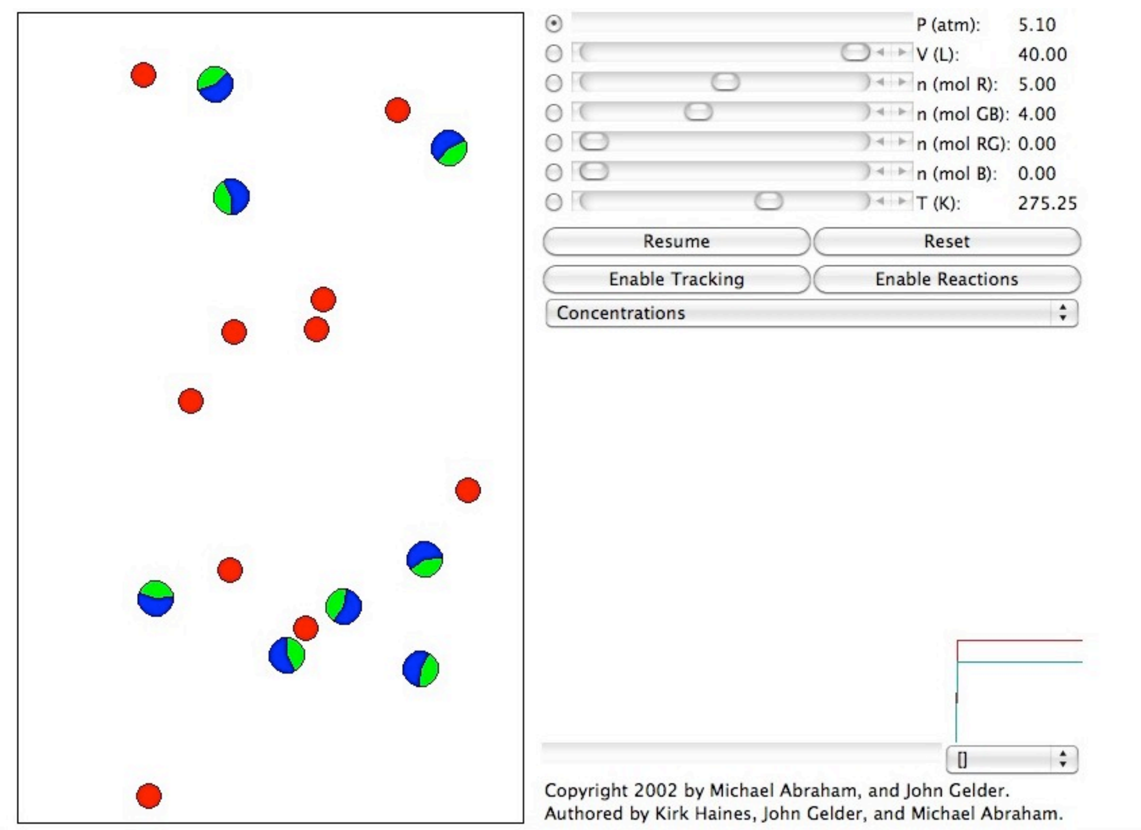
Shifting Reactions A

Name_______________________________Lab Section_____________________________

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

http://introchem.chem.okstate.edu/DCICLA/ERGBM.htm

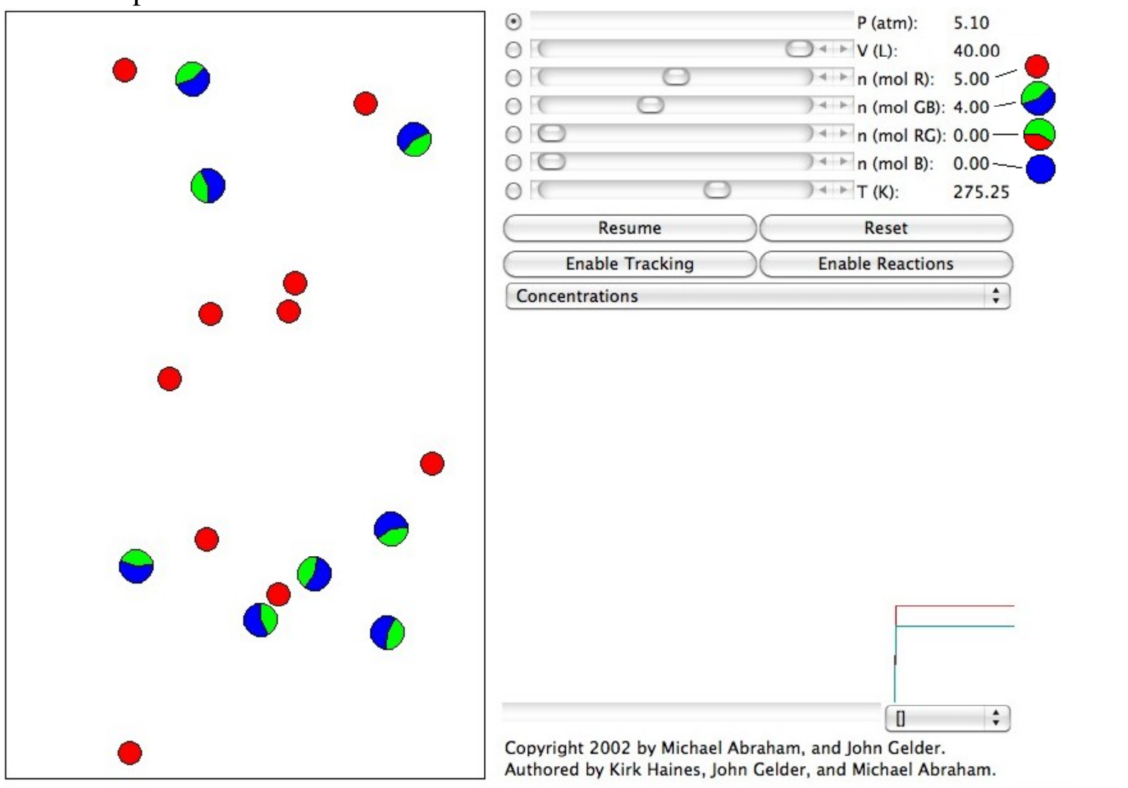
This will load a Particulate Simulation. Once you have the simulation running your screen will look like what is shown in Figure 1 below. If you haven't already done so, read the Particulate Simulation section of the Introduction to MoLEs Activities to learn how to use the simulation.



Problem Statement: What are the characteristics of a hypothetical chemical reaction?

I. Data Collection:

A. Open the Particulate Simulation. Use the pause button in the Control Bar region to stop the action of the particles. In the diagram below record the conditions of your sample as shown in the simulation.



B. Use the reset button to refresh the screen. Determine the concentration (mol liter^{-1}) of each substance in the control bar region. (Show your work.) Click on the pause button to stop the motion of the particles. In the Control Bar region, change the number of moles of one of the substances present by adding one half a mole to the amount already there. Resume motion and describe what you observe in the strip chart and the Sample Window.

Concentration of R:

$$\frac{\textbf{5.00 mol R}}{\textbf{40.00 L}} = \textbf{0.125 M}$$

Concentration of BG:

