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Molecular Dynamics Simulations in First-Semester General Chemistry: Visualizing Gas Particle Motion and Making Connections to Mathematical Gas Law Relationships

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Implementation of a freely available molecular dynamics (MD) software program in a general chemistry class to assist students in learning the relationship among particle motion, macroscopic properties, and mathematical gas laws is described. In this activity, students acquire skills in data analysis while developing a deeper understanding of the origin of macroscopic physical properties of gases. The activity is easy to implement and does not require significant expertise in computational chemistry on the part of the instructor.

Introduction

The transition from novice to professional chemist requires not only acquisition of content knowledge but also development of chemical intuition grounded in that content knowledge. Visualization of atomic and molecular level processes is a valuable tool in an instructor's toolbox for helping students at all levels acquire content knowledge and use that knowledge to develop accurate chemical intuition (1). Many types of visualizations exist, ranging from interactive laboratory simulations to mathematically accurate computational techniques (2–6). The former are traditionally used in introductory level courses while the latter are often reserved for higher-level courses after students have additional subject-specific content knowledge. This chapter will argue that students at the General Chemistry level can benefit from introduction to and use of mathematically accurate models of chemical behavior to develop a better understanding of molecular-level behavior via both visualization of particle motion and confirmation of mathematical relationships typically taught in the General Chemistry curriculum.

Readers of this book are likely already aware of the value of using computational techniques in the curriculum, but for some instructors, the barrier to introducing a new technology, particularly one not in their area of expertise, is too great. The activity described in this chapter is accessible for students and instructors at all knowledge levels. At the introductory level, the addition of computational tools to the course provides another mechanism for students to learn the required

content in a way that appeals to visual learners and to those who are ready for more advanced understanding of molecular-level behavior. Many students, even those at the upper-level, consider molecules to be stationary images of Lewis structures they learn to draw in general chemistry. Early introduction to molecular motion helps students with topics such as kinetics and reaction mechanisms in a way that stationary images cannot.

Visualization Activities

In each semester of my general chemistry lecture course of approximately thirty students, I assign students five “Visualization” activities, one of which is described in this chapter. The Visualization assignments are independent of each other, vary in complexity and technique, and often make use of PhET (7) or Jmol (8) resources. The primary objective is to help students understand molecular-level phenomena, so I select activities that allow students to visualize concepts such as dissociation (comparing electrolytes and nonelectrolytes as well as building skills for understanding spectator ions) (9), molecular geometry (10), and crystal structures (11). Many students report that the Visualization activities are the most helpful assignments for learning chemistry (more than homework, weekly quizzes, daily on-the-fly clicker questions, or daily warm-up questions). I use the freeware *Virtual Substance* molecular dynamics simulation software (12) as one of the Visualization assignment to teach gas laws, data analysis, and relationships between kinetic energy and temperature. Other software programs can be used to accomplish the same goals depending on access (purchased from companies such as Wavefunction (13)) or instructor familiarity (other freeware such as NAMD (14)).

Using Molecular Dynamics Software To Aid Student Learning

With the complementary goals of improving content knowledge and assisting students in the transition from novice to professional chemists, I have implemented assignments using the molecular dynamics (MD) software package *Virtual Substance* (12) in both my General Chemistry and Physical Chemistry courses. I have written about using the software in the Physical Chemistry curriculum on the first day of the lecture course (15) and in a lab situation (16) where students develop mathematical relationships that describe the physical behavior of real and ideal gases.

In this chapter, I describe how I have used an activity in the General Chemistry course where students conduct MD simulations on ideal gases, collect data on the physical properties (Temperature, Pressure, Volume, Kinetic Energy, and Potential Energy) of the system during the simulation, and use spreadsheet software (Excel, for example) to understand the relationships among these properties by plotting their data and using the trendline feature to determine physical constants. This activity addresses a number of course learning goals including understanding mathematical relationships among physical properties of ideal gases, representing and interpreting data graphically, and relating kinetic energy to temperature and particle motion. These learning goals are three of the most difficult for novice students. They can easily memorize and grind through the ideal gas law, but they do not really understand the origin of these physical properties at the atomic or molecular level. They also struggle with interpreting data graphically as well as using a spreadsheet program to clearly represent the data they have collected, particularly if this is the first time they are asked to do so.

There are a number of places in the general chemistry curriculum where data analysis skills can be developed, particularly in the laboratory component of the course. Students frequently collect, plot, and analyze data. Performing a similar activity in the lecture course further cements the importance of graphical analysis and interpretation of data, skills students need on their path from

novice to professional chemist. This connection may be particularly valuable when students have different instructors for the lecture and lab components of the course. As students are somewhat familiar with the application of these skills, and explicit instructions for constructing plots can be provided, it is somewhat more challenging for students to understand that particle interactions determine macroscopic physical properties and the mathematical relationships between those properties. Molecular dynamics simulations provide a perfect opportunity for students to learn each of these content topics and skills.

