Rates of Chemical Reactions

Name_________________________________ Lab Section________________________

Log on to the Internet. Type the following address into the location-input line of your browser:

http://cheminfo.chem.ou.edu/~mra/CCLI2004/KRGO1N.htm

This will load a Graphics Simulation. Once you have the simulation running your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Graphics Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.

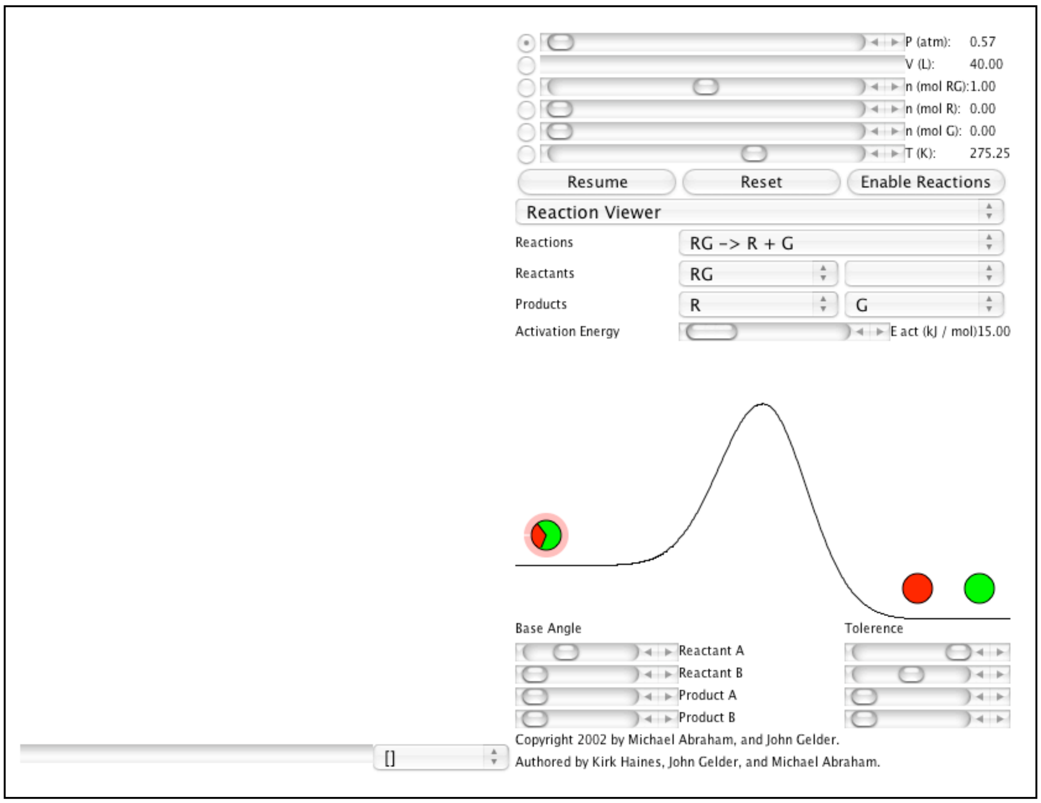


Figure 1.

Problem Statement: How is the rate of a chemical reaction related to the initial concentration of the reactants?

I. Data Collection:

Open the graphic simulation KRGO1N:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/KRGO1N.htm

A. Use the information there to write a balanced equation for the reaction you will be studying in this activity. Use the information in the Control Bar Region to determine the initial concentrations of the reactants and products in the reaction. Record this information in the space below.

B. Click on the Reset button. Click on the Enable Reactions and then the Resume buttons to begin the reaction. When the concentrations stop changing, click Pause to stop the action. In the space below, draw the appearance of the strip chart graph and label the axes. If necessary, use the scrollbar located under the strip chart to move the chart back to the beginning of the reaction. Identify the chemical substances that correspond to each of the colored lines. Interpret the meaning of the shape of the lines on the graph? What do these lines tell you about the rate of the reaction?

C. Click on the Reset button. In the drop down menu in the Module Control Region select Kinetics. Record the value for the initial concentration of RG, $[RG]_0$. Click on the Enable Reactions button and then the Get Data button. and record the rate at t = 0, the initial rate, for this set of conditions in the table below.

Experiment #	$[RG]_0$ (M)	Initial Rate (M $time^{-1}$), - Δ[RG]/Δtime
1		

D. Click on the Resume buttons to begin the reaction. The first 5 data points of the graph are displayed. Collect some additional time and amount data for RG by repeatedly clicking on the Get Data button while the reaction is proceeding. Graph the time vs. the amount of reactant on a piece of graph paper. (The easiest way to do this is to highlight and copy the data on the screen and then paste it into a graphing program. Microsoft Excel© is one possibility.) Describe the form of the graph.

