

# KINETICS LAB

## Part A: Background Information

Kinetics is a branch of chemistry or biochemistry concerned with measuring and studying the rate of reactions. In this lab you will look at three different situations, and analyze the graphs to determine which order the reaction that took place was. You can determine the order a reaction is by looking at the x and y axis. If the measurements on the x and y axis give you a straight line, then that will be the order of the reaction. The basic equation to determine the rate law is below:



where the rate =  $k[A]^m[B]^n$  and  $k$  is the term for the rate constant.

**Zero Order:** The process that takes place at a constant rate independent of drug concentration involved in the process. It is a constant rate process, and the process does not depend on the concentration. With a zero order equation, the rate =  $k$ , and this is because the rate constant does not depend on concentration. In order to get a straight line for the graph for a zero order equation the plot is  $[A]$  vs.  $t$ , and the slope is  $-k$  from this graph.

**First Order:** A first order reaction depends on the concentration of only one reactant (a unimolecular reaction). Other reactants can be present, but each will be zero order and would not affect the concentration. Concentration within a first order equation effects the rate constant because if the concentration doubles the rate doubles. Within a first order equation, the rate =  $k[A]$  where  $k$  is the rate constant and  $[A]$  is the concentration. The plot for a straight line with a first order equation is  $\ln[A]$  vs.  $t$ , and the slope based off of this graph is  $-k$ , which means the rate constant would be opposite of the slope of your graph.

**Second Order:** A second order reaction can come from two first order reactants or one second order reactant. Within a second order, the rate =  $k[A]^2$  and this shows that when the concentration doubles, the rate will quadruple. The plot for a straight line with a second order equation is  $1/[A]$  vs  $t$ . The slope of the graph equals  $k$  for a second order equation.

In this lab you will graph three different cases, and using the information above be able to determine by the line of best fit, and the graph that has the straight line, which order that your data represents. You will do so by looking at different commands that you have learned throughout the year.

## Part B:

1. Create a time vector called "t" using the linspace command that has 16 values and starts at 0 and ends at 10.
2. Create a variable called A that starts at zero increments by 0.1 and ends at 1.5
3. Enter these two lines of code after you create your time vector:  

```
A1 = sort(A, 'descend');
```
4. Create two new variables in order to look at all the orders of the graphs  
First Order Graph:  $\ln[A]$  vs.  $t$   
Second Order Graph:  $1/[A]$  vs.  $t$
5. Now plot all three graphs on separate figures:

Include a linear line on the graph which you think is a representation of the order of this certain data set that include the equation to 4 significant figures.

6. Based off the graphs, which order does this data represent? What is the rate constant for this equation?

### Part C:

1. Create a new section within your script.
2. Create a concentration vector that starts at 0.00730, increments by 0.005 and ends at 0.0172.
3. Place the variable below in your script file: (This is the rate constant)  

```
k = 1.3*10^-2;
```
4. Place this next line of code below your concentration vector:  

```
A1 = sort(A, 'descend');
```
5. Create variables for time, ln[A], and 1/[A]
  - a. Remember that in a second order equation that time will equal 1/A divided by the rate constant.
6. Now plot all three graphs on separate figures:  
Include a linear line on the graph which you think is a representation of the order of this certain data set that include the equation to 4 significant figures.
7. Based off the graphs, which order does this data represent? What is the rate constant for this equation?

### Part D:

1. Download the excel file titled "Run1" so that it is in the same folder as your current MATLAB script.
2. Create a new section within your script
3. Pull the time from the excel file into its own variable.
4. Pull the Base from the excel file into its own variable as well
5. Use the following commands:  

