

Credits

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Chapter 1: Gas Laws

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1.0 Overview

This is a 2 ½ week unit designed to cover high-school and introductory college level topics in the properties of gases and gas particle behavior. The unit includes thirteen activities. Seven of the activities use computer models to explore these topics in greater depth and using a greater degree of student inquiry and guided discovery than would be typically possible through other learning activities in the same amount of time.

The computer models enable students to investigate what causes pressure in a gas, how it is measured, and how it is affected by the properties of the particles that make the gas and the characteristics of the container they are in. Students are encouraged to understand how the principles and effects of pressure are generated from specific interactions between many particles (or simplified gas molecules) and with their environment. To do this, students gain a familiarity with a microscopic view of the gas particles by running many different computer models of systems of gas particles. Some initial models are designed for orienting the student to the NetLogo interface, others are designed for specific data gathering and data analysis tasks, and others are designed for more open ended inquiry and experimental design.

The later computer models focus on how particles behave in a variety of conditions. Such conditions include varying the number of particles, the size of the particles, the speed of the particles, and the location of solid walls they bounce off. These variations support students explorations of the models to design new variations into the model (adding new rules for particle behavior, designing new system boundaries), designing experiments and testing predictions with the models, and deriving mathematical models (symbolic representations of relationships that they find in graphs and table they build from data they gather in their experiments). The mathematical modeling of relationships between variables such as the number of gas particles, the temperature of a gas, the volume of the gas container, gas constants, and the pressure of the gas, helps students to progressively expand and derive the gas laws from experimental data. This mathematical modeling focus, helps students bridge the symbolic representations of the gas laws, to experimental data, to particle behavior.

The non-computer based activities ask students to apply ideas and relationships learned in class, extend the predictions of these relationships to new situations that they experience every day, and connect previous and upcoming concepts to their understanding of particle behavior (Kinetic Molecular Theory) and to broader cross cutting themes in science. Some of the broad cross cutting themes include building and using scientific models, systems thinking, data analysis, and change and equilibrium.

These activities will build a deep and intuitive sense of particle behavior that will extend readily to other chemistry topics. In particular, the behavior of particles in chemical reactions becomes easy to envision and predict the outcome of the interactions of molecules, even when the reactants are in solid or liquid form. This is because many of the concepts related to chemical reactions rely on an understanding of the number of molecules, volume, and temperature, and pressure.

2.0 Unit Organization

Activity One: Everyday Objects

This Activity introduces students to three real-world events/objects that will serve as anchoring activities for the rest of the Activity. An explanation of the behavior of these event/objects requires an understanding of gas particle behavior, which students will develop throughout the unit.

The first object is a bike tire. The bike tire is inflated with air. Students are asked to consider what is happening inside the bike tire as it is being inflated. The bike tire serves as the system which will be initially modeled and explored on the computer. The second object is an air filled syringe, sealed at both ends. It exhibits discrepant behavior as the plunger is depressed. Students are asked to consider why the syringe can be partially depressed, but can't be fully depressed. The third object is an open and nearly empty soda can that is heated and subsequently dunked upside down into cold water. When this happens the soda can implodes.

Each of the event/objects introduced in class and in the student homework help elicits student preconceptions about pressure, gasses, and molecular models of matter.

Activity Two: Modeling A Tire

This Activity introduces students to the representations of gas particles used in the computer models. The Activity explains the assumptions of the computer model and enables students to investigate the rules that underlie individual gas particle behaviors, while constructing a representation of a bike tire filled with air.

Students first focus on the objects and parts of the bike tire system. Then they look at a simple model of the bike tire, observing the particles that make up the gas inside the bike tire. They then learn the rules that govern their behaviors and interactions by adding the rules into the model one-by-one. While observing the consequences of "running" these rules and the resulting motion of the particles.

In this model students gain a familiarity with a microscopic view of the system and with the NetLogo model interface they will use again in later activities. This familiarity is a critical learning goal in the first Activity, since the use of computer interface (buttons, sliders, switches, etc...) becomes progressively more sophisticated in future activities.

Finally, students compare the assumptions of the computer-based model with those of Kinetic Molecular Theory and are introduced to the concept of gas pressure and real-world pressure measurements.

Activity Three: Changing Pressure

Students investigate what causes pressure at a microscopic level and how it is measured in the computer model. Students observe the effects of pumping up a tire with air by adding particles through a valve in the tire. They notice how this particle addition effects pressure, paying particular attention to the dynamics of the system, including changes, stability, and equilibrium in the system and how these are related to the particles' behaviors.

This type of complex systems thinking is prevalent in all NetLogo particle models and is necessary in later activities. For example, students learn to interpret time series data from graphs and make estimates of average values from these in NetLogo. Students learn to watch for and interpret delayed effects in the response of the system. Students consider the tradeoffs of building approximate models of systems versus more detailed models of systems. And students are introduced to the concept of scientific visualizations.

Activity Four: Experimenting with Particles

Students are first introduced to an array of new tools that enable the control and visualization of very specific particle properties. For example, these tools allow the students to track individual particles, control the direction and speed of particles, and color and label the particles.

Collisions of individual particles are investigated up close in this Activity, so that students can see how the outcome of particle collisions is dependent on the particles' speeds and directions. The outcome of the collision is connected to the concept of conservation of kinetic energy.

Students are then guided through an Activity of whether the particles' individual and average speed affects the pressure. Lastly, students design their own Activity related to particle pressure, such as exploring the effects of changes in particle mass on pressure or direction of travel on pressure. Students are asked to propose an explanation of particle actions and interactions that would explain this. This explanation builds on the dynamic nature of the system and the cascading chain of cause and effect in multiple particle collisions.

Activity Five: Number and Pressure

Students investigate the quantitative relationship between the number of particles in a container and the pressure inside. Students collect data from the model and develop a mathematical model of the relationship. From a graph they create, they note that the relationship between this number and pressure is a linear one and develop an algebraic representation (a linear equation) of this relationship.

Students are introduced to the idea of the average number of wall hits per particle and they find out that this value is independent of the number of particles. This finding is connected back to the linear equation the student discovered and shown that such a finding is predicted by the previous equation. The connection between the average number of wall hits per particle and the slope of the linear equation is explained and students are shown how such constants can be calculated in a linear relationship. Students then use the equation to predict and test their prediction for new pressure values.

Lastly, students reflect on many of the assumptions that they are now more familiar with in the computer model vs. the real system (a real bike tire) at this point.

Activity Six: Temperature and Pressure

Students investigate the quantitative relationship between temperature and pressure. Students explore the connection between the temperature of the gas and the average particles' speed, the connection to the concept of thermal equilibrium, and are introduced to the Kelvin temperature scale.

Students collect data and develop a mathematical model of the relationship between temperature and pressure, noting that the relationship is a linear one. Students note the similarities between this relationship and the one for the number of particles and the pressure of the gas. They then explore how both the number of particles and their temperature simultaneously affect the pressure of the gas and see how a more complex equation relating temperature, number, and pressure might be reasoned out. Students use the equations they develop to make predictions about what the pressure will be for different number and temperature combinations. Students make connections to conduction and convection as heat transfer mechanisms and begin to predict what would happen to gas pressure in a situation where there is a smaller volume gas container.

Activity Seven: Measuring and Modeling the Syringe

Students conduct a real world data gathering laboratory with they syringe. They measure the volume of the syringe and the weight or load on the syringe plunger. Then they develop a mathematical model of the relationship between volume and weight on the plunger, noting that the relationship is a not a linear one.

Lastly they try to develop mental models of what the particles are doing in the syringe that could account for the observed relationship. This is the first Activity where students are trying to explain real world phenomena using their particle model, before seeing a computer model that explains it.

Activity Eight: Volume and Pressure

Students continue their Activity of the quantitative relationship between volume and pressure, now with a computer model. Students are introduced to how the volume of a container is represented in the model. Particle density is used as a way to relate what students can easily visually observe in the model to the number of gas particles and the volume of the container.

Students also explore the temperature gradient that emerges from adiabatic expansion, again connecting these phenomena back to fundamental properties and interactions between the particles.

Students collect data and develop a mathematical model of the volume and pressure relationship, noting that the relationship is an inverse one (Boyle's Law). Students extend this mathematical model, by collecting data from a computer model of a container with a variable volume to develop both an algebraic equation that relates volume and pressure and then also one that relates number of particles and volume to pressure.

Students use the equations they develop to make predictions about what the pressure will be for different number and pressure combinations. Lastly students calculate pressure for a real world problem without the model.

