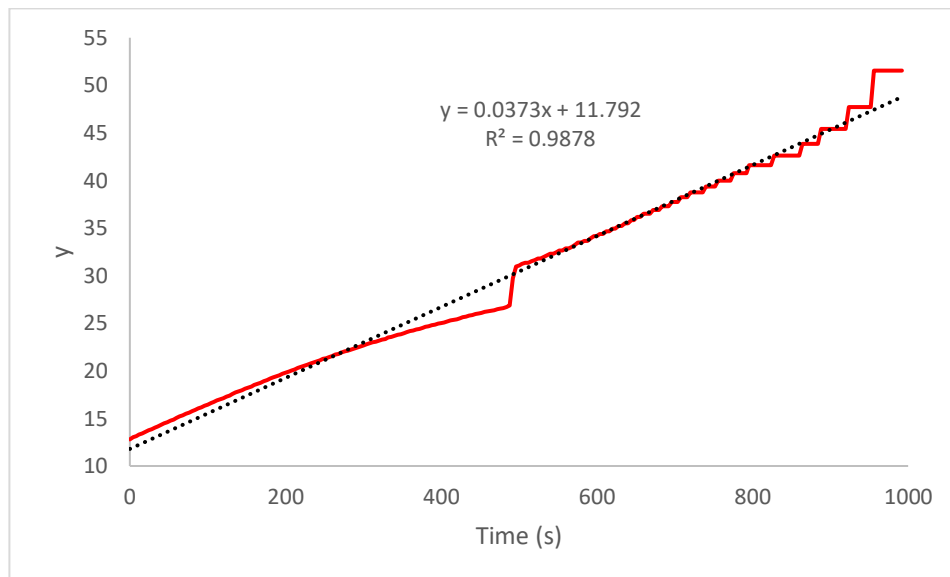
| Trial # | $\Delta H^{\circ\dagger}$ (J/mol) | $\Delta S^{\circ\dagger}$ (J/K) |
|---------|-----------------------------------|---------------------------------|
| 1 | 6560 | -264 |
| 2 | 21900 | -188 |
| 3 | 6260 | -265 |
| 4 | 21600 | -189 |

The thermodynamic data calculated above shows how the reaction is meant to proceed. Since the $\Delta S^{\circ\dagger}$ values calculated are all negative, that means that the entropy of the system decreases as the products are formed in the reaction. This in turn verifies that the mechanism tends to favor creating the products, which drives the reaction to produce ethanol and acetate ions.

