Name ____ Period ______ Date ______________

Partner ____

Molecules and pressure

Using the Boltzmann 3D program

Purposes of worksheet: Learn the molecular level relationship between pressure, temperature, mass, number of particles, and volume using a molecular view simulation program.

Introduction

In this lesson, you will use a program called **Boltzmann 3D** to study how pressure is affected by some factors. **Boltzmann 3D** demonstrates the principles of *Kinetic Molecular Theory* (KMT) in a visual and understandable way by simulating the motion of particles in a *very* small box. You control the number, size, mass and temperature of particles and watch them move in the box just like real gas atoms.

Remember that KMT has the following assumptions

1. Gases are made from tiny particles (atoms or molecules).
2. The volume (size) of individual particles is neglected compared to the volume of the container.
3. Particles are constantly moving, occasionally colliding with the walls of the container to cause the pressure felt by the walls. All collisions are elastic (no energy is lost)
4. Particles don't attract or repel each other except during brief collisions.
5. The average kinetic energy for the particles is directly proportional to the temperature (in Kelvin) of the gas.

Instructions

1. Load the program (*enter here the local source of the program or use http://people.chem.byu.edu/rbshirts/research/boltzmann_3d*).

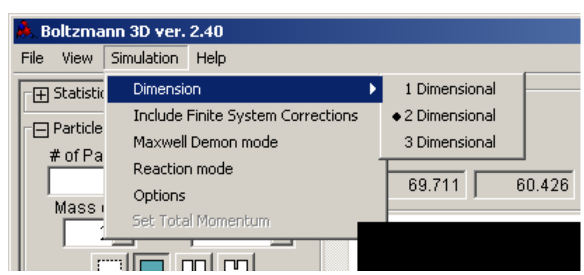
   The program window is divided into four main areas

   a) *Input/Output* area which includes three smaller areas, *Statistics*, *Particle Info* and *Advanced*

   b) *Viewing* window (called the "arena")

   c) *Pressure* area

   d) *Program Control* area



Understanding the arena

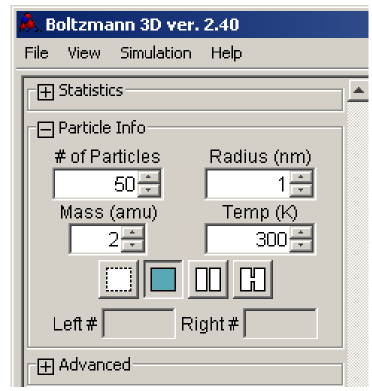
2. From the top menu, select *Simulation/Dimensions/3 Dimensional*. Describe in writing what you see.

3. While a 3-D view is the more realistic simulation, you will better understand your results if you reselect the *two-dimensional view*.
4. Switch back to the 2-D view and note the arena dimensions. They are _____ nm tall and _____ nm wide.
    a. What does the abbreviation “nm” mean?

    b. How many “nm” fit in 1 meter?

    c. What is a typical atom size in nm?

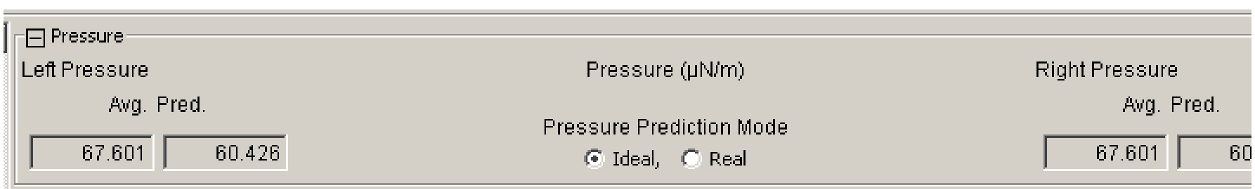
5. For this lesson, hide the *Statistics* area by clicking on the “**—**” box by the word, *Statistics*. The top left side of your screen should look like the figure to the right.



Notice there are four variables. These are:

a. number of particles
b. radius
c. mass
d. temperature.

You will be studying the effect of these variables on pressure as shown in the top right window (see below). Notice there are four pressure values. Right now, just focus on the *Left Pressure Pred* (predicted left pressure). For most exercises, left and right pressures will be the same.