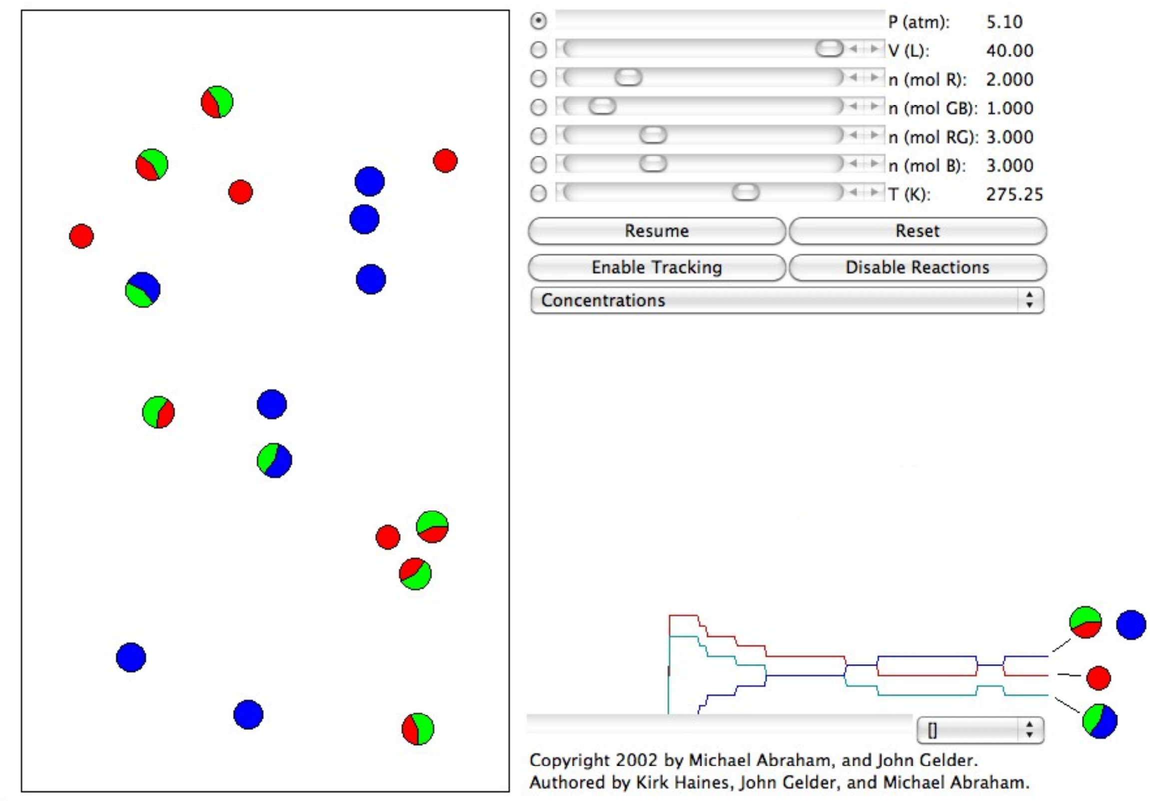
$$\frac{\textbf{4.00 mol BG}}{\textbf{40.00 L}} = \textbf{0.100 M}$$

Concentration of RG and B:

$$\frac{\textbf{0 mol}}{\textbf{40.00 L}} = \textbf{0 M}$$

The chart recording is showing the relative concentrations of the substances that are present in the container over time.

C. Use the reset button to refresh the screen. Click on the Enable Reactions button. After a short period of time has elapsed click the Pause button. In the space below draw a picture of the strip chart. Label the lines of the strip chart with their identity (R, GB, RG, and B).



NOTE: Since the products began with equal concentrations, the concentration of RG and B are the same and are superimposed on each other.

D. Resume the action. Observe how the concentrations of the particles in the sample change over time. How can you tell when the reaction is completed? What particles are present when the reaction is completed?

It appears that the reaction never stops. It certainly is not going completely to the products of the reaction. It appears to be shifting back and forth.

Some of all of the reactants and products are present.

E. Use the reset button to refresh the screen. Use the pull down menu to change the graphical representation to the replay function. Click the Enable Reaction button to begin the reaction. Allow the reaction to proceed for a short period of time (10 sec – 20 sec). Click the Pause button. Scroll the time index bar back to the point where only the reactant particles are present. Click on the forward arrow to roll the reaction forward in a step-wise manner to the point where the first new particle appears. Explain, in detail, the nature of that interaction. Include drawings and specify the orientation of all of the atoms in the interaction.

When using the replay feature it is possible to follow the movement of particles more easily. It is also possible to see when collisions occur between molecules. The only collisions that were effective, and by that it is meant the collision between reactants that result in the formation of products, occur when the red atom collides with green portion of the BG molecule. Sometimes that collision is not effective. When the collision between the R atom and the BG molecule have the correct orientation, but do not produce products it appears that the particles are not moving as fast as those collisions with the correct orientation that produce products. After a while the product concentrations increased and collisions between a blue atom and an RG, when the blue atom collided with the green side of the molecule, would produce an R atom and a BG molecule.