E. Plot the first two data points of your graph and determine the slope of the graph (include the units for the slope). Record this value below. Show your work on the graph paper and submit it with your report. What does the slope represent? Compare this value with the initial rate of the consumption of RG in the table above.

F. Use the drop down menu for the Compound to see the data points for the formation of G. Record the initial rate for the production of G. Graph the time vs. the amount of product on a piece of graph paper. Describe the form of the graph. Plot the first two data points of your graph and determine the slope of the graph. Show your work on the graph paper and submit it with your report. What does the slope represent? Compare this value with the initial rate of the production of G. What is the initial rate for the production of the other product, R?

II. Data Analysis and Interpretation:

A. What happens to the rate of the reaction as time passes? Use both the strip chart graph and your data points as evidence for your conclusion.

B. Compare the rate of the consumption of RG with the production of G and R. How are they related? How do you account for this relationship?

C. Under what circumstances are you justified in using the slope of a straight line to determine the initial rate of a chemical reaction with the data you have collected?

III. Data Collection:

In the table below record the concentration and the initial rate of the consumption of RG you measured in section I.C. Reset the simulation. Adjust the Compound setting to monitor the kinetics of the reactant RG. Change the amount of RG to 2 mols. Click on the Enable Reactions, the Get Data, and finally the Resume buttons to begin the reaction. Record the initial concentration and the initial rate of the consumption of RG for this new concentration. Collect sets of rate data for 0.25 mols of RG, 0.5 mols of RG, and 1.5 mols of RG.

Experiment #	$[RG]_0$ (M)	Initial Rate (M $time^{-1}$), $-\Delta[RG]/\Delta time$

IV. Data Analysis and Interpretation:

A. How does doubling the concentration of RG affect the rate of the reaction?

B. Construct a mathematical relationship (called a rate law) between the rate of the reaction and the initial concentration of RG. (Hint: Write a proportionality equation based on the data you collected in section III. Determine how the concentration changes for any two trials and then what is the corresponding change in the rate.)

C. Using your data from section III., determine the value for the proportionality constant (called the rate constant, k) for the equation you generated in section IV.B. for each set of data you collected in section III.

D. Propose a reason for calculating the rate constant for your reaction. Why not just use the value of the rate?

E. (Optional) Another way to express the rate law is to determine the mathematical relationship between the concentration of the reactant and the time. This form of the rate law for the reaction you are studying can be determined from the kinetics data you previously generated from the simulation. Using a graphing program plot the amount of RG vs. the time. Then use the curve fitting function of your graphing program to draw the best line through all of the points. Try each of the available functions and see which gives you the best fit. Record the equation of your best-fit line. Compare the equation of this best fit line with the data you collected in previous sections.

F. Click on the Reset button. Click on the Enable Reactions, Get Data, and then the Resume buttons to begin the reaction. As the reaction proceeds across the Strip Chart Region window, click on the Get Data button several times to collect additional data, and then pause the reaction. There is a drop down menu below the Strip Chart Region. The default position shows that concentration (symbolized as []) is being plotted on the y-axis against time on the x-axis. The y-axis can be changed to two other options: the natural logarithm of the concentration (symbolized as ln[]), and the reciprocal of the concentration (symbolized as 1/[]). Use your observations of these three options to plan the function of the amount of RG you will graph vs. time to generate a mathematical equation for your data. Graph that function of amount vs. time and determine the equation of the line. Compare the values in the equation with the values you developed in the equations from previous sections (Sections IV.B., IV.C., and IV.E.).

G. Do you think the rate law you determined for the reaction you are studying would be the same for all reactions? Why or why not?

V. Data Collection:

Open the graphic simulation K2RN:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/K2RN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar region to construct the overall chemical equation for the reaction you are studying.

B. Reset the simulation. In the drop down menu in the Module Control Region select Kinetics. Design experiments to investigate the relationship between the rate of consumption of reactant and the initial concentrations of the reactants of the reaction. (Refer to section III.) Fill in the concentrations and the name of the reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[ ]	Initial Rate Reactant, $-\Delta[\ ]/\Delta t$
1	1.0mol/40L = 0.0250M	
2	2.0mol/40L = 0.0500M	
3	0.333mol/40L = 0.008325M	

C. Reset the simulation. In the drop down menu in the Module Control Region select Kinetics. Click on the Enable Reaction, Get Data, and finally the Resume buttons. As the reaction proceeds across the Strip Chart Region window, click on the Get Data button several times to collect additional data, and then pause the reaction. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes. How is this graph different from the one you sketched in section I. B.

D. Graph the time vs. the amount of reactant on a piece of graph paper. Describe the form of the graph. Using the suggestions in section IV. F., determine the mathematical equation for the best-fit line.

VI. Data Analysis and Interpretation:

A. How does doubling the concentration of R affect the rate of the reaction?

B. How does tripling the concentration of R affect the rate of the reaction?

C. Determine the rate law for the reaction you are studying in terms of the rate and the concentration of reactant (see section IV. B.). Determine the rate constant for the reaction (see section IV. C.).