Activity Nine: Ideal Gas Law

In this Activity, students connect all their previous mathematical modeling work. Students are asked to design an experiment to maximize the pressure in a container, where they can change the number of particles, the temperature of the gas, and the volume of the container. They are then guided through a qualitative and quantitative development of the ideal gas law through reasoning about particle behavior, studying their recent data, looking at previously developed equations, and reflecting on their findings from the first experiment in this Activity which gives a qualitative sense of how the variables are related. Students compare their derivation with the actual equation and they then use the Ideal Gas Law to predict pressure values for different variable combinations. Lastly they test their predictions using the model.

Activity Ten: Modeling New Systems

Students are asked to use an open interface in the model to construct a representation of diffusion of perfume from a bottle. After orientation to this "sketch up" style interface that permits a wide range of ways to draft out new system representations, students are given the opportunity to draw a model of a real world system (or create a model and then argue what

real world system it might model). After drawing the model, students can then run the model and gather observations about the behavior of the particles in this system.

This Activity encourages students to start thinking about modeling almost any system with gas particles in it, with the computer, and thinking about how such modeling could be done. This mental construction of a particle based representation of a system is a key milestone to having achieved a thorough sense of what particles would do in any system that undergoes some state change.

Activity Eleven: Modeling Engines

This Activity poses some exciting challenges for students to apply their growing literacy of the particle model. They are asked to connect their understanding of temperature and volume effects on pressure to gas behavior in a new context. They learn about the historical evolution of engines and then are asked to explore and explain steam engines and internal combustion engines using their particle model of gas pressure, volume, and temperature.

Lastly they try to show a model of what the particles are doing in the syringe that could account for the observed relationship. This is the first Activity where students are trying to explain real world phenomena using their particle model, before seeing a computer model that explains it. It is also the first Activity which encourages the students to think about the system transitioning between different "system states/stages".

Activity Twelve: Modeling Discrepant Events

Students review the first two discrepant events they saw in the first Activity (the bike tire and syringe) and activate their previous knowledge about particle behavior, but this time think about the system from a "macroscopic change" results in what microscopic change in the system that accounts for a new macroscopic change. This thinking serves as a conceptual bridge between thinking about what particles do as a system moves between different systems states/stages.

Students use the "system state/stage" thinking to break down the imploding soda can phenomena from the first Activity into five states/stages. At each stage students use both symbolic manipulation of the ideal gas law to solve the predicted change that would occur in the system and use a semi-quantitative particle behavior based reasoning to predict what would happen.

Activity Thirteen: Ideal Gas Applications

Students explain the particle behavior and solve the predicted outcome of various ideal gas applications using both symbolic manipulation of the Ideal Gas Law and a visual representation of what gas particles are doing in these new applications.

3.0 Learning Objectives and National Standards

Alignment to National Math and Science and Mathematics Standards (NSES – National Science Education Standards, and AAAS – Project 2061 Benchmarks for Science Literacy, and NCTM – National Council of Teachers of Mathematics)

The learning objectives in this unit describe what the students should be able to know and do in the unit and the manner in which they are doing it. They were designed from an alignment of one or more content standards and to one or more inquiry standards in science and mathematics. Content standards describe important ideas that students should understand. Inquiry standards describe important skills and processes that students should be engaged in. Each of the learning objectives, and the related alignment to content standards and inquiry standards, are categorized into one of seven related strands. These strands are:

- 1) The Nature of Matter
- 2) Connecting Microscopic and Macroscopic Understanding
- 3) Systems Thinking
- 4) Scientific Models
- 5) Energy
- 6) Mathematical Models
- 7) Algebra, Scale, and Ratio

THE NATURE OF MATTER:

Learning Objectives:	Content Standards:	Inquiry Standards:
Draw and describe molecular epresentation of various states of matter, particularly gasses.	students should become familiar with characteristics of different states of matter-now including gases All matter is made up of atoms, which are far too small to see directly	Regardless of the scientific investigation performed, students must use evidence, apply logic, and construct an argument for their
Compare and contrast the behavior of gas particles in a computer model to those of an ideal gas.	through a microscope. The atoms of any element are alike but are different from atoms of other elements. Atoms may stick together in well-defined molecules or may be packed together in large arrays. Different arrangements	proposed explanations.
Describe the behavior and interactions of gas particles through time in a variety of situations.	of atoms into groups compose all substances.	

CONECTING MICROSCOPIC AND MACROSCOPIC UNDERSTANDING:

Learning Objectives:	Content Standards:	Inquiry Standards:
Describe how particle density is related to number of particles and size of gas container	High-school students develop the ability to relate the macroscopic properties of substances that they study in grades K-8 to the microscopic structure of substances. This	Solve simple problems involving rates and derived measurements for such attributes as velocity and density.
Describe how frequency of wall hits is related to particle speed, number of particles, and size of gas container, and the pressure of the gas.	development in understanding requires students to move among three domains of thoughtthe macroscopic world of observable phenomena, the microscopic world of molecules, atoms, and subatomic particles, and	Formulate a testable hypothesis and demonstrate the logical connections between the scientific concepts guiding
Connect real-world representations of force	the symbolic and mathematical world of chemical formulas, equations, and symbols.	a hypothesis and the design of an
and pressure to representations in the models.	The relationship between properties of matter and its structure continues as a	Regardless of the scientific investigation performed, students must
Connect particle behavior to macroscopic properties of the gas.	major component of study in 9-12 physical science	use evidence, apply logic, and construct an argument for their proposed
Connect symbolic representations of pressure, temperature, volume, and particle number to model representations and to real-world measurements.		Student inquiries should culminate in formulating an explanation or model. Models should be physical, conceptual, and mathematical

SYSTEMS THINKING:

Learning Objectives:	Content Standards:	Inquiry Standards:
Explore and describe the relationships between the objects and properties in the model to understand changes, stability, and other emergent behaviors and interrelationships in particle based systems.	Physical and [biological] systems tend to change until they become stable and then remain that way unless their surroundings change.A system may stay the same because nothing is happening or because things are happening but exactly counterbalance one another.	Use representations to model and interpret physical, social, and mathematical phenomena. Weigh the evidence and examine the logic so as to decide which explanations and models are best.
Describe how changes in the properties, boundary conditions, and parameters affect the behavior of the particles (macro→ micros) Describe how changes in the objects and relationships between objects in the system affect the system properties. (micro→ macro)	A system can include processes as well as things; A system usually has some properties that are different from those of its parts, but appear because of the interaction of those parts. A system in equilibrium may return to the same state of equilibrium if the disturbances it experiences are small. But large disturbances may cause it to escape that equilibrium and eventually settle into some other state of equilibrium. Things can change in detail but remain the same in general (the players change, but the team remains; cells are replaced, but the organism remains). Sometimes counterbalancing changes are necessary for a thing to retain its essential constancy in the presence of changing conditions.	Regardless of the scientific investigation performed, students must use evidence, apply logic, and construct an argument for their proposed explanations. Implement solutions using computer software. The investigation may also require student clarification of the question, method, controls, and variables.

SCIENTIFIC MODELS:

Learning Objectives:	Content Standards:	Inquiry Standards:
Explain the rules of the computer model. Compare and contrast	Students should be introduced to the roles of models and simulations	Demonstrate thoughtful planning for a piece of technology or technique.
the computer models rules and limitations with those of a real life situation.	Models are often used to think about processes that happen too slowly, too quickly, or on too small a scale to observe directly, or that are too vast to be changed	Use representations to model and interpret physical, social, and mathematical phenomena.
Create and test computer model for new real world situations.	deliberately, or that are potentially dangerous. Different models can be used to represent the same thing. What	Weigh the evidence and examine the logic so as to decide which explanations and models are best.
	kind of a model to use and how complex it should be depends on its purpose? The usefulness of a model may be limited if it is too simple or if it is needlessly complicated.	Regardless of the scientific investigation performed, students must use evidence, apply logic, and construct an argument for their proposed explanations.
	Computers have greatly improved the power and use of mathematical models by	Implement solutions using computer software.
	performing computations that are very long, very complicated, or repetitive. Therefore computers can show the consequences of applying complex rules or of	The investigation may also require student clarification of the question, method, controls, and variables.
	changing the rules. The usefulness of a model can be tested by comparing its predictions to actual observations in the real world.	demonstrate the logical connections between the scientific concepts guiding a hypothesis and the design of an experiment.
		Demonstrate appropriate procedures, a knowledge base, and conceptual understanding of scientific investigations.
		A variety of technologies, should be an integral component of scientific investigations. The use of computers for the collection, analysis, and display of data
		Student inquiries should culminate in formulating an explanation or model.