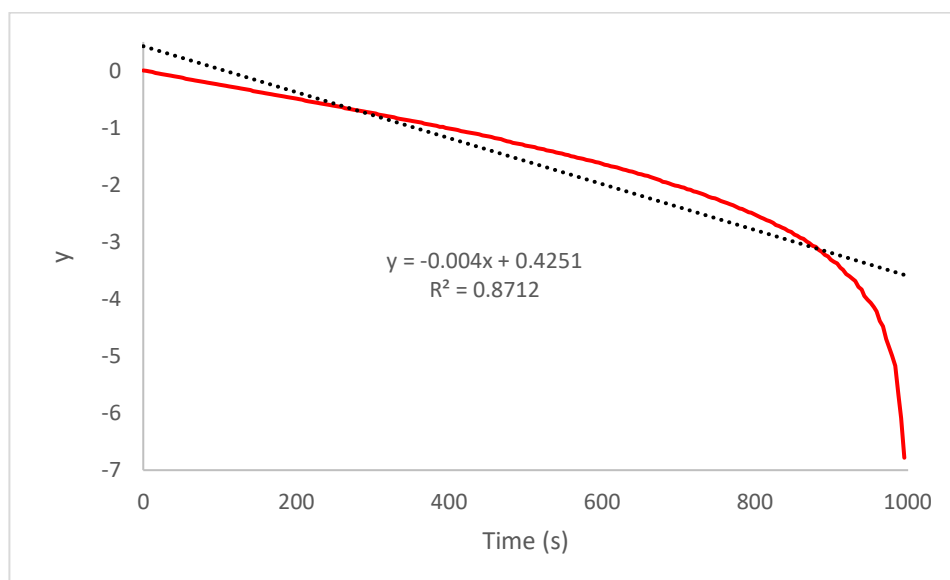
Supporting Data



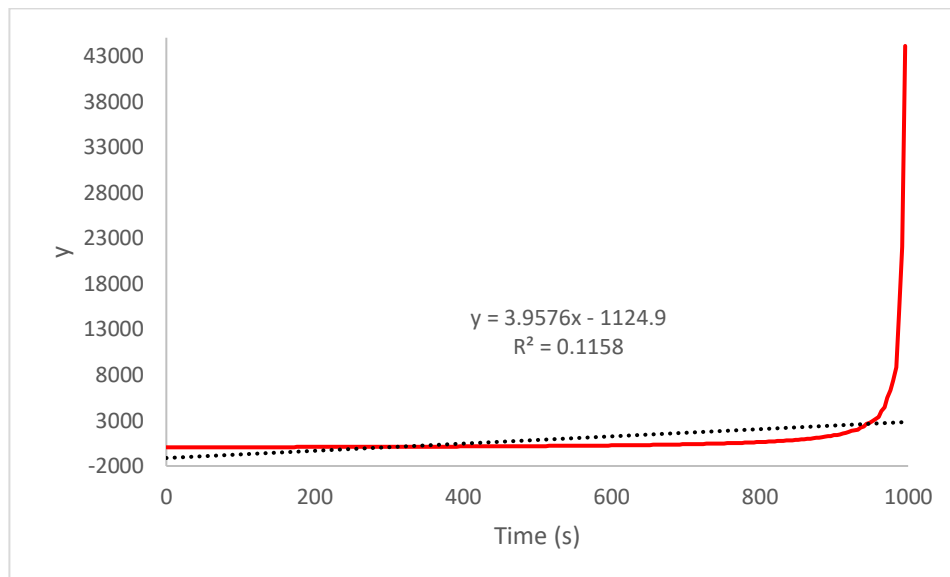
SD 1 – Linear Regression of Trial 1 for a one reactant second order reaction. The plot is constructed by plugging **Calculation [3]** into the y-axis of **Figure 5**.



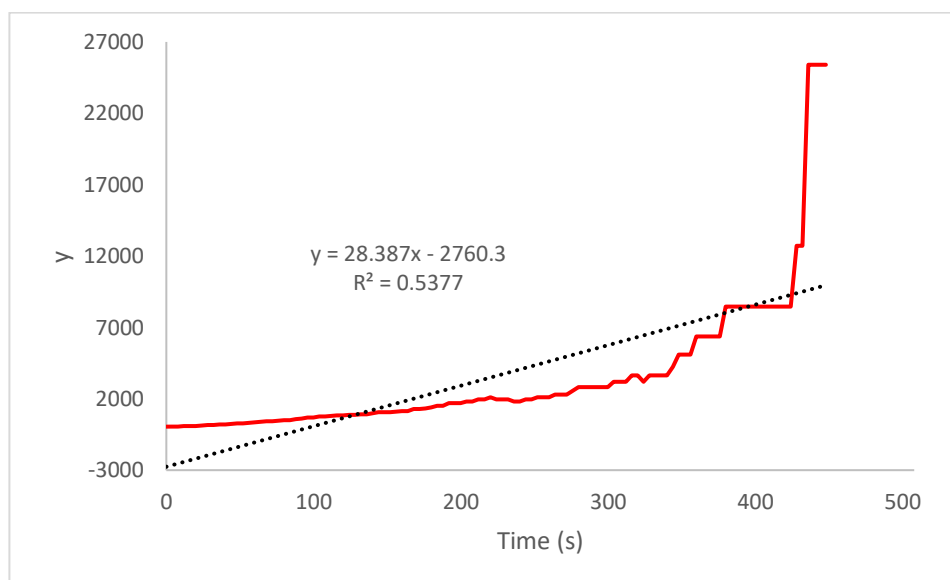
SD 2 – Linear Regression of Trial 1 for a two reactant second order reaction. The plot is constructed by plugging **Calculation [4]** into the y-axis of **Figure 5**.



