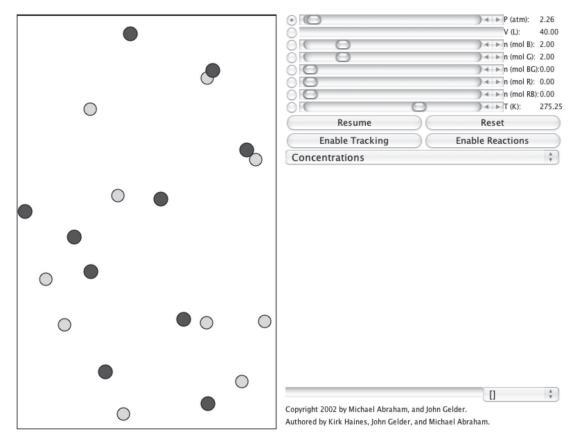
# CATALYSTS

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/KCatBGM.htm

This will load a Particulate 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 Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.





Problem Statement: What factors influence how fast a chemical reaction proceeds?

## I. Data Collection

Open the molecular simulation KCatBGM:

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

A. Record what you observe in the sample region of the screen. Indicate the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run until no more changes occur. Click on the Pause button and record the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

C. Reset the simulation. Calibrate the time axis (x-axis) of the Concentration Strip Chart. To do this, click on the Resume button and with a stopwatch time how long it takes for the strip chart line to proceed across the graphing space. Measure the length of the line in millimeters (mm) with a ruler. Record your data in the spaces below. Do this two more times and calculate an average. Use the average to develop a formula for converting mm to seconds.

	Trial 1	Trial 2	Trial 3	Average
Time (in sec)				
Time (in mm)				

Formula: 1 mm = \_\_\_\_\_seconds

D. Click on the Reset button. Click on the Enable Reactions button and then click on the Resume button. Pause the reaction when eight product particles are formed and measure the time elapsed by measuring the time on the strip chart's x-axis using the length (in cm) as a measure of time. Repeat this experiment two more times and record your results in the following table. Calculate the average time.

	Trial 1	Trial 2	Trial 3	Average
Time (in sec)				
Time (in mm)				

# II. Data Analysis and Interpretation

A. Write a balanced equation for the reaction you observed in this simulation.

B. Determine the average rate of the reaction to produce eight product particles. Express this rate with respect to the appearance of product BG in units of [BG]/s.

## III. Data Collection: Add particle R as a reactant

A. Reset the simulation. Add 2.000 moles of particle R to the reactants. Record what you observe in the sample region of the screen. Indicate the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

B. Click on the Resume button and then the Enable Reactions button and allow the simulation to run until no more changes occur. Click on the Pause button and record the number and the concentration of the particles.

	В	G	BG	R	RB
# of Particles					
Concentration (M)					

Collisions	Collisions Between						
Particle 1	Particle 2	Result	Comments				
В	G						
В	R						
G	R						
В	RB						
G	RB						

C. Study the details of this reaction by observing the interactions between the following pairs of particles.

D. Click on the Reset button. Add 2.000 moles of particle R to the reactants. Click on the Enable Reactions button and then click on the Resume button. Pause the reaction when eight product particles are formed and measure the time elapsed by measuring the time on the strip chart's x-axis using the length (in cm) as a measure of time. Repeat this experiment two more times and record your results in the following table. Don't forget to add the 2 moles of particle R each time. Calculate the average time.

	Trial 1	Trial 2	Trial 3	Average
Time (in mm)				
Time (in sec)				

# IV. Data Analysis and Interpretation

A. Taking into account the data from sections III.A. and III.B., compare the amount of particle R before the reaction with that after the reaction. What conclusions can you draw from this information?

B. Write a balanced chemical equation for the overall reaction you observed. How does this reaction compare to the equation you wrote for section II.A.?

C. Using the data you collected in section III.C., propose the series of steps that describes the route taken (called the mechanism) by the reaction as it proceeds from reactants to products.

D. Describe what happens to particle R and RB as the reaction proceeds from reactants to products.

E. Determine the average rate of the reaction to produce eight product particles. Express this rate with respect to the appearance of product BG in units of [BG]/s.

F. Compare the rates of the reactions from sections II.B. and IV.E. How do you account for any differences you observe? What role do any of the reacting particles play in this difference?

G. A chemical substance that increases the rate of a chemical reaction but is neither a reactant nor product in the overall equation for the reaction is called a catalyst. Identify the catalyst in the reaction studied in this experiment. How does a catalyst increase the rate of a chemical reaction?