ENERGY:

Learning Objectives:	Content Standards:	Inquiry Standards:
Learning Objectives: Describe what it means for kinetic energy to be conserved in a particle collision. Describe how heat/energy is transferred through particle collision (conduction) with other particles or with heated surfaces and through bulk movement (convection) of particles to new locations.	Content Standards: Energy can be transferred by collisions However, it can never be destroyed. All energy can be considered to be either kinetic energy, which is the energy of motion; or Heat consists of random motion and the vibrations of atoms, molecules, and ions. The higher the temperature, the greater the atomic or molecular motion. Everything tends to become less organized and less orderly over time. Thus, in all energy transfers, the	Inquiry Standards: Regardless of the scientific investigation performed, students must use evidence, apply logic, and construct an argument for their proposed explanations.
	overall effect is that the energy is spread out uniformly. Examples are the transfer of energy from hotter to cooler objects by conduction, radiation, or convection and the warming of our surroundings	

MATHEMATICAL MODELS:

Learning Objectives:	Content Standards:	Inquiry Standards:
Sketch and graph changes in properties of a system over time. Describe reasons for	Most systems above the molecular level involve so many parts and forces and are so sensitive to tiny differences in conditions that their precise behavior is unpredictable, even if all	Understand line graphs use them to display data The use of computers for the collection, analysis,
Describe reasons for why larger samples result in less error in measurement or estimation in general Graph two variable data from experiments. Describe the relationship between the two variables in data in a table, graph, and equation. Identify the best fit parent function of a relationship of two variables from experimental data on a graph Reason about the meaning of the y- intercept and the slope of a linear relationship for gas system properties (number and pressure, temperature and pressure)		the collection, analysis, and display of data build new mathematical knowledge through problem solving; solve problems that arise in mathematics and in other contexts; apply and adapt a variety of appropriate strategies to solve problems perform ransformations such as arithmetically combining, composing, and inverting commonly used functions, interpret representations of functions of two variables analyze functions of one variable by investigating rates of change, intercepts, The use of computers for the collection, analysis, and display of data Student inquiries should culminate in formulating an explanation or model. Models should be physical, conceptual, and mathematical Recognize and apply
		mathematics in contexts outside of mathematics.

ALGEBRA, SCALE, AND RATIO:

Learning Objectives:	Content Standards:	Inquiry Standards:
(Algebra, Scale, and		
Ratio)	Symbolic equations can be used to	build new mathematical
_	summarize how the quantity of	knowledge through
Develop, manipulate,	something changes over time or in	problem solving; solve
and solve for unknown	response to other changes.	problems that arise in
values in symbolic		mathematics and in other
representations	Symbolic statements can be	contexts; apply and adapt
between the number of	manipulated by rules of mathematical	a variety of appropriate
particles, temperature	logic to produce other statements of	strategies to solve
of a gas, the volume of	the same relationship, which may	problems
a gas container, and the	show some interesting aspect more	
pressure of the gas.	clearly. Symbolic statements can be	Student inquiries should
	combined to look for values of	culminate in formulating
Use ratios between two	variables that will satisfy all of them at	an explanation or model.
variables to reason	the same time.	Models should be
about the how another		physical, conceptual, and
variable or constant	Any mathematical model, graphic or	mathematical
would change and test	algebraic, is limited in how well it can	Lice retice and
the values predicted by their calculations in a	represent how the world works. The usefulness of a mathematical model	Use ratios and proportions, including
model.	for predicting may be limited by	constant rates, in
model.	uncertainties in measurements, by	appropriate problems.
Use symbolic	neglect of some important influences,	appropriate problems.
representations and/or	or by requiring too much computation.	Find answers to problems
quantitative reasoning	or by requiring too match computation.	by substituting numerical
to predict the change in	When a relationship is represented in	values in simple algebraic
pressure, with a change	symbols, numbers can be substituted	formulas and judge
in one variable (e.g.	for all but one of the symbols and the	whether the answer is
number), two variables	possible value of the remaining symbol	reasonable by reviewing
(e.g. number and	computed.	the process and checking
temperature), and three	•	against typical values.
variables (e.g. number	Judge the meaning, utility, and	5 71
and temperature and	reasonableness of the results of	Consider the possible
volume)	symbol manipulations	effects of measurement
		errors on calculations
Apply appropriate	Recognize and apply mathematics in	
strategies to solve and	contexts outside of mathematics.	
predict the outcome of		
state changes in ideal		
gas situations.		

4.0 Suggested Timeline

This twelve to fourteen activity sequence is designed to allow a 45-50 minute class period for each activity. This puts the length of the unit at 12-14 class periods. The computer icon next to each activity represents that the activity will need to occur in a computer lab (recommended two to a computer) and/or on a classroom set of computers. The following represents a suggested timeline:

Week One:

One class period – Activity 1: **Everyday Objects** One class period – Activity 2: **Modeling A Tire**** Homework 2: approx. 20 minutes

One class period – Activity 3: **Changing Pressure** Homework 3: approx. 30 minutes

One class period – Activity 4: **Experimenting with Particles** Homework 4: approx. 5 minutes

One class period – Activity 5: **Number and Pressure** Homework 5: approx. 30 minutes

Week Two:

One class period – Activity 6: **Temperature and Pressure** Homework 6: approx. 30 minutes

Two class periods – Activity 7: **Volume and Pressure** Homework 7: approx. 30 minutes

One class period – Activity 8: **Ideal Gas Law** Homework 8: approx. 45 minutes ***

One class period – Activity 8: Use a class period to review Ideal Gas Law Homework

Week Three:

One class period – Activity 9: **Modeling Real World Systems** Homework 9: approx. 20 minutes

One class period – Activity 10: **Ideal Gas Applications** Homework 10: approx. 45 minutes ***

One class period – Activity 10t: Use a class period to review Ideal Applications Homework

**Classes already familiar with NetLogo, may wish to compact or skip Activity 2: Modeling A Tire.

*** Questions similar to the qualitative and quantitative questions in both of these homework assignments could also be created as a student assessment.

5.0 Using Homework

Homework assignments in this unit are designed to apply, connect, and extend important ideas and skills between lessons. Teacher's may wish to assign additional supplemental homework, but each of the homework assignments provided, cue students into ways to think about and reflect on what they are learning in class. The connection between microscopic behavior of particles and macroscopic mathematical relationships is stressed in the homework. And the connection between in class labs and computer activities and real world applications is also stressed.

It is important that students review the homework before beginning each lesson. One very effective way to do this is to provide students approximately five minutes to review their answers to the homework with a partner. It is important to make this review a required part of the homework assignment, as consensus with another student helps provide students a sense of certainty and self-confidence, that what they are discovering in in-class investigations, is being applied correctly when they try to apply those discoveries independently.

Only questions that the partner and they can not resolve should be set aside by the students for further whole class discussion. Then, at the end of this period, students can ask about homework problems that they are still uncertain about. A brief review of answers for those problems should take only a few more minutes.

This sort of homework review is an excellent primer for the class activities, since many of the homework questions are designed to help students organize their ideas and mental models they will need to use in the upcoming activity in class.

6.0 Technology

The models used in this unit are included with the latest **NetLogo** release. **NetLogo** is a programmable modeling environment for simulating natural and social phenomena. It is particularly well suited for modeling complex systems developing over time. Modelers can give instructions to hundreds or thousands of independent "agents" all operating concurrently. This makes it possible to explore the connection between the micro-level behavior of individuals and the macro-level patterns that emerge from the interaction of many individuals.

NetLogo lets students open simulations and "play" with them, exploring their behavior under various conditions. It is also an authoring environment which enables students, teachers and curriculum developers to create their own models. NetLogo is simple enough that students and teachers can easily run simulations or even build their own. And, it is advanced enough to serve as a powerful tool for researchers in many fields.

NetLogo has extensive documentation and tutorials. It also comes with a Models Library, which is a large collection of pre-written simulations that can be used and modified. These simulations address many content areas in the natural and social sciences, including biology and medicine, physics and chemistry, mathematics and computer science, and economics and social psychology. Several model-based inquiry curricula using NetLogo are currently under development.

NetLogo can also power a classroom participatory-simulation tool called HubNet. Through the use of networked computers or handheld devices such as Texas Instruments (TI-83+) calculators, each student can control an agent in a simulation.

NetLogo is the next generation of the series of multi-agent modeling languages that started with StarLogo. It builds off the functionality of this product and adds significant new features and a redesigned language and user interface. NetLogo is written in Java so it can run on all major operating systems on most types of computers (Macs, Windows, Linux, et al). It is run as a standalone application. Individual models can be run as Java applets inside a web browser.