Implementation and Results

Keeping in mind that the purpose of the activity is student learning, students at the general chemistry level do not need to understand how an MD simulation works beyond knowing that the particles are following the laws of physics that govern their motion. These topics can be adequately explained at the instructor's discretion as the Virtual Substance (16) MD software program is introduced and the activity to be completed is distributed. The first steps in using the software require selecting the substance to use (He, Ne, Ar, Kr, Xe, or user defined), the type of boundary conditions (Fixed Walls or Periodic Boundary Conditions), and the Potential Model (No potential = ideal gas, soft sphere, Lennard-Jones, and options for adding finite extensible nonlinear elastic models for treating polymers) as seen in Figure 1.

Figure 1. Screenshot of Virtual Substance initial set up for 128 Argon atoms treated as an ideal gas and using periodic boundary conditions.

Depending on the goals of the instructor for use of this activity, these selections can be explained fully or minimally. My preference is that the students understand that periodic boundary conditions are a mechanism for replicating the box in all dimensions, therefore mimicking bulk-like behavior by allowing particles to pass through one edge of the box and reappear on the other side as if the boundary did not exist. I also explain that the other Potential Models in the software allow modeling of real gas behavior and how real gases differ from ideal gases on a general chemistry level, i.e. real gases have volume and experience intermolecular forces. Beyond that, I do not discuss in detail the different options for real gas potential models.

Once the Virtual Substance is built using the process outlined in the previous paragraph, the next step is to run the simulation. Once again, the instructor can choose how much or how little detail is necessary for the student to understand the simulation. The user must select the type of simulation (constant energy, constant volume and temperature, or constant temperature and pressure), targets for that selected simulation type, time step (0.5, 1.0, 2.0, 5.0, or 10.0 fs), number of steps (500, 1000, 2000, 5000, 10000, 20000), and how frequently the calculations should be reported to the user.

After building the Virtual Substance and selecting the simulation settings, the user selects Run Simulation, and the data appears in an output screen (Figure 2a) while the movement of the substance is observed in another part of the screen (Figure 2b). A typical simulation of an ideal gas on a personal computer will take under a minute.

Figure 2. Screenshot of Virtual Substance a) simulation parameters for 128 Argon gas particles treated as an ideal gas with periodic boundary conditions after 120 ps of Molecular Dynamics Simulation under conditions of constant volume (1.0 L/mol) and temperature (298 K) and b) static image at the conclusion of the simulation. Instantaneous and average values of the temperature, pressure, volume, and total, kinetic, and potential energy are reported.

In the assigned activity, all students are required to run five separate simulations at a fixed temperature and a series of molar volumes. They are then required to prepare Pressure versus molar Volume, V_m , (see Figure 3) and Pressure vs V_m^{-1} plots and determine the value of the gas constant, R . I do not tell them how to numerically determine R , which results in guided discussion in class as students ask about that part of the assignment. How to proceed after making plots is not immediately obvious to many students. After our in-class discussion, students typically choose to use a linear fit of their Pressure vs V_m^{-1} plot to determine R (the slope of the trendline is RT), but some students will perform a fit to the curve from their Pressure vs V_m^{-1} plot and determine R from the equation of that fit. For example, in Figure 3, the fit yields $P = (24.375) V_m^{(-1.003)}$ for simulations conducted at 298 K. Using $P = RT/V_m$, the calculated value of R would be $0.0818 \text{ L atm mol}^{-1} \text{ K}^{-1}$, an error of less than 1% from the accepted value of $0.0821 \text{ L atm mol}^{-1} \text{ K}^{-1}$. This level agreement is the norm, which does give students some comfort that they are on the right track.

Students are subsequently asked to perform additional simulations of argon gas at either a fixed volume and a series of temperatures (still using a constant volume and temperature simulation) or a fixed pressure and a series of temperatures (using a constant pressure and temperature simulation). In both cases, students are again asked to determine the gas constant, R . In addition, students are required to plot the average kinetic energy as a function of temperature. See Figure 4. If appropriate to the class, instructors could point out that the slope of the energy vs temperature plot is $3/2 R$ and discuss the equipartition theorem demonstrating the three translation degrees of freedom each contributing $1/2 R$.

Students are also asked to submit a coherent paragraph that includes their observations of the gas motion, how visualizing this motion impacted their understanding of gas behavior, an interpretation of their results (are they consistent with what was expected), and any unusual results. The paragraph was evaluated holistically for patterns of both clarity and misunderstandings.

Figure 3. Student-submitted plot for Virtual Substance simulation of Argon at 298 K and a series of molar volumes. The line, which is the best fit by least squares regression, is $y = 24.375x^{-1.003}$, where y is pressure in atmospheres and x is volume in L/mol, with correlation coefficient 0.9999.

Figure 4. Student-submitted plot for Virtual Substance simulation of Argon at fixed pressure and a series of temperatures. The line, which is the best fit by least squares regression, is $y = 12.372x + 12.535$, where y is average kinetic energy in J mol^{-1} and x is temperature in Kelvin, with correlation coefficient 0.9999.

Conclusions

Impact on Student Learning

Student learning was evaluated using three measures: 1) the submitted assignments, 2) a pre/post set of 6 clicker questions (see Table 1), and 3) relevant questions on the final exam. The results showed distinct improvements in students' understanding of gas motion and the connection between that motion and the physical properties of pressure, temperature, volume, and kinetic

energy. There were clearly areas where student misconceptions were still evident even after the visualization activity, however.

