Students' foraging through the complexities of the particulate world in the Connected Chemistry (MAC) curriculum

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ABSTRACT

In this paper, we describe five design principles that governed the design of the Connected Chemistry Curriculum and describe classroom research we conducted to evaluate the design. In the Modeling Across the Curriculum (MAC) project, high-school students explore computer models in science that are embedded in a supporting script. The Connected Chemistry curriculum focuses on topics in chemistry and employs multi-agent NetLogo models (Wilensky, 1999) to enable students in self-directed inquiry: manipulating and observing interactions between objects at the molecular level in order to gain insight into emergent patterns and macroscopic phenomena. We describe the curriculum, using examples to illustrate its design principles in action with a particular focus on three design principles: the importance of the process of modeling, making connections between different levels of description, differentiating between equilibrium and processes of change in the system.

INTRODUCTION

In this paper, we describe a set of design heuristics gleaned from classroom experiments conducted with the first unit in the Connected Chemistry curriculum. In the Modeling Across the Curriculum (MAC) project (Gobert et al, 2003), high-school students explore computer models in science that are embedded in a supporting script. The Connected Chemistry curriculum (Levy & Wilensky, 2004; Levy, Novak & Wilensky, 2005) focuses on topics in chemistry and employs multi-agent NetLogo models (Wilensky, 1999) to enable students to conduct self-directed inquiry: manipulating and observing interactions between objects at the molecular level in order to gain insight into emergent patterns and macroscopic phenomena. This curriculum has grown out of previous work in the domain of physics and chemistry (Wilensky, Hazzard & Froemke, 1999; Wilensky, 2000; Stieff & Wilensky, 2003), in which agent-based models are used to explore scientific phenomena.

BACKGROUND

A body of science education literature points to student's difficulties in understanding the gaseous phase of matter (Lin & Cheng, 2000; Maz & Perez, 1987). Some of these difficulties 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. The macroscopic properties of gases are easy 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' difficulties in understanding the Kinetic Molecular Theory as it applies to gases: students view molecules as being pushed down by atmospheric pressure, staying away from heat and expanding when they are heated. All three of these views can be related to our macroscopic daily experiences: gravitation towards the earth, boiling water rising out of a pot and expansion of substances upon heating. Mas and Perez (1987) have found that high-school students regard gases as weightless, reasoning from the macroscopic behavior that gases (such as boiling water) rise, and therefore cannot have weight.

The learning research community has recognized a disconnect 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 to use 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 employed a variety of conceptual models to build 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; 2003; Wilensky, Hazzard & Froemke, 1999) have shown that multi-agent models can be powerful avenues for learning about gases and, more generally, about statistical mechanics. In their studies, students used the GasLab (Wilensky, 2000) package. Students were involved at three levels: exploring existing GasLab models, modifying those models, and constructing new such models.

The work 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 but are guided and constrained by a script. The script is designed to guide but also to enable freedom and exploratory flexibility. But, in addition to the scripted activities the Connected Chemistry curriculum is "glass box" -- it enables students to depart from the script and examine directly the mechanism or rules underlying the model. This feature enables students to view the model as changeable, and not a prepared "movie" over which they have no control.

FRAMEWORK

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). A free-form version of Connected Chemistry was created by Stieff and Wilensky (2003). In the current project, the models are embedded within a Pedagogica script (Horwitz, 2002) that structures the interaction of the students with the models.

The 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, the CC curriculum targets several important chemistry-related strands: (a) modeling (scientific and mathematical); (b) microscopic-to-macroscopic connections; (c) change and equilibrium. More generally, the chemistry topics are set within a wider perspective of complex systems (Holland, 1995; Kauffman, 1995; Jacobson & Wilensky, 2006), by including concepts such as the relationship between randomness and the system's robustness, and the global effects of small-scale changes. Over the course of the design experiment cycle with these activities, we have developed a number of guiding principles for designing agent-based science modeling activities. We outline here three primary and two subsidiary principles. In following sections we will illustrate each of these principles with examples from curricular activities. The three focal principles of the curriculum are:

1) Microscopic-to-Macroscopic Connections - Integration of a two-level perspective of the system, by providing several explorations that focus alternatively on the micro and macro views, as well as micro-to-macro and macro-to-micro transitions;

2) Dynamics of Change in a Complex System - Developing students' powers of observation by calling their attention to the subtle local interactions and discrepant events, key phenomena in forming a causal understanding of the complex phenomena at hand. The explorations of complexity can be categorized into two themes: *Change and Equilibrium* and *Randomness and Stability*.