D. What does the equation you constructed in section V. D. represent? What does the numerical amount (slope) in the equation represent?

E. Propose a mechanism to explain and describe how the reactant particles for this reaction interact to form product particles. ? (You can also view the mechanism with the molecular simulation of this reaction at http://cheminfo.chem.ou.edu/~mra/CCLI2004/K2RM.htm.)

F. How would you characterize the mechanism in terms of the number of the original reactant particles necessary for each individual reaction to occur? How is this related to the rate law you proposed?

G. Compare the rate law and conclusions concerning the number of necessary reactant particles in this section with that of the rate law and number of necessary reactant particles for the reaction in section IV. B.? (You can view the mechanism of this reaction with the molecular simulation of this reaction at http://cheminfo.chem.ou.edu/~mra/CCLI2004/KRGO1M.htm. How would you account for the differences in the rate laws?

VII. Data Collection:

Open the graphic simulation K2GBN:
http://cheminfo.chem.ou.edu/~mra/CCLI2004/K2GBN.htm

A. Click on the Resume and then the Enable buttons and observe the changes that occur in the strip chart. Use this information and the information from the Control Bar region to construct the overall chemical equation for the reaction you are studying.

B. Reset the simulation. Change the Module Control Region to view the kinetics table. Adjust the compound setting drop down menu so that you will gather data for the production of compound G_2B. Click on the Enable Reaction button, Click on the Get Data, and finally the Resume buttons. Sketch the curves traced out in the strip chart. Label the lines and discuss what is happening as time passes.

C. Determine the initial rate of production of the product G_2B, $\Delta[G_2B]/\Delta$time, for the reaction. (See section I.E.)

D. Design experiments to investigate the relationship between the rate of production of the product G_2B and the initial concentrations of the reactants of the reaction you are studying. (Refer to section III.) Make sure you choose concentration combinations that will isolate the effect of each reactant on the rate. Fill in the concentrations and the name of each reactant in the following table. Use the simulation to run each combination and determine the rate and record these values in the table.

Experiment #	[ ]	[ ]	Initial Rate, $\Delta[G_2B]/\Delta$time

VIII. Data Analysis and Interpretation:

A. What effect does doubling the concentration of G have on the initial rate of the reaction?

B. What effect does doubling the concentration of B have on the initial rate of the reaction?

C. Determine the rate law comparing the rate of the reaction with the initial concentrations of the reactants B and G (see section IV.B.). Determine the rate constant for the reaction.

IX. Data Collection:

Return to the simulation and use the pull down menu in the Module Control Region to expose the Reaction Viewer. Use the Reactions pull down menu to view the step-by-step process (the mechanism) showing how the reaction proceeds from reactants to final products. (You can also view the mechanism with the molecular simulation of this reaction at http://cheminfo.chem.ou.edu/~mra/CCLI2004/K2GBM.htm.) Record the mechanism below and show how the steps in the mechanism are related to the overall reaction.

X. Data Analysis and Interpretation:

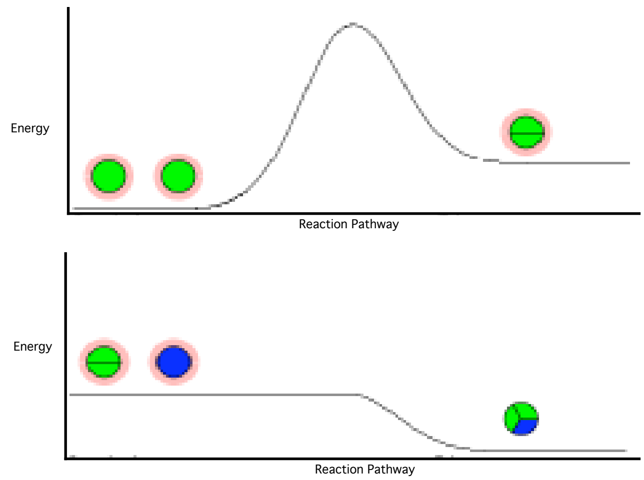
A. How would you characterize each step in the mechanism in terms of the number of the original reactant particles necessary for the stoichiometry of the reaction? How is this related to the rate law you proposed in section XI.?

B. How would you characterize the number and kind of reactant particles necessary to determine the rate of the overall reaction?

C. Below is the reaction profiles for step one and step two of the mechanism of the reaction you are studying.. Each profile shows how the energy of that step changes as the reaction proceeds from reactants to products. Compare the profiles with each other and use them to explain why each reactant particle is necessary or not necessary to determine the rate of the reaction.

Step One

Step Two



D. Identify any particles not part of the overall reaction but that are present in the mechanism. What role do these particles play in the reaction?