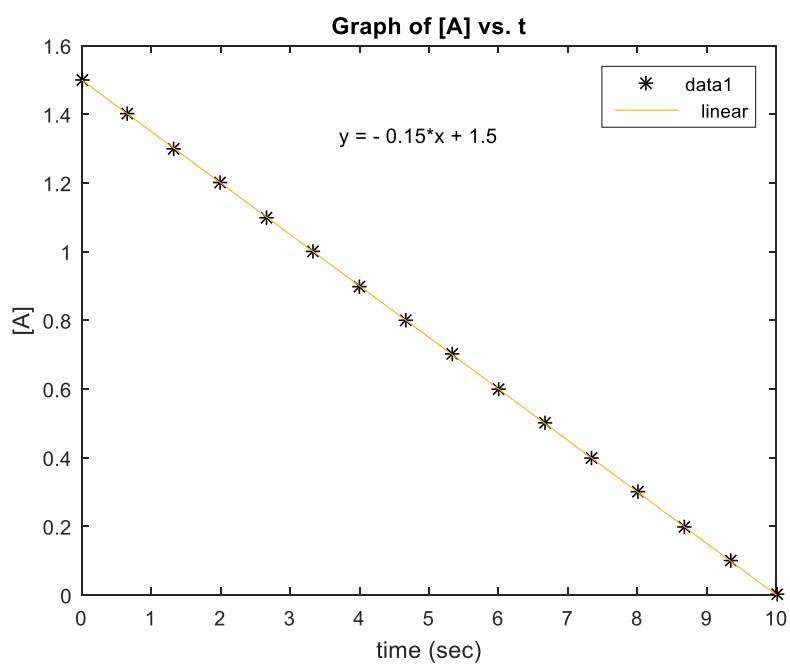
```
Base = Base';  
Time = Time';
```

This transfers your variables from 22 x 1 to a 1 x 22 vector
6. Now using three separate for loops calculate the following
  - a. The total base added
  - b.  $V_{\infty} - V_t / V_{\infty}$  (Where  $V_{\infty}$  is the total base added, and  $V_t$  is the amount of base added at that time)
    - i. Hint: For example, if you had  $t = 1, 2, 3, 4$  and  $Base = 2, 3, 4$ . Your amount of base added at  $t=2$  is 5, and your total base is 7.
  - c. Calculate the natural log of the step above
7. Now plot all three graphs on separate figures:  
Include a linear line on the graph which you think is a representation of the order of this certain data set that include the equation to 4 significant figures.
8. Based off the graphs, which order does this data represent? Is this data a perfect fit for this order? What is the rate constant for this equation?