II. Data Analysis:

Write a chemical equation representing the chemical interaction you observed.

$$\mathbf{R + BG \rightarrow RG + B}$$

III. Data Collection:

A. Use the reset button to refresh the screen and the pause button to stop the action. Using the controls in the Control Bar region, fix the amounts of R and GB at zero, of RG at 3, and B at 4. Set the graphics display to Concentrations, and resume the interaction. Calculate the concentrations of the particles. Calculate the initial concentrations of all the substances (R, GB, RG and B).

Concentration of B:

$$\frac{4.00 \text{ mol B}}{40.00 \text{ L}} = 0.100 \text{ M}$$

Concentration of RG:

$$\frac{3.00 \text{ mol RG}}{40.00 \text{ L}} = 0.075 \text{ M}$$

Concentration of R and BG:

$$\frac{0 \text{ mol}}{40.00 \text{ L}} = 0 \text{ M}$$

B. Click on the Enable Reactions button. When the reaction is complete, click on the Pause button. Calculate and record the final concentrations of all of the substances.

Just as before it was a little difficult to determine when the reaction was 'over' because the reaction just keeps on going. So I decided to calculate the concentrations of R, GB, RG and B using the numbers below.

Concentration of B:

$$\frac{\text{2.50 mol B}}{\text{40.00 L}} = \text{0.0625 M}$$

Concentration of RG:

$$\frac{\text{1.50 mol RG}}{\text{40.00 L}} = \text{0.0375 M}$$

Concentration of R and BG:

$$\frac{\text{1.50 mol}}{\text{40.00 L}} = \text{0.0375 M}$$

C. Use the reset button to refresh the screen. Using the controls in the Control Bar region, fix the amounts of R and GB at zero, of RG at 3, and B at 4. Use the pull down menu to change the graphical representation to the replay function. Click the Enable Reaction button to begin the reaction. Allow the reaction to proceed for a short period of time (10 sec – 20 sec). Click the Pause button. Scroll the time index bar back to the point where only the reactant particles are present. Click on the forward arrow to roll the reaction forward in a step-wise manner to the point where the first new particle appears. Explain, in detail, the nature of that interaction. Include drawings and specify the orientation of all of the atoms in the interaction.

When using the replay feature it is possible to follow the movement of particles more easily. It is also possible to see when collisions occur between molecules. The only collisions that were effective, and by that it is meant the collision between reactants that result in the formation of products, occur when the blue atom collides with green portion of the RG molecule. Sometimes that collision is not effective. When the collision between the B atom and the RG molecule have the correct orientation, but do not produce products it appears that the particles are not moving as fast as those collisions with the correct orientation that produce products. After a while the product concentrations increased and collisions between a R atom and an BG, when the R atom collided with the green side of the BG molecule, would produce an B atom and a RG molecule.

IV. Data Analysis:

A. Write a chemical equation representing the chemical interaction you observed

$$\mathbf{RG + B \rightarrow R + BG}$$

B. Compare and contrast the two equations you wrote in sections II. and IV. A.

The two equations are exactly the opposite of each other. In Section II the equation is;

$$\mathbf{R + BG \rightarrow RG + B}$$

In Section IV A the equation is;

$$\mathbf{RG + B \rightarrow R + BG}$$

V. Interpretation and Conclusions:

A. Chemists refer to the type of reaction you have been investigating as a reversible reaction. Using the chemical system you investigated explain what is meant by reversible reaction.

A reversible reaction is a reaction that can occur in either direction. Initially, assuming no products are present, the reaction proceeds from left to right. However, after the concentration of the products reaches a high enough value the reverse reaction begins to occur.

Reversible reactions will have some concentrations of all reactants and products after a period of time.

At the particulate level reversible reactions appear to never stop, the reaction continues in both directions, for ever.