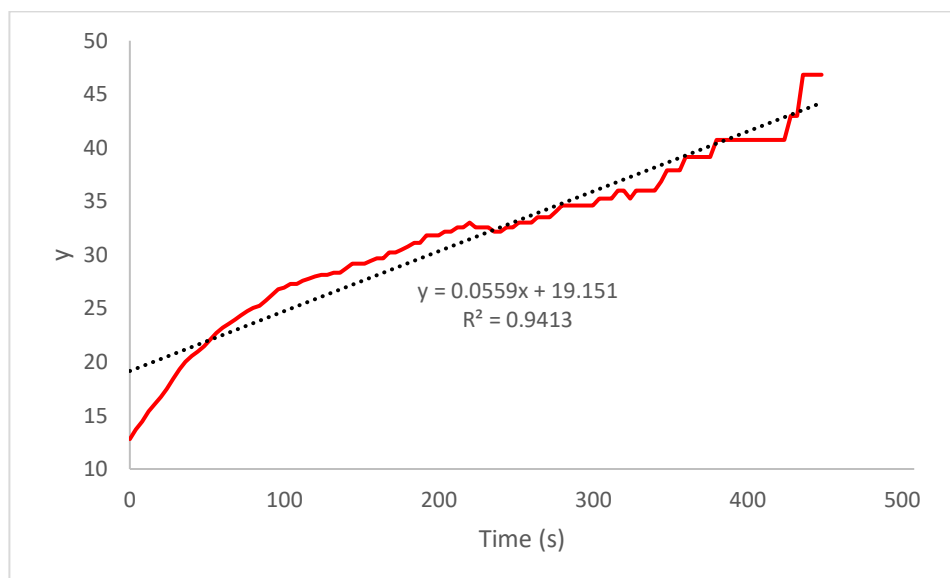
SD 3 – Linear Regression of Trial 2 for a first order reaction. The plot is constructed by plugging **Calculation [2]** into the y-axis of **Figure 6**.



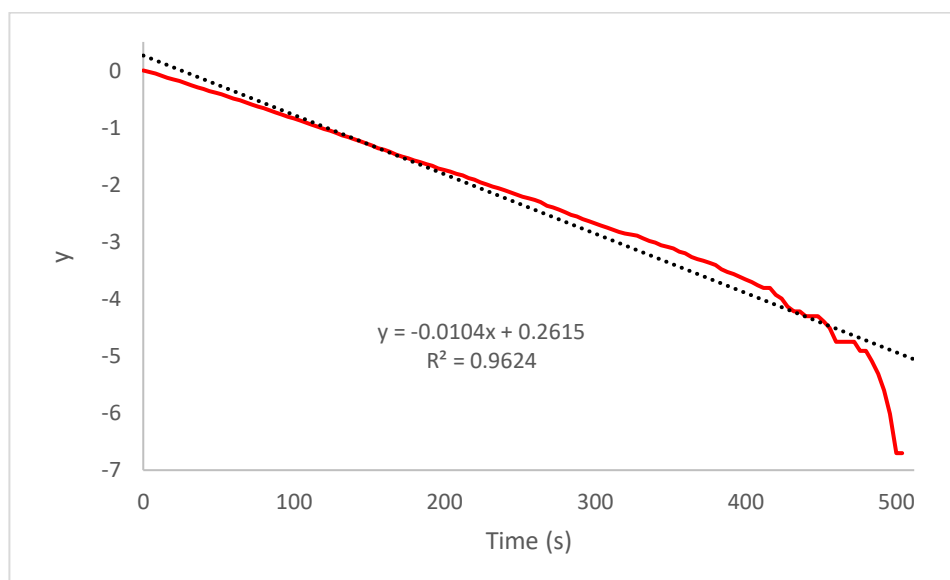
SD 4 – Linear Regression of Trial 2 for a one reactant second order reaction. The plot is constructed by plugging **Calculation [3]** into the y-axis of **Figure 6**.