Each computer that is used by the class will need to have this installation of NetLogo on them. It is recommended to have one computer for every two students.

Please see <u>http://ccl.northwestern.edu/netlogo</u> to download the latest version of the software.

It is highly recommended that the teacher complete the tutorials that come in **NetLogo** become familiar with the interface and operation of the program, before looking at the section on General Model Information. These tutorials are included with the software when it is installed on your computer and are also available at http://ccl.northwestern.edu/netlogo/docs/

All the models for this unit can be found in the Models Library of **NetLogo** under the folder for Curricular Models/ConnectedChemistry

6.1 General Model Information

LIST OF THE MODELS:

Connected Chemistry Modeling A Tire.nlogo – used in Activity Two Connected Chemistry Changing Pressure.nlogo – used in Activity Three Connected Chemistry Experimenting with Particles.nlogo – used in Activity Four Connected Chemistry Number and Pressure.nlogo – used in Activity Five Connected Chemistry Temperature and Pressure.nlogo – used in Activity Six Connected Chemistry Volume and Pressure.nlogo – used in Activity Seven Connected Chemistry Ideal Gas Law.nlogo – used in Activity Eight Connected Chemistry Gas Particle Sandbox.nlogo – used in Activity Nine

Each NetLogo computer model has the information shown below listed in the information tab in the model. For easy reference, we have included a screen shot of each model interface when the model loads and the information tab for that model.

LOCATION OF THE MODELS:

The models are located in the NetLogo Models Library. To open a model:

- 1. Start NetLogo
- 2. Under the File option menu, select Models Library.
- 3. In the dialog window that opens, select: Curricular Models > Connected Chemistry

The models are located in this folder. Select a model and it will open.

HOW THEY WORK:

Most of the models in the curriculum use the same basic rules for simulating the behavior of gases. And, each model highlights different features of how gas behavior is related to gas particle behavior.

The basic principle gas particle behavior in all of the models is that gas particles are assumed to have two elementary actions: they move and they collide - either with other particles or with any other objects such as walls.

Particles behave according to the following rules:

1. A particle moves in a straight line without changing its speed, unless it collides with another particle or bounces off the wall.

2. Two particles "collide" if COLLIDE switch is on and they find themselves on the same patch (the world is composed of a grid of small squares called patches).

3. A random axis is chosen, as if they are two balls that hit each other and this axis is the line connecting their centers.

4. They exchange momentum and energy along that axis, according to the conservation of momentum and energy. This calculation is done in the center of mass system.

5. Each turtle is assigned its new velocity, energy, and heading.

6. If a turtle finds itself on or very close to a wall of the container, it "bounces" -- that is, reflects its direction and keeps its same speed.

NETLOGO FEATURES, EXTENDING THE MODEL, AND CITATIONS:

These topics are not summarized here. They are provided, however, in the information tab in each model file.

6.2 Specific Information About Each Model

CONNECTED CHEMISTRY BIKE TIRE.NLOGO MODEL

MODEL INTERFACE:

🖗 setup 🖗 place-box	▲ ↔ \$
number-of-particles-to-add 10	
👻 place-particles 👩	
🗑 go/stop 😄	
TOn collide?	
clock Number	
0 0	

WHAT IS IT?

This model introduces the behavior of gas particles in a simple of condition: trapped in a container with a fixed volume, such as a bike tire or free and unbounded.

In this model, the fixed volume container (represented by a box), can be drawn in different sizes and proportions. The number of particles added to the inside or the outside of the box can be changed by painting particles. And the rules of particle interactions (do they bounce off the walls? and do they collide with each other?) can be easily turned on and off).

This model helps students become acclimated to the user interface of NetLogo and evaluate modeling assumptions and representations, before they begin more analytical data analysis and mathematical modeling tasks associated with later models.

HOW IT WORKS

When the COLLIDE? switch is on, the particles are modeled as hard balls with no internal energy except that which is due to their motion. Collisions between particles are elastic. When the BOUNCE? switch is on, the particle will then bounce off the wall in an elastic reflection (angle of incidence equals the angle of reflection).

HOW TO USE IT

- 1. Press the SETUP button
- 2. Press the PLACE-BOX button. (A small gray dot will be drawn)

3. Click anywhere in the black portion of the WORLD & VIEW and a yellow box will be drawn to make a corner of it where you click.

- 4. Repeat steps 1-3 to draw different boxes.
- 6. If there is no yellow box in your model, repeat steps 1-3.
- 7. Press the PLACE-PARTICLES button. The button will remain a dark black color.
- 8. Click anywhere in the WORLD & VIEW to draw in some particles.
- 9. Press GO/STOP and observe what happens.

- 10. Turn the COLLIDE? switch off and repeat steps 7-9 and observe the effect.
- 11. Turn the BOUNCE? switch off and repeat steps 7-9 and observe the effect.

Initial settings:

- NUMBER-OF-PARTICLES-TO-ADD: the number of gas particles in the box when the simulation starts.

Monitors:

- CLOCK: the number of times the go procedure has been run
- NUMBER: the number of particles in the box

THINGS TO NOTICE

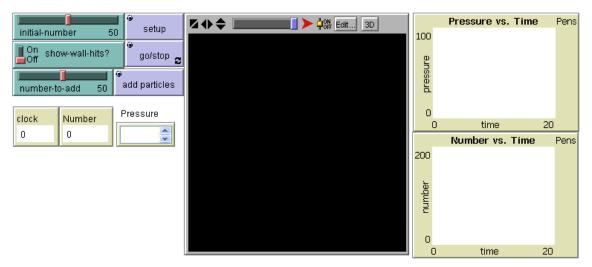
- Can you observe collisions with the walls as they happen (you can pendown a particle or slow down the model)? For example, do the particles change their color? Direction?
- In what ways is this model a correct idealization of kinetic molecular theory (KMT)?
- In what ways is this model an incorrect idealization of the real world?

THINGS TO TRY

- Turn the COLLIDE? switch off and repeat steps 7-9 and observe the effects.
- Turn the BOUNCE? switch off and repeat steps 7-9 and observe the effects.

CONNECTED CHEMISTRY CHANGING PRESSURE.NLOGO MODEL

MODEL INTERFACE:



WHAT IS IT?

This model explores the relationship between the number of gas particles and the pressure of a gas in a container with a fixed volume. The model simulates the effects of pumping up a bike tire.

In this model, the gas container (a bike tire represented by a box) has a fixed volume. The number of particles can be varied initially and by "pumping up the bike tire" by adding particles through a valve on the left wall of the box.

This model helps students study the representations of gas pressure in the model and the dynamics of the gas particles that lead to increases and decreases in pressure. In this model, students can also look at the relationship between number of particles and pressure. When the particles hit the walls they change their color temporarily. These models have been adapted from the model GasLab Pressure Box.

HOW IT WORKS

Particles are modeled as perfectly elastic particles with no energy except their kinetic energy - which is due to their motion. Collisions between particles are elastic.

HOW TO USE IT

-----Buttons:

SETUP - sets up the initial conditions set on the sliders.

GO/STOP - runs and stops the model.

ADD-PARTICLES - when pressed releases particles into the box while the simulation is running.

Sliders:

INITIAL-NUMBER - sets the number of gas particles in the box when the simulation starts. NUMBER-TO-ADD - the number of gas particles released into the box when the ADD-PARTICLES button is pressed. Choosers:

SHOW-SPEED-AS-COLOR? allows you to visualize particle speed using a color palette. The "blue-green-red" setting shows the lower half of the speeds of the starting population as blue, and the upper half as red.

The "violet shades" setting shows a gradient of dark violet to light violet for slow to fast particle speed.

The "all green" setting does not show a different color for each particle based on its speed.

Monitors:

CLOCK - number of clock cycles that GO has run.

NUMBER - the number of particles in the box.

PRESSURE - the total pressure in the box.

WALL HITS PER PARTICLE - the average number of wall hits in one clock tick

Plots:

PRESSURE VS TIME - plots the pressure in the box over time. NUMBER VS TIME - plots the number of particles in the box over time.

Initially, the particles are not moving. Therefore the initial pressure is zero. When the particles start moving, they repeatedly collide, exchange energy and head off in new directions, and the speeds are dispersed -- some particles get faster, some get slower. When they hit the wall they change their heading, but not their speed.

