Introduction to MoLEs Activities
Computer Simulations[*]

Molecular Level Experiments (MoLEs) are chemistry laboratory experiments based on computer simulations. There are two types of simulation programs that you can be used in these activities: Particulate Simulations and Graphic Simulations.

To begin an activity you must be able to log on to the Internet using Internet Explorer (Microsoft) 4.5 or higher or Safari with OSX for macs.

Particulate Simulations

Once the browser is running, type the following address into the location-input line of your browser:

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

This should load a sample Particulate Simulation. Once you have the simulation running your screen should look similar to what is shown in Figure 1. below.
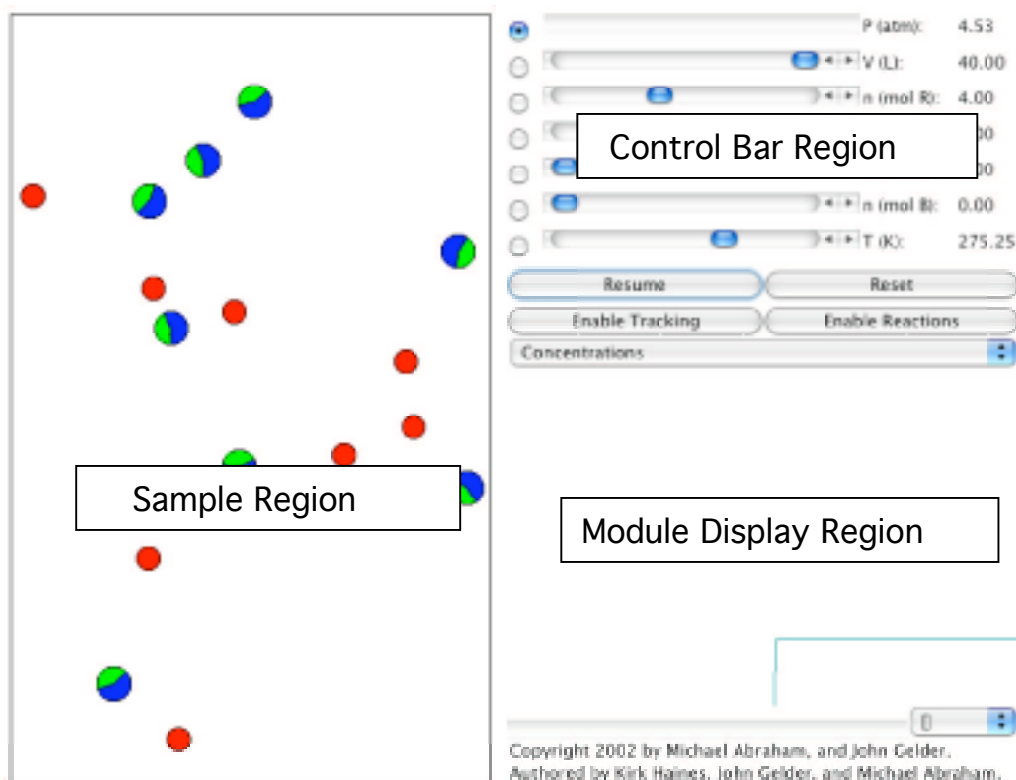

Figure 1

Although the details of the screen you will see will vary with different MoLE activities, all Particulate Simulations have three important regions. The Sample Region has the most activity. It is a container with different kinds of particles. To explore the behavior of the sample you can change the variables located in the Control Bar Region. The Control Bar Region has scrollbars that allow you to change the variables of the experiment. There are scrollbars for pressure (in units of atmospheres), for volume (in units of liters), for the amounts amount of each substance that is active in the Sample Region (in mols), and for temperature (in units of Kelvins). The concentration of each substance can be calculated by dividing the number of mols by the volume of the container. To the left of each scrollbar is a radio button. When selected, that particular variable (called the dependent variable) is calculated based on the value of the other variables. In the default mode the pressure scrollbar's radio button is selected so the pressure of the sample is varied.

As a simple exploration try moving each of the scrollbars and observe the effect on the sample. These effects will be address in more detail in each experiment. You can click the mouse on the Reset button located below the temperature scrollbar to return to the original conditions. The Pause button will suspend the motion in the gas sample while the Enable Tracking button will turn the red tracking line on and off.