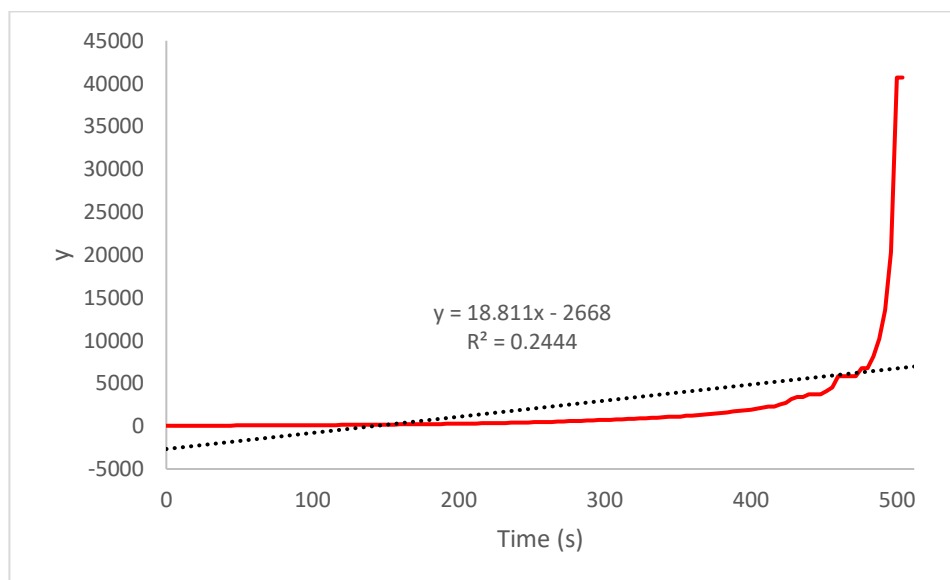
SD 5 – Linear Regression of Trial 3 for a one reactant second order reaction. The plot is constructed by plugging **Calculation [3]** into the y-axis of **Figure 7**.



SD 6 – Linear Regression of Trial 3 for a two reactant second order reaction. The plot is constructed by plugging **Calculation [4]** into the y-axis of **Figure 7**.



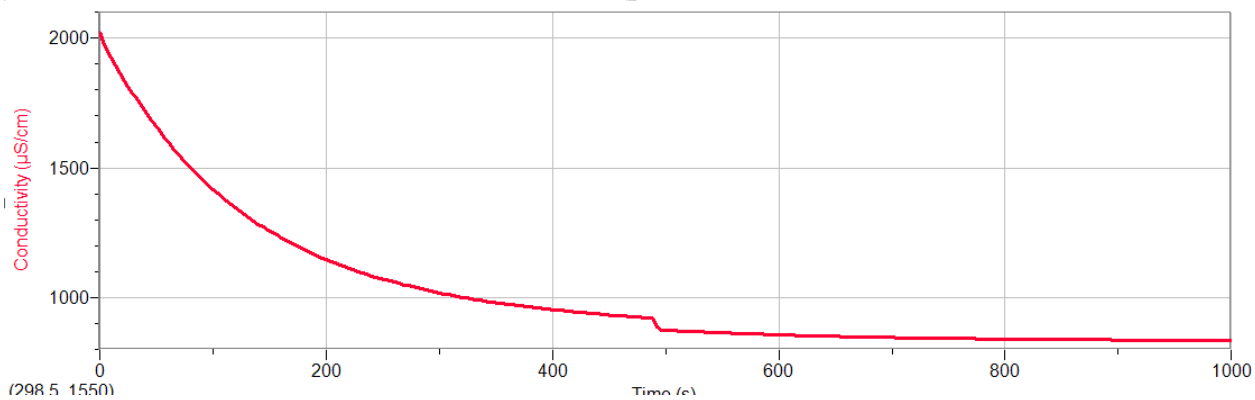
SD 7 – Linear Regression of Trial 4 for a first order reaction. The plot is constructed by plugging **Calculation [2]** into the y-axis of **Figure 8**.