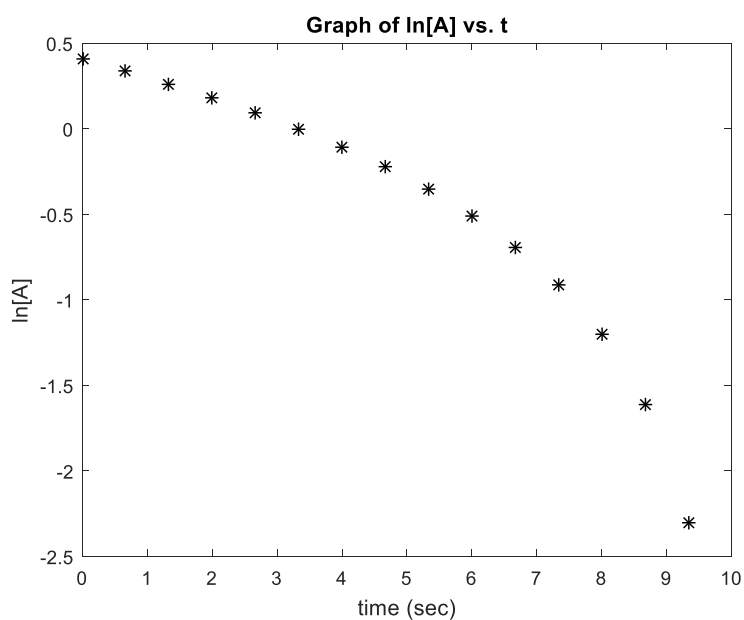
**Answers:**

**Part B: Zero Order**

Rate Constant Figure 1:  $k = 0.15$



**Figure 1: Graph of Zero Order based upon Data in Part B**



**Figure 2: Graph of First Order based upon Data in Part B**

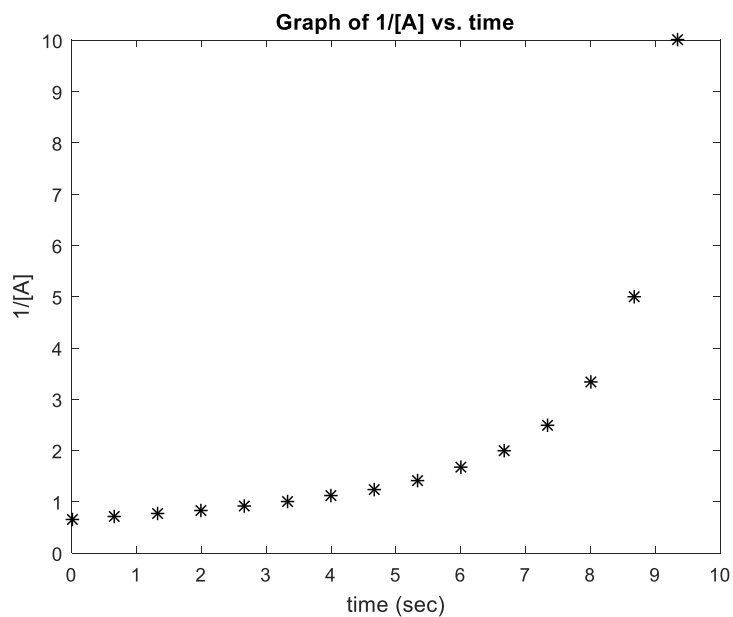