B. An example of a non-reversible reaction is:

$$2KClO_3(s) \rightarrow 2KCl(s) + 3O_2(g)$$

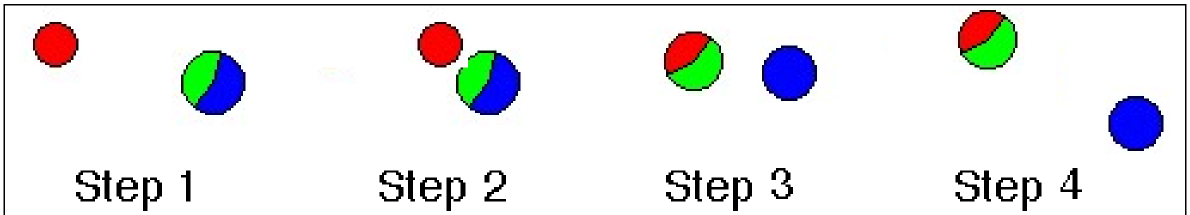
What is meant when the term non-reversible is used to describe this reaction?

In this reaction non-reversible would mean that the reverse reaction does not occur, measurably. That is, we would not expect to see oxygen gas reacting with potassium chloride to form potassium chlorate. We would only see potassium chlorate decomposing to potassium chloride and oxygen gas.

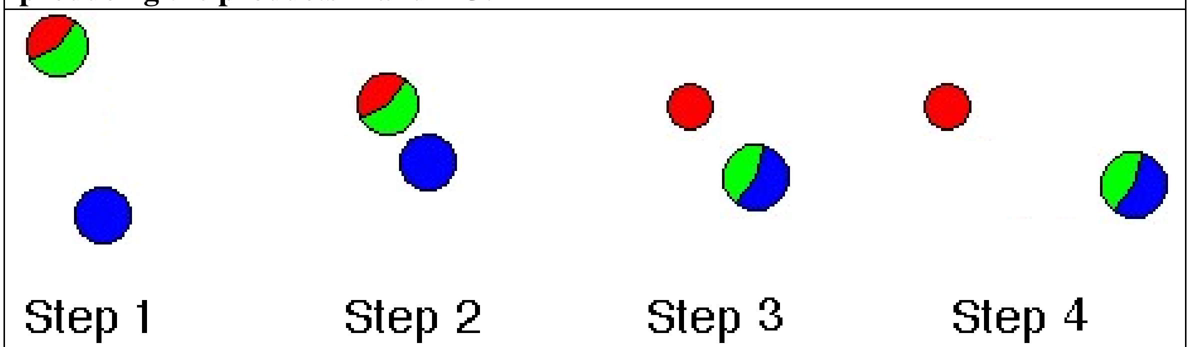
C. When viewed at the macroscopic level in the laboratory, chemical reactions seem to stop after a period of time. How does this compare to your molecular observations in this activity? How do your observations at the molecular level explain what happens at the macroscopic level?

At the macroscopic level reversible reactions appear to stop. If we assumed that one of the reactants or products absorbed in the visible region of the electromagnetic spectrum, then for a reversible reaction at the macroscopic level the color with reach a point where it is no longer changing. That would be the end of the reaction. At the particulate level, the reversible reaction would still be occurring, however, to keep the color of the solution constant any forward reaction would have to be exactly balanced by a reverse reaction somewhere else in the mixture.

D. Mental Modeling: Using the Particulate Simulation program see if you can observe both chemical reactions studied in this activity to occur in the same window. Illustrate your observation by drawing a sequence of interactions that result in both reactions occurring sequentially.



In this sequence an R and BG approach each other with the R atom colliding with G portion of the BG molecule with sufficient energy for a reaction to occur and producing the products B and RG.



In this sequence an B and RG approach each other with the B atom colliding with G portion of the RG molecule with sufficient energy for a reaction to occur and producing the products R and BG.

E. Summarize in a few statements what are the characteristics of chemical reactions of the type studied in this activity.

A reversible reaction is a reaction that can occur in either direction. Initially, assuming no products are present, the reaction proceeds from left to right. However, after the concentration of the products reaches a high enough value the reverse reaction begins to occur.

Reversible reactions will have some concentrations of all reactants and products after a period of time.

At the particulate level reversible reactions appear to never stop, the reaction continues in both directions, for ever.