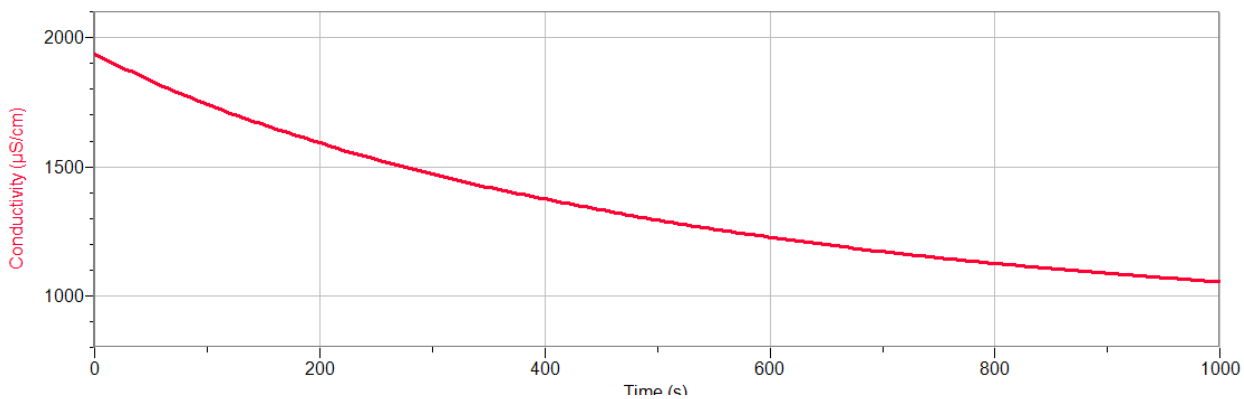
SD 1 – Linear Regression of Trial 4 for a one reactant second order reaction. The plot is constructed by plugging **Calculation [3]** into the y-axis of **Figure 8**.

Lab Notebook (5 pts)

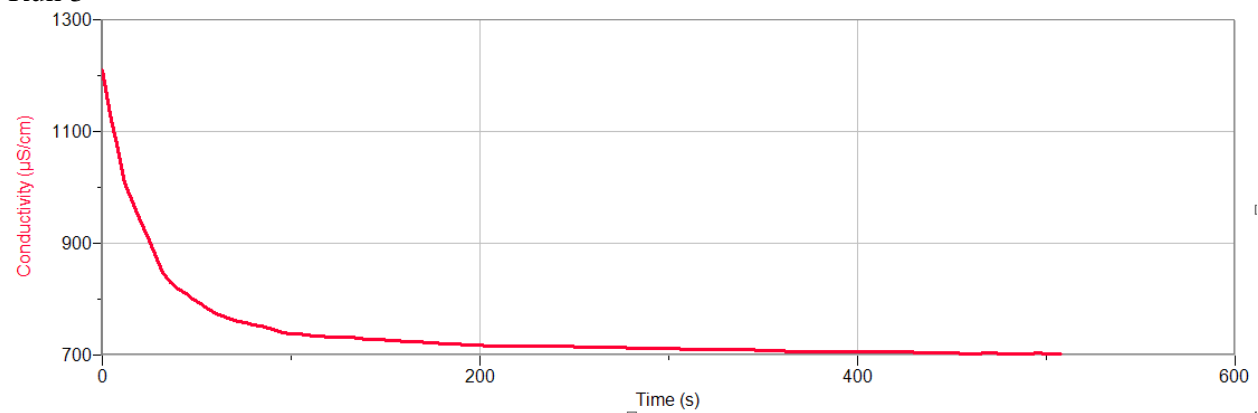
Run 1



Run 2



Run 3



Run 4