Figure 3: Graph of Second Order based upon Data in Part B

Part C: Second Order

Rate Constant (given in the instructions/also from the graph/Figure 6)= 0.013

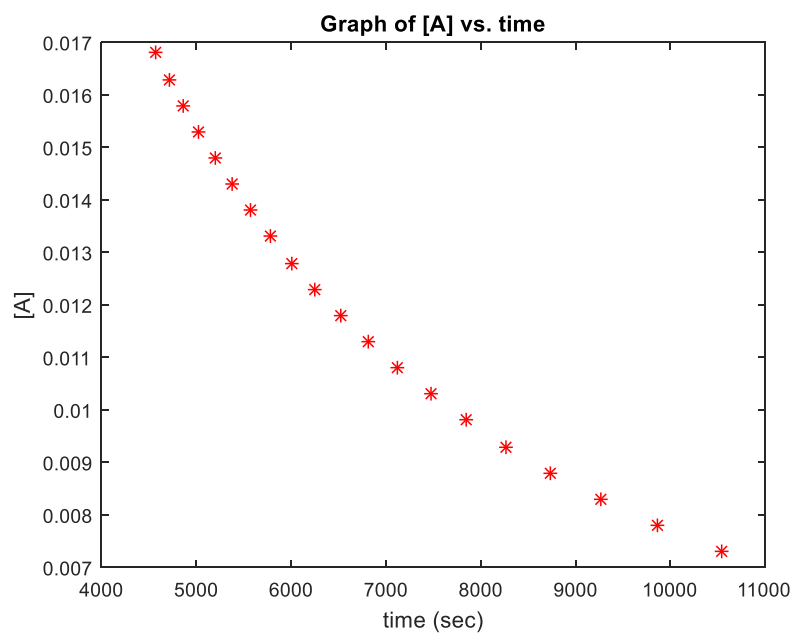
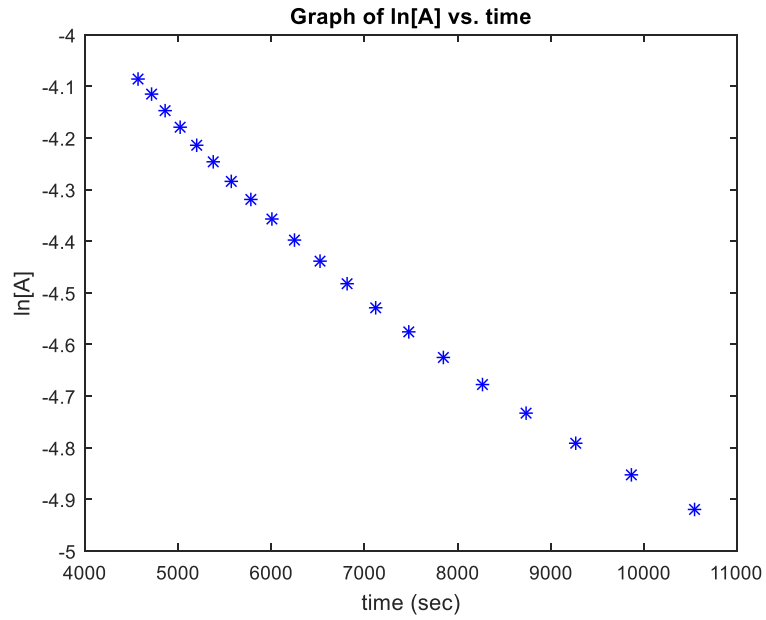
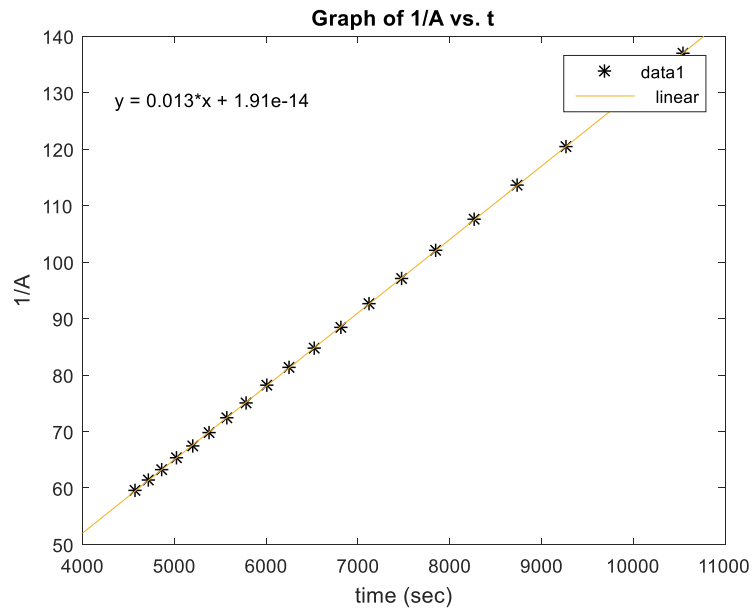