3) Exploring, Extending and Critiquing Models - Engaging students in a process of planning the design of models, evaluating the behavior of computer models and the predictive power of mathematical models, critiquing modeling assumptions, and predicting the outcome of changing the modeling assumptions.

In addition to these three focal principles, we endeavor to integrate scaffolds into the curriculum by using 1) a variety of visualization tools to help students view a single entity's behavior among a multitude and to move back and forth between micro- and macro- views. 2) Gradual fading of text scaffolds as the students become adept in using the model, integrating its representations and observing the complex phenomena. As the supports are withdrawn, student's interactions with models transition from guided to independent inquiry.

The Connected Chemistry unit consists of a sequence of seven activities. The sequence of activities is as follows:

(1) **Modeling a Tire**: A rule-by-rule construction of the gas model, leading up to a focus on the Kinetic Molecular Theory (KMT) assumptions.

(2) **Changing pressure**: Introduces the concept of pressure, elaborating on processes of change, delays between perturbing the system until the system reacts and then re-equilibrates, relations between the randomness of the gas particles' motion and the stability of pressure.

(3) **Experimenting with particles**: New tools are offered in this activity – the use of several NetLogo commands to change the particles' properties (such as their speed and direction), enhance and change the visual representations; propagating global effects from a local change; The students design and conduct an experiment of their choice, determining their course of action and using NetLogo commands to conduct their exploration.

(4) **Number and pressure**: The relationship between the number of particles in a fixed container and the pressure is explored, both qualitatively and quantitatively – deriving the equation that relates the two variables.

(5) **Temperature and pressure**: The concept of energy is elaborated upon via the changes to the gas temperature; the qualitative and quantitative relationship between temperature and pressure is investigated as well as the interrelationship between concurrent changes to the number of particles, the temperature of the gas, and the pressure.

(6) **Volume and pressure**: The concept of pressure is further explored in this activity, as it relates to the area of the container's surface; the qualitative and quantitative relationship between the two variables is probed and summarized as well as the interrelationship between concurrent changes to number of particles, volume of the container, and the pressure.

(7) **Ideal gas law**: Through both open investigation of a more complex gas model, and a guided mathematical derivation, the unit culminates in the Ideal Gas Law and extensions into the nature of scientific modeling.

To illustrate the way the above principles play into the curriculum, we portray a number of examples.

Building and Critiquing Models *(scientific and mathematical)*

Scientific modeling is introduced from the very first activity, even before students interact with the first NetLogo model. The activity is set within a real-world context of pumping up a bicycle tire. Several questions elicit students' noticing central features, both at a macroscopic and microscopic level. They are first asked to construct (in theory) a model of this phenomenon, as seen in the following screenshot (Figures 1a), from the selected parts and their properties to a mental simulation changes taking place. The model is introduced, part-by-part (Figure 1b), rule-by-rule (Figure 1c), where each object is mapped and compared to its real-world counterpart. Only after most of the rules underlying the gas particles behavior have been explored and outlined, is the Kinetic Molecular Theory presented and further investigated (Figure 1d).

Modeling A Tire: Activity 1

Exploration 1: Modeling a Bike Tire

screen
5 of 23

In a real bicycle tire you cannot see the air particles. We will build and then use a NetLogo model to simulate and visualize air particles inside the bicycle tire as it is being pumped up with air. A model is something that helps you understand very complicated or difficult to observe processes. It is based upon a set of assumptions that are usually much simpler or more exagerated than what actually may be taking place.

To build a useful model, we will need to consider the important objects or parts that need to be included. We also need to consider the important properties of the objects or parts and the interactions between them that we want to include.
Take a moment to describe what you would include in a model of pumping up a bicycle tire.

Question 3. What objects or parts need to be included?

A pump, a tire, air

Question 4. What are the properties that need to be included in your model?

A property describes an object or part (for example: the color, shape, or material it is made of).

Question 5. Describe how pumping up the tire would change what is happening inside it:

Modeling A Tire: Activity 1

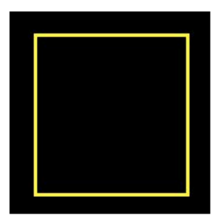
Exploration 1: Modeling a Bike Tire

screen
6 of 23

The model you will be using in the remainder of the activity will include only two types of objects: the walls of the tire and the air particles.

In a bike tire there are often other parts besides the tire wall and the air inside (such as the rim and the inner tube).

If you drew a picture of the inside of the bike tire in this photo, you might draw the walls of the bike tire as an uneven circle, oval, or teardrop shape.



In this picture the bike tire is represented as a yellow box. Although a real bike tire is not box shaped, using a box shaped container is a simplified model of the walls of the bike tire.