READ THIS CAREFULLY:

General suggestions for using the program.

a. After you change any setting, click on the  button in the bottom left corner to activate your changes.
b. After changing a setting, wait 20 seconds before reading the pressure or observing the arena.   It takes a little while for the values to average over enough wall collisions to settle down.
c. When changing a setting, check and reset the temperature if needed.   The temperature is calculated from the average kinetic energy and sometimes changes when another value is altered.

Qualitative Behavior of Individual Molecules

Your *Particle Info* values should be set to: # of particles = 50, radius = 1 nm, mass = 2 amu. If not, enter these values. Set the temperature to 50 K and press the restart button:

Observe the arena and answer these questions

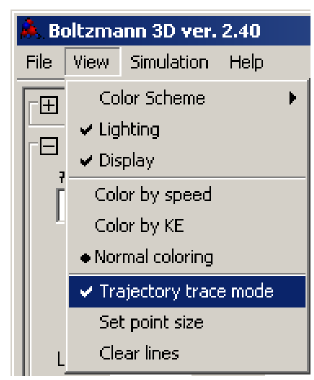
1. Between collisions, are the molecules slowing down or keeping the same speed?

2. Do the molecules travel in straight-line motion between collisions?

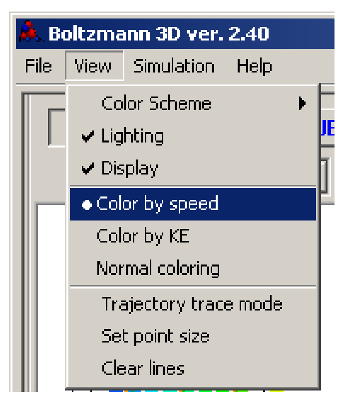
3. Are all molecules traveling at the same speed? *Explain*

4. Click in the arena with the mouse. This will drop a blue molecule into the simulation. Follow this molecule for at least 20 seconds. Does the given molecule always travel at the initial speed or does its speed vary? *Explain*.

5. Reset the temperature to 300 K. From the *View* menu, select the *Trajectory trace mode*. Over 30 seconds, watch the blue molecule trace. Is there a pattern to its movements? Or does it follow a random motion?



6. Turn off the *Trajectory trace mode*. Set *# of Particles* = 5. From the *View* menu, select the *Color by speed*. Over 40 seconds, watch the molecules. When do their colors (speed) change? When you are done, select *Normal coloring.*



Effects of radius, mass, temperature, and number of particles on wall pressure

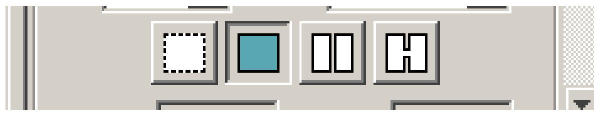
7. Try changing each of the four variables and note the effect on pressure and on the molecules in the arena.

	Pressure	***Description of arena conditions***
Original settings *# of particles = 50* *Radius = 1 nm* *Mass = 2 amu* *Temperature = 300 K*		
Double the number of particles *# of particles = 100* *Radius = 1 nm* *Mass = 2 amu* *Temperature = 300 K*		
Cut the particle radius in half *# of particles = 50* *Radius = 0.5 nm* *Mass = 2 amu* *Temperature = 300 K*		
Double the particle mass *# of particles = 50* *Radius = 1 nm* *Mass = 4 amu* *Temperature = 300 K*		
Double the temperature *# of particles = 50* *Radius = 1 nm* *Mass = 2 amu* *Temperature = 600 K*		

8. From your observations, what conclusions would you reach about the factors that affect gas pressure? Which ones do? Which ones don't?

9. Given what you have learned about temperature, pressure, and kinetic energy (look up the formula) does this make sense? *Use KMT assumptions to support your explanation.*

Relationship of volume and pressure



10. Under *Particle Info*, look for the four icons like those shown to the right.

    Input the following settings

    # of particles = 50
    Radius = 1 nm
    Mass = 2 amu
    Temperature = 300 K

    Record the pressure ______________

    Click on the two vertical bars (3rd icon from the left). What did it do to the arena?

    Record the pressure ______________

    Click on the single solid rectangle (2nd icon from the left). What did it do to the arena?

    Record the pressure ______________

    Using the data you just gathered, *describe* what you think is the relationship between *pressure* and *volume*.

    Given what you know about KMT, *explain* this relationship between volume and pressure on a molecular level. Use KMT assumptions, 1, 3 and 5 to support your explanation.