In the submitted assignments, students were able to collect the appropriate data and generate the requested plots (representative plots shown in Figures 3 and 4). They were able to follow the instructions in the assignment sheet easily. In their summary paragraph, many students stated that they were able to understand and make connections more clearly as a result of visualizing gas particle behavior and the relationship between physical properties. Representative statements from students include the following

- “Being able to watch the simulations enhanced my ability to understand the concepts behind the math associated with the ideal gas law.”
- “It was helpful to me because I am a visual learner and when I see things it makes me understand them more thoroughly.”
- “The visualization of the movement of gasses showed the random nature of the movement of the gases in a way that describing it does not.”
- “I could see the relationships in the gas law physically in action which helped me to form more realistic connections in understanding the material.”

In the post-activity clicker questions, most students were able to identify the correct static image of gas particles distributed throughout a container, select the correct relationships between volume and pressure (inversely proportional) and volume and temperature (directly proportional), and relate pressure to macroscopic and molecular-level relationships. In the 2017 class, 65% of students showed improved scores on the clicker questions after completing the MD activity. As shown in Table 1, improved scores were primarily due to increased understanding of relationships between gas properties.

Parts of their paragraphs describing their observations along with the questions they answered incorrectly on the post-activity clicker questions highlighted their continued misunderstandings on some of the important physical relationships, particularly among kinetic energy, average velocity, and temperature. While they were able to make a plot showing that kinetic energy and temperature are directly proportional (Figure 4), they did not understand that kinetic energy was related to particle velocity. We had not yet studied the Maxwell-Boltzmann distribution relating particle velocity to temperature, and some students made incorrect statements that the particles were moving faster or slower when pressure or volume changed while temperature was held constant. These statements are, of course, incorrect. Perhaps the computer was refreshing less frequently or they felt that they were seeing the particles move more slowly, but the average kinetic energy at constant temperature was constant, so their perceptions were incorrect. This misconception was very enlightening to me as an instructor. When we arrived at kinetic-molecular theory and the Maxwell-Boltzmann distribution, I opened the Virtual Substance program and ran a simulation for the entire class. We talked about the distribution of particle speeds and how that depended solely on temperature for an ideal gas. They had a context for understanding the new material, which is always helpful for learning and retaining knowledge.

Table 1. Clicker Question Summary. Note that this clicker set allows multiple selections per question.

Clicker Question	Pre- to Post-Test Results
1. Which image represents particles distributed in a container?	No change: most answered correctly in pre-test.
<p>A) B) C) D)</p>	
2. What happens to particle speed when gas is added isothermally to a container?	Increase in correct answers
A) Increase, B) Decrease C) Remain the Same	
3. Which is the correct plot of <i>volume</i> vs <i>pressure</i> ? A) Linear plot B) Inverse relationship	Increase in correct answers
4. Which is the correct plot of <i>volume</i> vs <i>temperature</i> ? A. Linear plot B. Inverse relationship	Increase in correct answers
5. What are the differences between real and ideal gases?	No change: many students had an extra response in addition to the correct options of C and D.
A) Real gases move faster B) Ideal gases have no collisions C) Real gases have size, where ideal gases are point masses D) Real gases have attractive and repulsive interactions	
6. Gas Pressure is	Increase in correct answers
A) a measure of force per unit area. B) independent of temperature. C) the result of collisions between particles and the walls of the container. D) the result of an external force.	

Extensions and Challenges

While my classes are relatively small, this activity can easily be used with larger classes. Most of the work is performed independently. The instructor will need to review student submissions, but there is no additional equipment or preparation required. Variations on data collected and plots prepared are endless depending on the goals of the instructor. As mentioned earlier, other topics at the general chemistry level can be clarified by use of Virtual Substance simulations, for example, how non-zero volume and intermolecular forces (i.e. those in real gases) impact physical properties of pressure and internal energy, or a more explicit understanding of internal energy as the sum of kinetic and potential energy, just to name two. If more insight into how the least squares fit is used to create a trendline, activities such as the Multi-Function Data Flyer (17) could be used.

The challenges associated with this activity are the same as those associated with teaching in general: students arrive with preconceived ideas about a topic. Some students are resistant to activities that challenge their preconceived ideas and will continue to cling to those instead. Technical difficulties have been relatively minimal. Access to a PC is required, but the software works on a variety of machines and operating systems, including Windows 10. Installing and running several

simulations of ideal gases should take less than 30 minutes. Simulations using a Lennard-Jones potential will take longer, and may be better suited to homework assignments or lab activities (16).

The activity itself is usually one students enjoy. When I ask what component of the course was most helpful for their learning, the visualization activities are consistently rated very highly. As I hope is clear from the collection of chapters in this book, computational chemistry is just one tool in the arsenal to improve student learning. It is not a magic bullet. It is another way to aid learners in developing a molecular-level understanding of chemical behavior that will serve them well as they move from novice to professional chemist.

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