The region below the Control Bar Region is the Module Display Region. This region allows the data in the other regions to be represented graphically or in tables in several ways depending on the particular activity you are doing. These might include simple graphs comparing variables, concentration strip charts showing concentrations vs. time, energy reaction profiles showing the relative energies of reactants and products of a chemical reaction, and a replay feature that allows you to replay and slow down a portion of the particulate interactions showing in the Sample Region. To utilize these different functions use the pull down menu located below the temperature scrollbar.

The Concentrations option shows the relative concentrations and changes in concentration vs. time for each substance studied in the simulation. Manipulate the concentrations using the Control Bars to see how the strip chart is affected. These effects will be addressed in more detail in experiments that utilize this function. You can click on the Reset button located below the temperature scrollbar to return to the original conditions.

The Replay option (see Figure 2) allows you to slow down the motion in the Sample Region and to replay portions of the reaction sequence. You can click on the Pause Button and using the forward or reverse arrows on the time index function, view the motion of the particles a step at a time. These effects will be addressed in more detail in experiments that utilize this function. You can click the mouse on the Reset button located below the temperature scrollbar to return to the original conditions.

Figure 2

The Kinetics option allows you to record quantitative information being generated by the strip chart. Three columns of data are generated: time, amount, and instantaneous rate. These data are generated by specifying the compound you want to follow and then clicking on the Get Data button. This can be done as many times during the reaction as you want. These effects will be addressed in more detail in experiments that utilize this function.

The Reaction Viewer shows the reaction profile for a chemical reaction as it proceeds from reactants to products. These effects will be addressed in more detail in experiments that utilize this function.

The Relations option reveals an xy graph with a dropdown menu on each axis. Selecting the dropdown menu on either axis provides a list of the variables shown in the Control Bar Region. The two buttons, Enable and Multiple are used when plotting pairs of variables. If you select pressure for the y-axis and volume for the x-axis, and then select "Enable," these same variables are activated in the Control Bar Region. By scrolling the volume slide bar in the Control Bar Region you will trace out a plot. The Multiple Button allows two or more plots to be superimposed.

The Velocities option is a plot of the speed distribution of the sample. The y-axis of this plot represents the number of particles. The x-axis represents the range of velocities starting at zero. The bars in this plot represent the velocities of the particles in the Sample Region. As the velocities of the particles change, the plot is redrawn. The smooth curved line in the plot represents the ideal distribution of the velocities for the gas sample. A vertical line represents the average (root-mean-square average) speed of the sample. This line is the same color as the particles. Observe the behavior of this region while changing each of the variables in the Control Bar Region. If you click on the Enable Tracking button, you can follow the path of a particle in the Sample Region. The length of the tail represents a fixed unit of time, and consequently can be used as a measure of the speed of the particle. This same particle is identified as a red line, labeled with the actual speed (in meters/second), in the speed distribution plot. If you pause the motion of the particles, you can click on different particles to get a measure of their speeds.

If you have any questions check with another student in the class, or your instructor.

Graphic Simulations

Once the browser is running, type the following address into the location-input line of your browser:

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

This should load a sample Graphic Simulation. Once you have the simulation running your screen should look similar to what is shown in Figure 3. Although the details of the screen you will see will vary with different MoLE activities, all Graphic Simulations have three important regions. The Strip Chart Region will plot the relative concentrations versus time of all the substances in the reaction to be studied. When you first load the program the Strip Chart Region is blank. It is activated when you click on the Resume button.
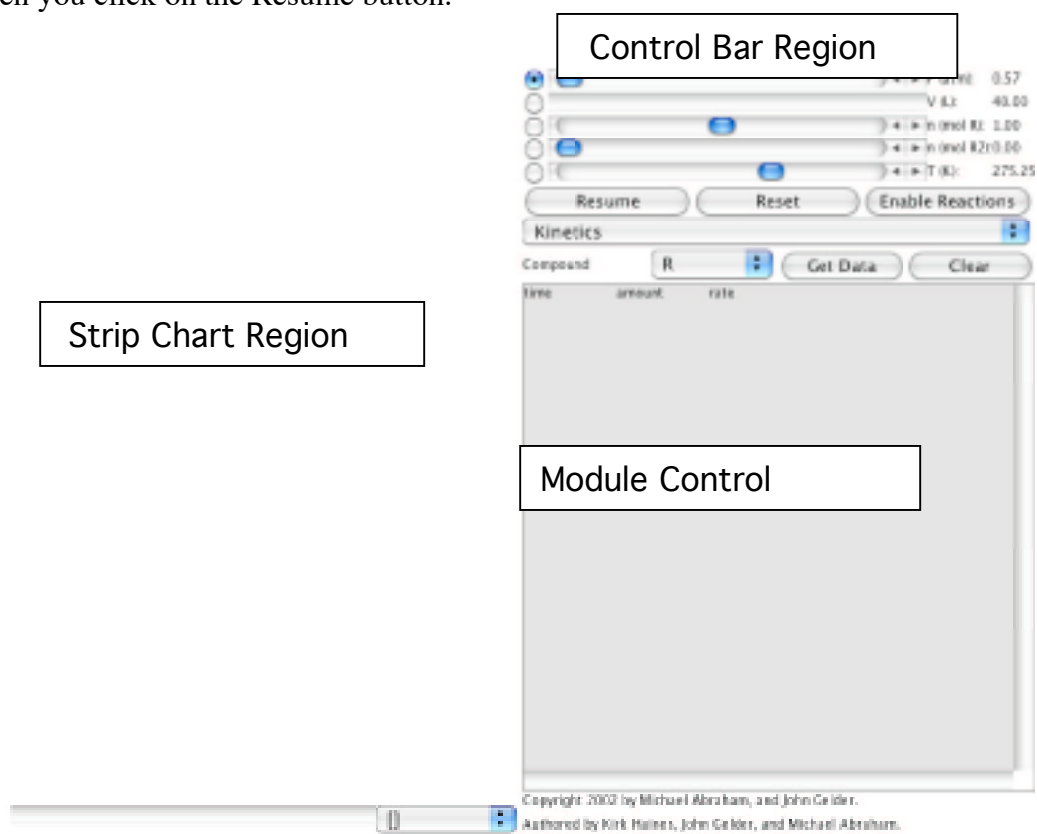
Figure 3

The Control Bar Region has scrollbars that allow you to change the variables of the experiment. There are scrollbars for pressure (in units of atmospheres), for volume (in units of liters), for the amounts amount of each substance that is active in the Sample Region (in mols), and for temperature (in units of Kelvins). The concentration of each substance can be calculated by dividing the number of mols by the volume of the container. To the left of each scrollbar is a radio button. When selected, that particular variable (called the dependent variable) is calculated based on the value of the other variables. In the default mode the pressure scrollbar's radio

button is selected so the pressure of the sample is varied.

As a simple exploration try moving each of the scrollbars and observe the effect on the strip chart. These effects will be address in more detail in each experiment. You can click the mouse on the Reset button located below the temperature scrollbar to return to the original conditions. The Pause button will suspend the motion in the gas sample.

The region below the Control Bar Region is the Module Display Region. As was the case for the Particulate Simulation this region allows the data in the other regions to be represented in several ways depending on the particular activity you are doing. These might include energy reaction profiles showing the relative energies of reactants and products of a chemical reaction, and simple graphs comparing variables. To utilize these different functions use the pull down menu located below the temperature scrollbar.

The Kinetics option allows you to record quantitative information being generated by the strip chart. Three columns of data are generated: time, amount, and instantaneous rate. These data are generated by specifying the compound you want to follow and then clicking on the Get Data button. This can be done as many times during the reaction as you want. These effects will be addressed in more detail in experiments that utilize this function.

The Reaction Viewer shows the reaction profile for a chemical reaction as it proceeds from reactants to products. These effects will be addressed in more detail in experiments that utilize this function.

The Relations option reveals an xy graph with a dropdown menu on each axis. Selecting the dropdown menu on either axis provides a list of the variables shown in the Control Bar Region. The two buttons, Enable and Multiple are used when plotting pairs of variables. If you select pressure for the y-axis and volume for the x-axis, and then select "Enable," these same variables are activated in the Control Bar Region. By scrolling the volume slide bar in the Control Bar Region you will trace out a plot. The Multiple Button allows two or more plots to be superimposed.

If you have any questions check with another student in the class, or your instructor.