Figure 4: Graph of Zero Order based upon Data in Part C



**Figure 5: Graph of First Order based upon Data in Part C**

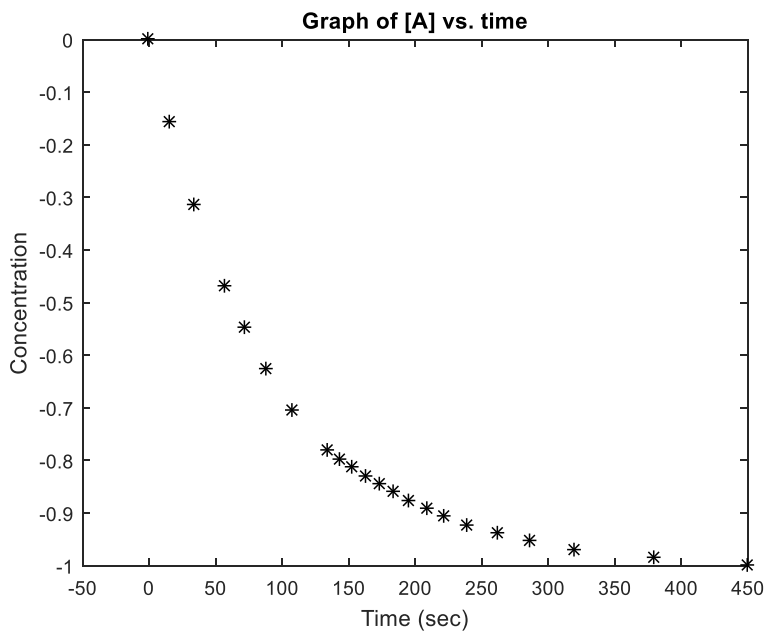


**Figure 6: Graph of Second Order based upon Data in Part C**

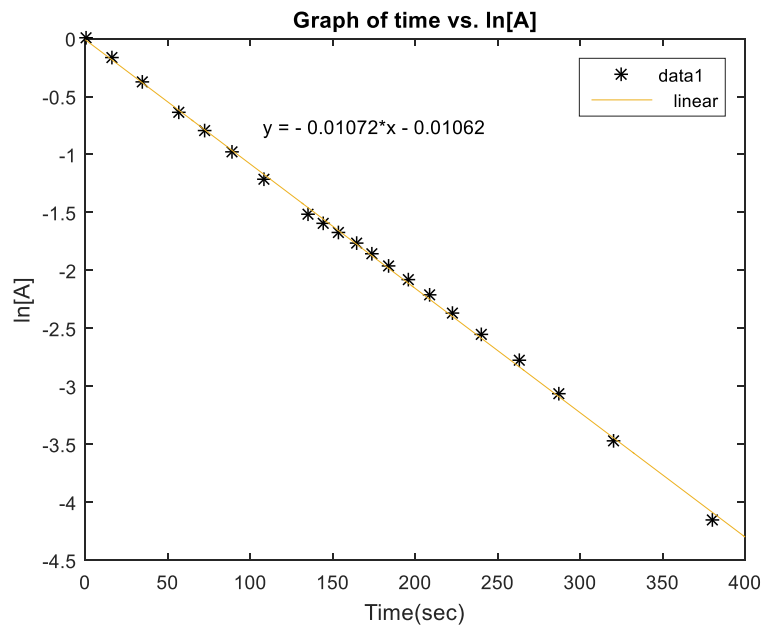
**Part D: First Order**

This is not a perfect fit. Can fit for this data- can look at the plot of residuals

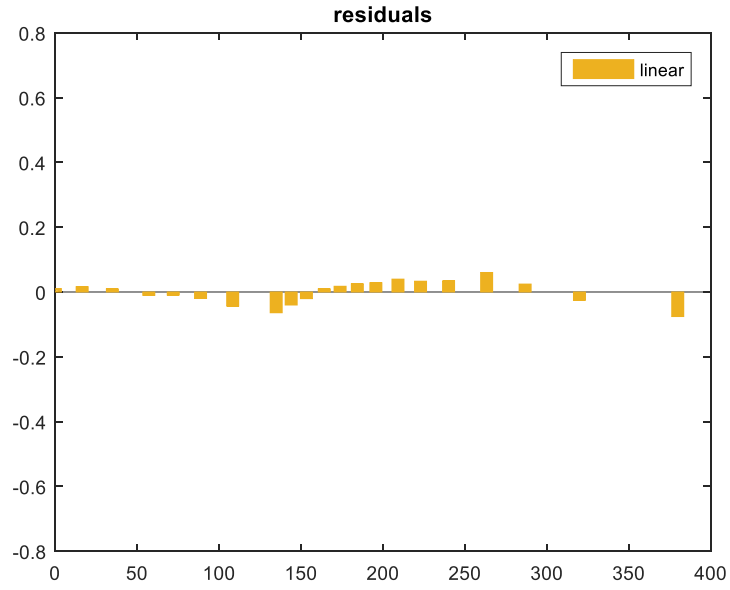
Rate Constant (Figure 8) = 0.01072



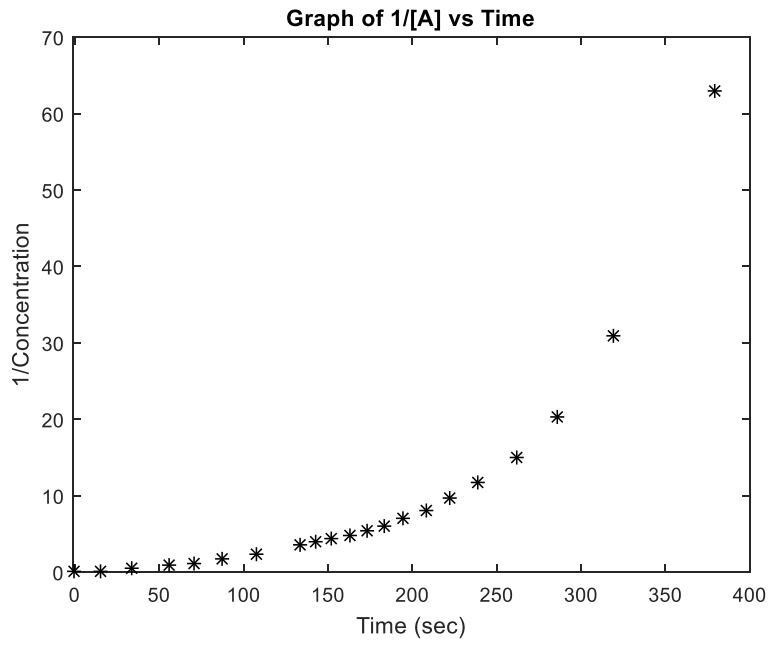
**Figure 7: Graph of Zero Order based upon Data in Part D**



**Figure 8: Graph of First Order based upon Data in Part D**



**Figure 9: Residuals Graph for First Order**



**Figure 10: Graph of Second Order based upon Data in Part D**