Name(s)	Project Number
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Project Title

The Molecular Model: A Computer Simulation of the Kinetic-Molecular Theory

Abstract

Objectives/Goals

How does a computer simulation of a gas, following kinetic-molecular theory, stack up against the ideal gas law? How do real gas conditions (molecular collisions and intermolecular attractions) change the situation?

Methods/Materials

The basic premise of the project is to create the computer model. In theory, the following steps are taken, although in practice, the lines are very much blurred. The foundation code was obtained from http://nehe.gamedev.net. From that, a "Molecule" object was added which could move around in an imaginary box and could draw itself, along with the environment, which could in turn contain several Molecules. The variables of pressure, volume, and number of molecules were introduced, and the real gas concepts of collisions and attractions were added. Finally, a script system was written which would churn out data points systematically for detailed analysis of the results.

Results

Under ideal conditions, the simulation came very close to the ideal gas law, generally with a correlation exceeding .99, and under real conditions, the model correctly deviates at very high pressures. There are a few noteworthy observations to be drawn: a "solid" state can be induced, and without collisions, intermolecular attractions can destabilize the model.

Conclusions/Discussion

The molecular model I built correctly (although not perfectly) mimics ideal and real gas behavior. It provides a useful visual for understanding how all the assorted variables come together to result in the equations for the gas.

Summary Statement

Using the kinetic-molecular theory, a computer model was built that would simulate gas molecules, allowing both intuitive grasp of the concepts used as well as detailed analysis of the results.

Help Received

Mother helped in cutting and pasting paper and in the placement of construction paper; other family members gave some assorted ideas and suggestions