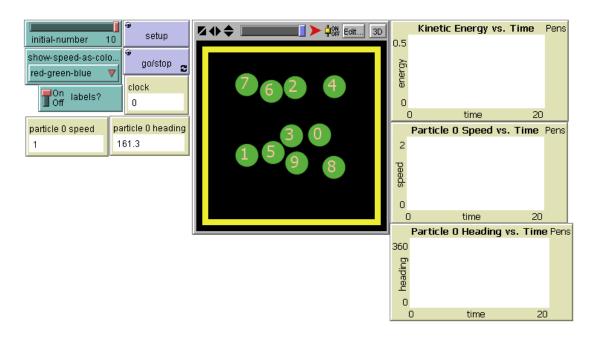
- 1. Adjust the INITIAL-NUMBER slider.
- 2. Press the SETUP button
- 3. Press GO/STOP and observe what happens.
- 4. Adjust the NUMBER-TO-ADD slider.
- 5. Press the ADD PARTICLES button.
- 6. Observe the relationship between the Number vs. Time graph and Pressure vs. Time.

THINGS TO NOTICE

- Can you relate what you can see happening to the particles in the box with changes in pressure?
- Why does the pressure change over time, even when the number of particles is the same? How long does it take for the pressure to stabilize?
- What happens to the wall hits per particle when particles are added to the box?
- In what ways is this model an incorrect idealization of the real world?

THINGS TO TRY

- You can pen-down a particle through the command center or by using the turtle menus. What do you notice about a particle's path when there more and less particles in the box?
- How can you make the measure monitor read 0?
- Why is there a delay between when particles are added (using ADD PARTICLES) and when the pressure goes up?
- Can you make the pressure graph smooth? Can you do it in more than one way?
- Sometimes, when going up in an elevator, airplane or up a mountain we feel a 'popping' sensation in our ears. This is associated with changes in pressure. Can you relate between this model and these changes in pressure? Are the temperature and volume constant in this situation?
- Pressure waves (expanding wavefronts of gas particles) are used to describe other phenomena in nature. What changes in the model could be made to represent pressure waves from explosions, sounds, breaking the sound barrier, etc...



CONNECTED CHEMISTRY CIRCULAR PARTICLES.NLOGO MODEL

WHAT IS IT?

This model explores the relationship between particle kinetic energies during particle collisions.

This model is different from the other Connected Chemistry and GasLab models in that the collision calculations take the circular shape and size of the particles into account, instead of modeling the particles as dimensionless points.

HOW IT WORKS

The model determines the resulting motion of particles that collide, with no loss in their total momentum or total kinetic energy (an elastic collision).

To calculate the outcome of collision, it is necessary to calculate the exact time at which the edge of one particle (represented as a circle), would touch the edge of another particle (or the walls of a container) if the particles were allowed to continue with their current headings and speeds.

By performing such a calculation, one can determine when the next collision anywhere in the system would occur in time. From this determination, the model then advances the motion of all the particles using their current headings and speeds that far in time until this next collision point is reached. Exchange of kinetic energy and momentum between the two particles, according to conservation of kinetic energy and conservation of momentum along the collision axis (a line drawn between the centers of the two particles), is then calculated, and the particles are given new headings and speeds based on this outcome.

HOW TO USE IT

INITIAL-NUMBER determines the number of gas particles used with SETUP. If the world is too small or the particles are too large, the SETUP procedure of the particles will stop so as to prevent overlapping particles.

SMALLEST-PARTICLE-SIZE and LARGEST-PARTICLE-SIZE determines the range of particle sizes that will be created when SETUP is pressed. (Particles are also assigned a mass proportional to the area of the particle that is created.)

Choosers:

SHOW-SPEED-AS-COLOR? allows you to visualize particle speed using a color palette. The "blue-green-red" setting shows the lower half of the speeds of the starting population as blue, and the upper half as red.

The "violet shades" setting shows a gradient of dark violet to light violet for slow to fast particle speed.

The "all green" setting does not show a different color for each particle based on its speed.

Monitors:

CLOCK - number of clock cycles that GO has run.

PARTICLE 0 SPEED - reports the speed for one of the particles (the first particle created that has a who value of 0)

PARTICLE 0 HEADING - reports the heading for one of the particles (the first particle created that has a who value of 0)

Plots:

KINETIC ENERGY VS TIME - plots the kinetic energy for two particles. If the model is run with only two particles for the INITIAL-NUMBER slider, then this graph will show that kinetic energy is conserved in collsions between these two particles.

PARTICLE 0 SPEED VS. TIME - plots the speed for one of the particles (the first particle created that has a who value of 0) over time.

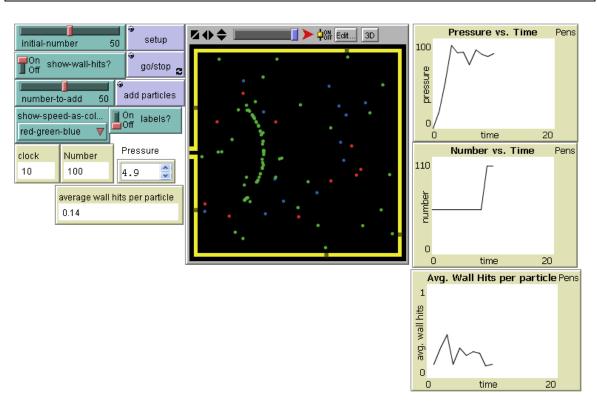
PARTICLE 0 HEADING - plots the heading for one of the particles (the first particle created that has a who value of 0) over time.

THINGS TO NOTICE

- Particles never overlap or penetrate into each other or the wall as they move about.
- For only two particles in the world, what do you notice about the kinetic energy of the particles before and after a collision?
- Does kinetic energy of a particle (e.g. particle 0) change when a particle hits the wall?

THINGS TO TRY

- Setting all the particles to have a very slow speed (e.g. 0.001) and one particle to have a very fast speed helps show how kinetic energy is eventually transferred to all the particles through a series of collisions and would serve as a good model for energy exchange through conduction between hot and cold gases.
- Try using the slow motion slider on the top of the WORLD & VIEW to run the model in slow motion.
- Use the command center to set the speed of all the particles to a very low number (but not zero e.g. 0.01) and set the speed of one particle to a very high number (e.g. 1000). Watch how the kinetic energy of the fast particle is distributed in collisions to the other particles.
- Use the command center to trace the path of a particle, using pendown.
- How is kinetic energy represented by color when you set the SHOW-SPEED-AS-COLOR? chooser to "blue shades"?



CONNECTED CHEMISTRY NUMBER AND PRESSURE.NLOGO MODEL

WHAT IS IT?

This model explores the relationship between the number of gas particles and the pressure of a gas in a container with a fixed volume. The model simulates the effects of pumping up a bike tire.

In this model, the gas container (a bike tire represented by a box) has a fixed volume. The number of particles can be varied initially and by "pumping up the bike tire" by adding particles through a valve on the left wall of the box.

This model helps students study the representations of gas pressure in the model and the dynamics of the gas particles that lead to increases and decreases in pressure. In this model, students can also look at the relationship between number of particles and pressure. In addition, one can follow the average number of wall hits in one model clock tick. When the particles hit the walls the walls change their color temporarily. These models have been adapted from the model GasLab Pressure Box.

HOW IT WORKS

Particles are modeled as perfectly elastic particles with no energy except their kinetic energy -- which is due to their motion. Collisions between particles are elastic. Particles speed can be visualized by color coding them according to speed -- for example: blue for slow, green for medium, and red for high speeds.

HOW TO USE IT

Buttons:

Settons: SETUP - sets up the initial conditions set on the sliders. GO/STOP - runs and stops the model. ADD-PARTICLES - when pressed releases particles into the box while the simulation is running.

Sliders:

INITIAL-NUMBER - sets the number of gas particles in the box when the simulation starts. NUMBER-TO-ADD - the number of gas particles released into the box when the ADD-PARTICLES button is pressed.

Monitors:

CLOCK - number of clock cycles that GO has run. NUMBER - the number of particles in the box. PRESSURE - the total pressure in the box. WALL HITS PER PARTICLE - the average number of wall hits in one clock tick

Plots:

PRESSURE VS TIME - plots the pressure in the box over time. NUMBER VS TIME - plots the number of particles in the box over time. AVG. WALL HITS PER PARTICLE - plots the average wall hits per particle over time.

Initially, the particles are not moving. Therefore the initial pressure is zero. When the particles start moving, they repeatedly collide, exchange energy and head off in new directions, and the speeds are dispersed -- some particles get faster, some get slower. When they hit the wall they change their heading, but not their speed.

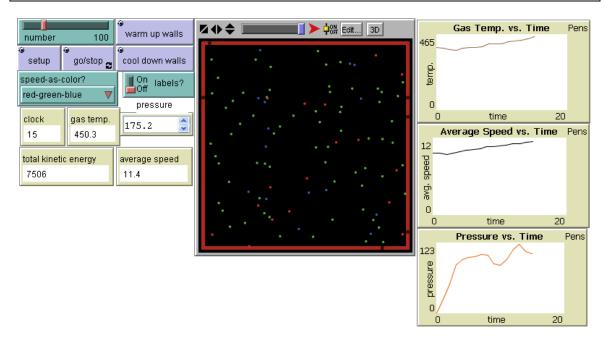
- 1. Adjust the INITIAL-NUMBER slider.
- 2. Press the SETUP button
- 3. Press GO/STOP and observe what happens.
- 4. Adjust the NUMBER-TO-ADD slider.
- 5. Press the ADD PARTICLES button.
- 6. Observe the relationship between the Number vs. Time graph and Pressure vs. Time.

THINGS TO NOTICE

- Can you relate what you can see happening to the particles in the box with changes in pressure?
- Why does the pressure change over time, even when the number of particles is the same? How long does it take for the pressure to stabilize?
- What happens to the wall hits per particle when particles are added to the box?
- In what ways is this model an incorrect idealization of the real world?
- What is the relationship between particle number and pressure? Is it reciprocal, linear, quadratic, exponential?
- Why is the average number of wall hits per particle, relatively constant, even if you change the number of particles in the model?

THINGS TO TRY

- -----
- Try different settings, especially the extremes. Are the particles behaving in a similar way? How does this affect the pressure?
- What is the relationship between particle number and pressure? Is it reciprocal, linear, quadratic, exponential?



CONNECTED CHEMISTRY NUMBER AND TEMPERATURE.NLOGO MODEL

WHAT IS IT?

This model explores the relationship between the temperature of a gas and the pressure of a gas in a container with a fixed volume.

In this model, the gas container (a bike tire represented by a box) has a fixed volume. The number of particles can be varied initially and the temperature of the gas can be varied by warming and cooling the gas container walls.

This model helps students study the representations of gas pressure in the model and the dynamics of the gas particles that lead to increases and decreases in pressure. In this model, students can also look at the relationship between number of particles and pressure, temperature of the gas and pressure. Alternatively they can make changes to both the number of particles and the temperature of the gas, and see what the combined affects of these changes are on pressure. In addition, one can follow the average number of wall hits in one model clock tick. These models have been adapted from the model GasLab Pressure Box.

These pressure models are part of a suite of models that students use to gain deeper insight on Gas Laws and particle behavior. In all of the Connected Chemistry Curriculum models, the same basic rules are used for expressing what happens when gas particles collide. Each model has different features in order to show different aspects of the behavior of gases.

HOW IT WORKS

The particles are modeled as hard balls with no internal energy except that which is due to their motion. Collisions between particles are elastic. Collisions between the walls are not.

As the walls of the box are heated, the sides of the walls will change color from a deep red (cool) to a bright red, to pink to a pale pink white (hot). The walls contain a constant heat value throughout the simulation.

The exact way particles gain energy from the walls of the box is as follows: 1. Particles check their state of energy (kinetic).

2. They hit or bounce off the wall.

3. They find wall energy and set their new energy to be the average of their old kinetic energy and the wall energy.

4. They change their speed and direction after the wall hit.

HOW TO USE IT

Buttons:

SETUP - sets up the initial conditions set on the sliders. GO/STOP - runs and stops the model. WARM WALLS - incrementally warms the box walls each time it is pressed. COOL WALLS - incrementally cools the box walls each time it is pressed.

Sliders:

NUMBER - sets the number of gas particles in the box when the simulation starts.

Choosers:

SHOW-SPEED-AS-COLOR? allows you to visualize particle speed using a color palette. The "blue-green-red" setting shows the lower half of the speeds of the starting population as blue, and the upper half as red.

The "violet shades" setting shows a gradient of dark violet to light violet for slow to fast particle speed.

The "all green" setting does not show a different color for each particle based on its speed.

Switches:

LABELS? turn particle id labels on or off

Monitors:

CLOCK - number of clock cycles that GO has run. PRESSURE - the total pressure in the box. GAS TEMP. - the temperature of gas. TOTAL KINETIC ENERGY - the total kinetic energy of the gas. AVERAGE SPEED - the average speed of the gas particles.

Plots:

- TEMPERATURE VS. TIME: plots particle temperature inside the box over time.

- AVERAGE. SPEEDS VS. TIME: plots average speed of the gas particles inside the box over time over time.

- PRESSURE VS. TIME: plots the average gas pressure inside of the box over time.

1. Adjust the INITIAL-NUMBER slider.

- 2. Press the SETUP button
- 3. Press GO/STOP and observe what happens.
- 4. Wait until the gas temperature stabilizes.
- 5. Press WARM WALLS or COOL WALLS a few times.
- 5. Wait until the gas temperature stabilizes

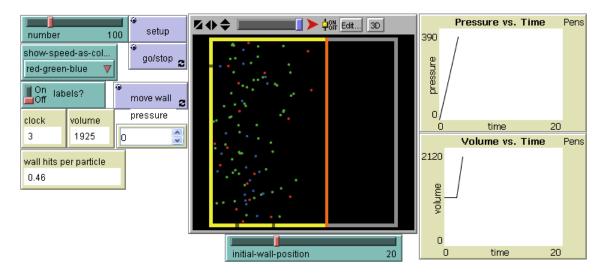
6. Observe the relationship between the Temperature vs. Time graph and Average Speeds vs. Time and Pressure vs. Time.

THINGS TO NOTICE

- It takes a while for the gas temperature to stabilize after you press WARM WALLS or COOL WALLS.
- Some particles move faster and slower than the average particles, at any gas temperature.

THINGS TO TRY

- Try to get the inside temperature to reach the outside temperature. Is this possible?
- How does adding heat to the box walls affect the speed of the particles?
- What do you think temperature is a measure of in a gas?
- How does adding heat to the box walls affect the pressure of the gas?
- Why can't you stop the gas particles completely by cooling the walls?
- How does the particle behavior or system response change with only one wall heated instead of all walls heated?
- Does the system reach an equilibrium temperature faster when the wall is heated or cooled the same amount in comparison to the temperature of the particles?



CONNECTED CHEMISTRY VOLUME AND PRESSURE.NLOGO MODEL

WHAT IS IT?

This model explores the relationship between the volume of a gas container and the pressure of a gas in a container at a constant temperature.

In this model, the gas container has an adjustable volume. The number of particles can also be varied initially.

This model helps students study the representations of gas pressure in the model and the dynamics of the gas particles that lead to increases and decreases in pressure. In this model, students can also look at the relationship between number of particles and pressure, volume of the gas container and pressure. Alternatively they can make changes to both the number of particles and the volume of the gas container, and see what the combined affects of these changes are on pressure.

HOW IT WORKS

Particles are modeled as perfectly elastic particles with no energy except their kinetic energy -- which is due to their motion. Collisions between particles are elastic. Particles speed can be visualized by color coding them according to speed -- for example: blue for slow, green for medium, and red for high speeds.

HOW TO USE IT

Buttons:

SETUP - sets up the initial conditions set on the sliders.

GO/STOP - runs and stops the model.

MOVE WALL -will temporarily "pause" the model when GO/STOP is running and wait until the user clicks in a new location in the World & View for the orange wall of the gas container. The new location must be to the right of the current orange wall location (so as to permit adiabatic free expansion of the gas)

Sliders:

NUMBER - sets the number of gas particles in the box when the simulation starts. INITIAL-WALL-POSITION helps adjust the initial volume by setting the location of the orange box wall. Switches:

LABELS? turn particle id labels on or off

Choosers:

SHOW-SPEED-AS-COLOR? allows you to visualize particle speed using a color palette. The "blue-green-red" setting shows the lower half of the speeds of the starting population as blue, and the upper half as red.

The "violet shades" setting shows a gradient of dark violet to light violet for slow to fast particle speed.

The "all green" setting does not show a different color for each particle based on its speed.

Monitors:

CLOCK - number of clock cycles that GO has run.

VOLUME - the volume of the box. Volume is computed based on what it would be using the 3D view. The can be visualized as the inner gas volume (yellow walls and orange wall) that is 1 patch width deep in the z direction.

PRESSURE - the total pressure in the box.

WALL HITS PER PARTICLE - the average number of wall hits in one clock tick

Plots:

- VOLUME VS. TIME: plots the volume of the gas container over time. Volume is computed based on what it would be using the 3D view. The can be visualized as the inner gas volume (yellow walls and orange wall) that is 1 patch width deep in the z direction.

- PRESSURE VS. TIME: plots the average gas pressure inside of the box over time.

1. Adjust the INITIAL-NUMBER and/or the INITIAL-WALL-POSITION slider.

2. Press the SETUP button

3. Press GO/STOP and observe what happens.

4. Press MOVE WALL. The particle motion will pause momentarily.

5. Then move your cursor to a spot inside the WORLD & VIEW, to the right of the current

position of the orange wall. Click on this spot and the wall will move and the particle motion will resume.

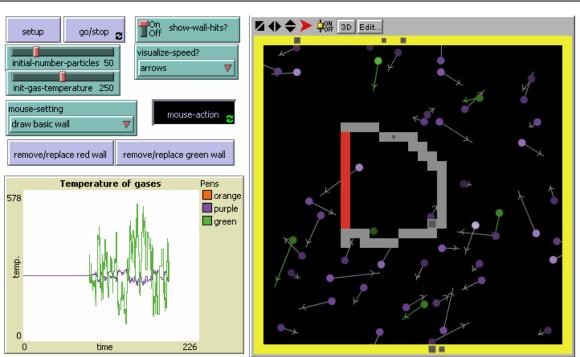
6. Observe the relationship between the Volume vs. Time graph and Pressure vs. Time graph.

THINGS TO NOTICE

- When you move the wall, the faster particles move toward it first. Does this type of diffusion occur in reality?
- There are combinations of NUMBER of particles and volumes for the container that yield the same pressure. What do you notice about the density of the gas particles in these situations: e.g. double the number of particles and double the volume?

THINGS TO TRY

- Find a mathematical model that related volume to pressure by recording and graphing various volume and pressure values in the model.
- What combination of volume and number of particles gives the highest pressure?



CONNECTED CHEMISTRY PARTICLE SANDBOX.NLOGO MODEL

WHAT IS IT?

This model supports a drawing style interface for "sketching" up representations of new systems to explore related to gas behavior and gas particles. This model is part of the "Connected Chemistry" curriculum

http://ccl.northwestern.edu/curriculum/ConnectedChemistry/ which explores the behavior of gases.

Most of the models in the Connected Chemistry curriculum use the same basic rules for simulating the behavior of gases. Each model highlights different features of how gas behavior is related to gas particle behavior.

In all of the models, gas particles are assumed to move and to collide, both with each other and with objects such as walls.

In this model, particles can be added, color coded, and sped up or slowed down, by drawing with the mouse cursor in the WORLD & VIEW. Also, additional types of removable and replaceable walls can be added to the WORLD.

This model enables students to draw a model of a real world system and then test that model. A wide range of real world systems can be modeled with this simple interface (e.g. diffusion of perfume from an uncapped container, hot gas mixed with a cold gas, mixtures of gases).

HOW IT WORKS

The particles are modeled as hard balls with no internal energy except that which is due to their motion. Collisions between particles are elastic. Collisions with the wall are not.

The exact way two particles collide is as follows:

1. A particle moves in a straight line without changing its speed, unless it collides with another particle or bounces off the wall.

2. Two particles "collide" if they find themselves on the same patch. In this model, two turtles are aimed so that they will collide at the origin.

3. An angle of collision for the particles is chosen, as if they were two solid balls that hit, and this angle describes the direction of the line connecting their centers.

4. The particles exchange momentum and energy only along this line, conforming to the conservation of momentum and energy for elastic collisions.

5. Each particle is assigned its new speed, heading and energy.

As the walls of the box are heated, the sides of the walls will change color from a deep red (cool) to a bright red, to pink to a pale pink white (hot). The walls contain a constant heat value throughout the simulation.

The exact way particles gain energy from the walls of the box is as follows:

1. Particles check their state of energy (kinetic).

2. They hit or bounce off the wall.

3. They find wall energy and set their new energy to be the average of their old kinetic energy and the wall energy.

4. They change their speed and direction after the wall hit.

HOW TO USE IT

-----Buttons:

SETUP - sets up the initial conditions set on the sliders.

GO/STOP - runs and stops the model.

MOUSE ACTION - press this down to use the mouse cursor to draw new objects or change properties of objects in the WORLD & VIEW. One depressed, select a MOUSE-SETTING action to use with the cursor. With a setting selected, click in the WORLD & VIEW to paint, erase, color, or add various objects and properties.

Sliders:

INITIAL-NUMBER-PARTICLES - sets the number of gas particles in the box when the simulation starts.

INITIAL-GAS-TEMPERATURE sets the initial temperature of the gas.

Switches:

SHOW-WALL-HITS? turn visualization of when particles hits the walls (as flashes) on or off

Choosers:

VISUALIZE-SPEED? allows you to visualize particle speeds. For example, selecting "arrows", creates a representation of each particle velocity using a scalar arrow. Selecting "shades" creates representation of each particle speed using a brighter (faster) or darker (slower) shade of the particle's color.

MOUSE-SETTING sets the action the user will enact when using the MOUSE ACTION in the WORLD & VIEW. Possible settings include:

"draw basic wall" - adds a gray wall under the mouse cursor

"draw red removable wall" - adds a red wall under the mouse cursor which can be alternatively removed and replaced (like a valve) using the REMOVE/REPLACE RED WALL. "draw green removable wall" - adds a green wall under the mouse cursor which can be alternatively removed and replaced (like a valve) using the REMOVE/REPLACE GREEN WALL. "big eraser" - erases all objects (except the yellow box boundary walls) under the mouse cursor.

"slow down particles" - increase the current speed of the particles by 10%.

"speed up particles" - reduces the current speed of the particles by 10%.

"paint particles green" - recolors the particles under the mouse cursor green (other settings include orange and purple)

"add green particles" - adds a couple of new particles under the mouse cursor (other settings include orange and purple)

Plots:

- 1: TEMPERATURE OF GASES VS. TIME: plots the temperature of the different gases in the model, as indicated by their color (orange particles, green particles, and purple particles)

THINGS TO NOTICE

The mouse interaction can be used while the model is running as well as when it is stopped.

THINGS TO TRY

Create a model of how odors move throughout a room. Why do some people smell the odor before others? Does the layout of furniture, large objects, and walls in the room effect the movement of the odor? How about the temperature of the air in the room?

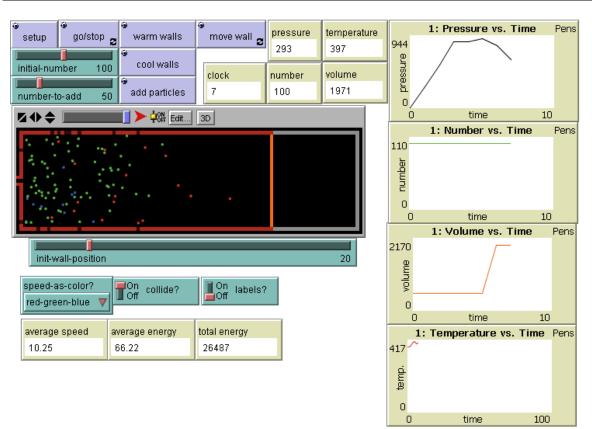
Create a model of diffusion of a perfume from a closed container. How would you represent the different gases (the perfume and the surrounding air)? What shape will the container be? How will you model a removable cap or lid?

Create a model of room filled with cold air and a different room filled with warm air. How will represent these different rooms of air? What could you add to show what happens when they mix?

Create a model of heat transfer that shows what happens to the energy of one very fast moving gas particle when it hits a bunch of very slow moving gas particles. What does this show happening to the energy of the initial gas particles?

RELATED MODELS

See GasLab Models See other Connected Chemistry models.



CONNECTED CHEMISTRY IDEAL GAS LAW.NLOGO MODEL

WHAT IS IT?

This model is one in a series of GasLab models. They use the same basic rules for simulating the behavior of gases. Each model integrates different features in order to highlight different aspects of gas behavior.

This model is illustrates the relationship between temperature and pressure in a fixed volume gas container.

HOW IT WORKS

The particles are modeled as hard balls with no internal energy except that which is due to their motion. Collisions between particles are elastic.

As the walls of the box are heated, the sides of the walls will change color from a deep red (cool) to a bright red, to pink to a pale pink white (hot). The walls contain a constant heat value throughout the simulation. If ONE-SIDE? is set to ON, only the left wall will be heated, while the other three walls remain yellow.

The exact way particles gain energy from the walls of the box is as follows:

- 1. Particles check their state of energy.
- 2. They hit or bounce off the wall.
- 3. They find wall energy and recalculate their new energy.
- 4. They change their speed and direction after the wall hit.

HOW TO USE IT

------Initial settings: - NUMBER-OF-PARTICLES: number of particles within in the box

Buttons: The SETUP button will set these initial conditions. The GO button will begin the simulation.

Other Settings:

OUTSIDE-TEMPERATURE: temperature of the outside of the box and the wall of the box. ONE-SIDE?: heats only the left wall if enabled. the other walls are colored yellow, and do not affect the energy of the particles that bounce into it.

- COLLIDE?: Turns collisions between particles on and off.

Plots:

- SPEED COUNTS: plots the number of particles in each range of speed.

- SPEED HISTOGRAM: speed distribution of all the particles. The gray line is the average value, and the black line is the initial average.

- ENERGY HISTOGRAM: distribution of energies of all the particles, calculated as $m^*(v^2)/2$.

- PRESSURE VS. TIME: plots average pressure of the inside of the box over time.

- TEMPERATURE VS. TIME: plots particle temperature inside the box over time and wall temperature over time.

- WALL HITS PER PARTICLE: plots average wall hits per particle over time.

THINGS TO NOTICE

- How does adding heat to the box walls affect the pressure?
- How does adding heat to the wall affect the particle behavior?
- How does the particle behavior or system response change with only one wall heated instead of all walls heated?
- Does the system reach an equilibrium temperature faster when the wall is heated or cooled the same amount in comparison to the temperature of the particles?

THINGS TO TRY

- Try to get the inside temperature to reach the outside temperature. Is this possible?
- Try to increase the wall hits per particle. Is this possible?

7.0 Prerequisite Knowledge

This activity assumes that students have a

- A conceptual understanding of Force and Motion (middle school level)
- A particulate view of the nature of matter that accounts for states of matter and molecular motion.
- Introduction to energy transfer and conservation of energy (middle school level).
- Completed a high school level algebra course.
- Developed mathematical models (graphs and equations) for linear and reciprocal relationships from experimental or messy real world data (in math or science).

If your students have not covered one of these topics, we suggest supplementing where needed before starting this unit

8.0 Student Prior Mental Models

Prior to using the models, most students know that pressure is involved in inflating a bicycle tire or a basketball. When encouraged to think of gas particles in this context, some of the students view inflating the tire as 'packing' the ball with particles or as increasing their speed.

Regarding the notion of packing, this is quickly resolved through the activities when they observe the particles moving randomly about the container. Thus, the particulate nature of a gas is brought forth, as well as the fact that a particle has a mass, speed and direction. Using the models and visualizing the particles and the empty space around them supports the students transition toward a more intimate understanding of the gas phase.

Some students view the action of pumping particles into a container as increasing their speed, which results from their collisions, which become more frequent with a greater gas density.

They tie this increase in speed to an increase in pressure. Some students employ an interesting idea -- that when the density of particles in the container increases, there is less room for each particle to move about -- but reason incorrectly that the many collisions with other particles slow the particles down.

9.0 Research Base

A body of science education literature points to student's misunderstandings of the gaseous phase of matter (Lin & Cheng, 2000; Maz & Perez, 1987). Some of these misunderstandings can be related to what Wilensky and Resnick call "levels confusion" (1999), where the properties of the macro-level are incorrectly ascribed to the micro-level (in the particular case of chemistry). The macroscopic properties of gases are easier to experience and perceive, such as when a kettle boils or a coke bottle produces a hiss when it's opened. However, the microscopic particles that are moving, colliding and bouncing off the walls are invisible. The literature reports a variety of alternative notions about gases such as ordered packing and weightlessness. Lin and Cheng (2000) describe high-school students' failures in understanding Kinetic Molecular Theory as it applies to gases: molecules are pushed down by atmospheric pressure, molecules stay away from heat and molecules expand when they are heated. All three can be related to our macroscopic daily experiences: our gravitation towards the earth, boiling water rising out of a pot and macroscopic expansion upon heating. Mas and Perez (1987) have found that high-school students regard gases as weight-less, reasoning from the macroscopic behavior that gases rise, and therefore cannot have weight. Similar problems have been reported in a variety of scientific domains, such as genetics (Marbach-Ad & Stavy, 2000) and basic electricity concepts (Frederiksen, White & Gutwill, 1999).

The learning research community has recognized the discontinuities between conceptual and algorithmic understandings of Chemistry (e.g., Kozma et al, 1990; Niaz & Robinson, 1992; Stieff & Wilensky, 2003). For example, Berg and Treagust (1993) point to the minimal use of qualitative relationships regarding teaching the gas laws both in a variety of textbooks they analyzed and in teaching approaches in schools. Students may be capable of solving problems that involve the procedures commonly taught in science classes. However, they do not necessarily do as well when approaching a similar problem that requires more qualitative, or conceptual reasoning.

A fruitful way of approaching the problem of bridging the conceptual and symbolic forms of representing chemical phenomena is the use of computer models that employ multiple representations and that have affordances that enable connecting the representations (see 4M:Chem, Kozma et al, 1996). Frederiksen, White & Gutwill (1999) have used a variety of models in computer simulations, to help students connect the different levels that can be used to describe basic electricity: a particle model, a circuit model and an algebraic model. Wilensky et al (Wilensky, 1999b; Wilensky, Hazzard & Froemke, 1999) have shown that NetLogo models can be powerful avenues for learning about gases and, more generally, about statistical mechanics. In their studies, students used the GasLab (Wilensky, 1999x) package. Students were involved at three levels: exploring existing GasLab models, modifying those models, and constructing new such models.

The unit reported here builds upon this previous work, but differs in that all students are involved only at the exploratory level and that their explorations are not entirely free (in most cases) but are guided by small and specific explorations (5-15 minutes in length).

The primary affordance for the students in using the computer models in the activities is the ability to connect the observed phenomena with the mechanism or rules underlying the model. This enables students to view the model as truly computational, and not a prepared "movie" selected by the designers and programmers.

Chemistry is a natural domain for an agent-based approach, as all chemical phenomena emerge from local interactions among a multitude of interacting individual molecules. The models used in the current project are a modified version of those originally created for the GasLab curriculum (Wilensky, 1999b; Wilensky, Hazzard & Froemke, 1999). A free-form version of Connected Chemistry was created by Stieff and Wilensky (2003). In an early version of the current project, the models were embedded within a script (Pedagogica, Horwitz, 2002) that structures the student interactions with the models. The software, called Pedagogica, necessary to run this earlier version of the scripted curriculum can be downloaded from <u>http://mac.concord.org</u>.

Through research of student responses and interactions with the Connected Chemsitry models We have found that through exploring the Connected Chemistry activities, the students gain a deeper understanding of the microscopic viewpoint and connect it with the macroscopic viewpoint (Levy, Kim & Wilensky, 2003). We have also observed their fine-tuning and adaptation of model exploration strategies as they become more fluent with the tools and domain (Levy & Wilensky, 2004).

This first set of activities in the Connected Chemistry curriculum is on the topic of gases: Gas laws, and Kinetic Molecular Theory (KMT). Kinetic Molecular Theory describes the behavior of individual particles (e.g., particles move in straight lines, they elastically collide with each other and with the walls). Gas laws describe the relationships among properties of the system of particles as a whole, when it is in equilibrium (e.g., Boyle's Law: the relationship between the volume of a box and the pressure inside, when temperature and the number of particles are constant). In addition to the traditional chemistry content, our curriculum also targets several important chemistry-related ideas: (a) Modeling: how a model is constructed, its assumptions, affordances and limitations, its relation with the target real-world phenomenon; (b) Thinking "from the molecule up" by focusing on micro-to-macro descriptions, transitions and connections; (c) Focus on processes of change in the system, such as perturbation and equilibration; (d) Mathematical modeling, deriving equations from data obtained through the students' NetLogo model explorations.

More generally, the chemistry topics are set within a wider perspective of complex systems. The domain of "complex systems" has evolved rapidly in the past 15 years, developing novel ideas and tools, and new ways of comprehending old phenomena, such as weather systems. Complex systems are made up of many elements (often named "agents", in our case, molecules), which interact among themselves and with their environment. The interactions of numerous elements result in a higher-order or collective behavior. Although such systems are not regulated through central control, they self-organize in coherent global patterns (Holland, 1995; Kauffman, 1995; Resnick & Wilensky, 1993). These patterns are often counter-intuitive and surprising. Exploring such patterns in a dynamic modeling environment can lead to profound and lasting discoveries about

10.0 Materials and Supplies

1 for class
1 for class
1-4 for class
* optional: 1 for class
1 per lab group/station
1 per lab group/station
Set of 8 per lab group/station
1 per lab group/station
1 per lab group/station
1 per lab group/station
1 per lab group/station

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12.0 Teachers Guide to Student Activities and Homework