The NetLogo model you will be using on the next page will represent the rubbery (but relatively rigid) walls of the tire as a yellow box that does not change its size at all. It will show the walls of the box as continous lines, instead of modeling them as being made of many molecules in a solid state.

TIP: In the bottom left corner is a button with a picture of a glossary on it. This is the Chemistry glossary. Click on this button to learn more about the meaning of words that you are unfamiliar with or want to review.

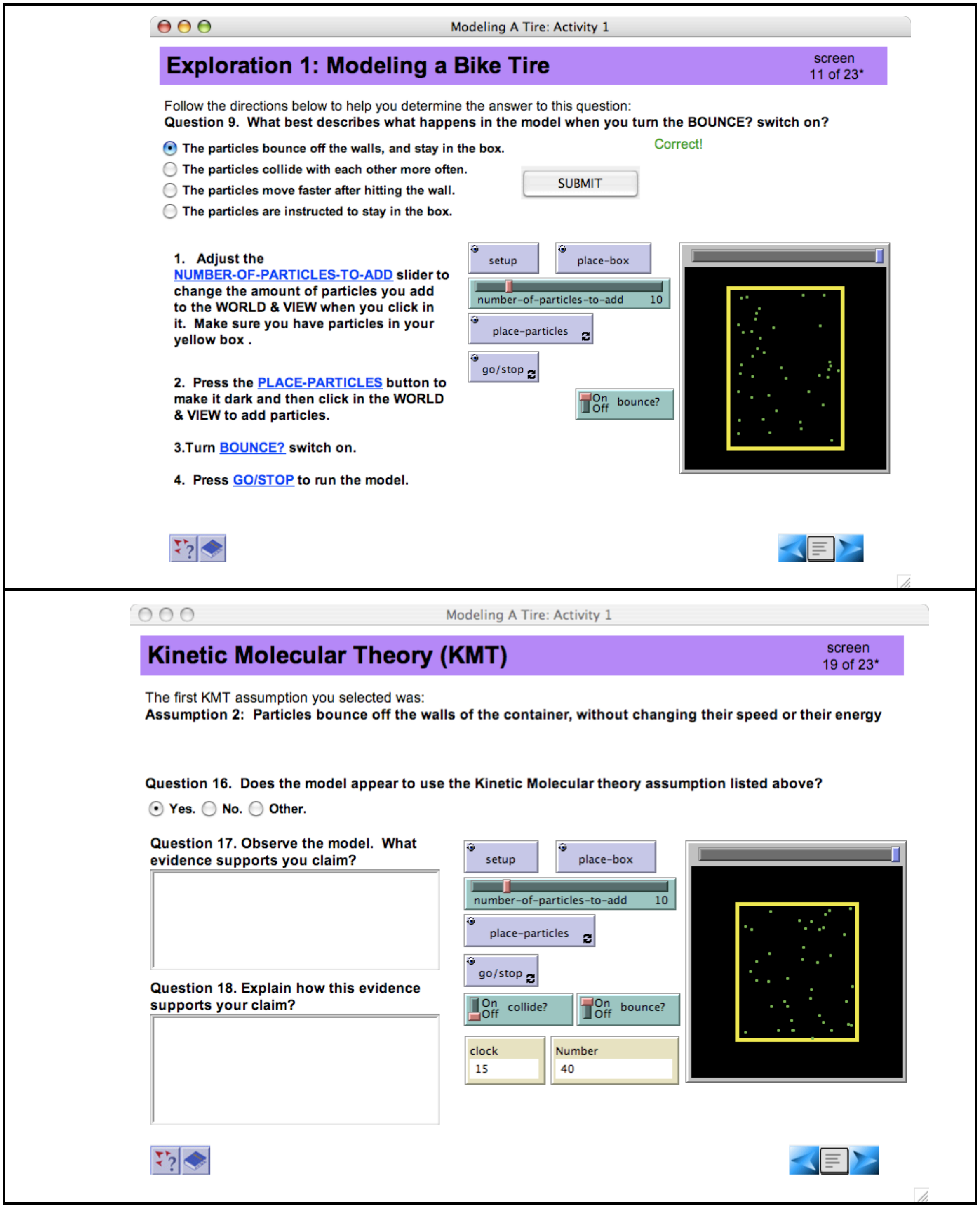


Figure 1: Modeling the Connected Chemistry curriculum

In a later activity, model construction and exploration is summarized with a comparison between the real bicycle tire and the model, encouraging the students to discuss the impact of such differences upon the validity of the model (Figure 2).

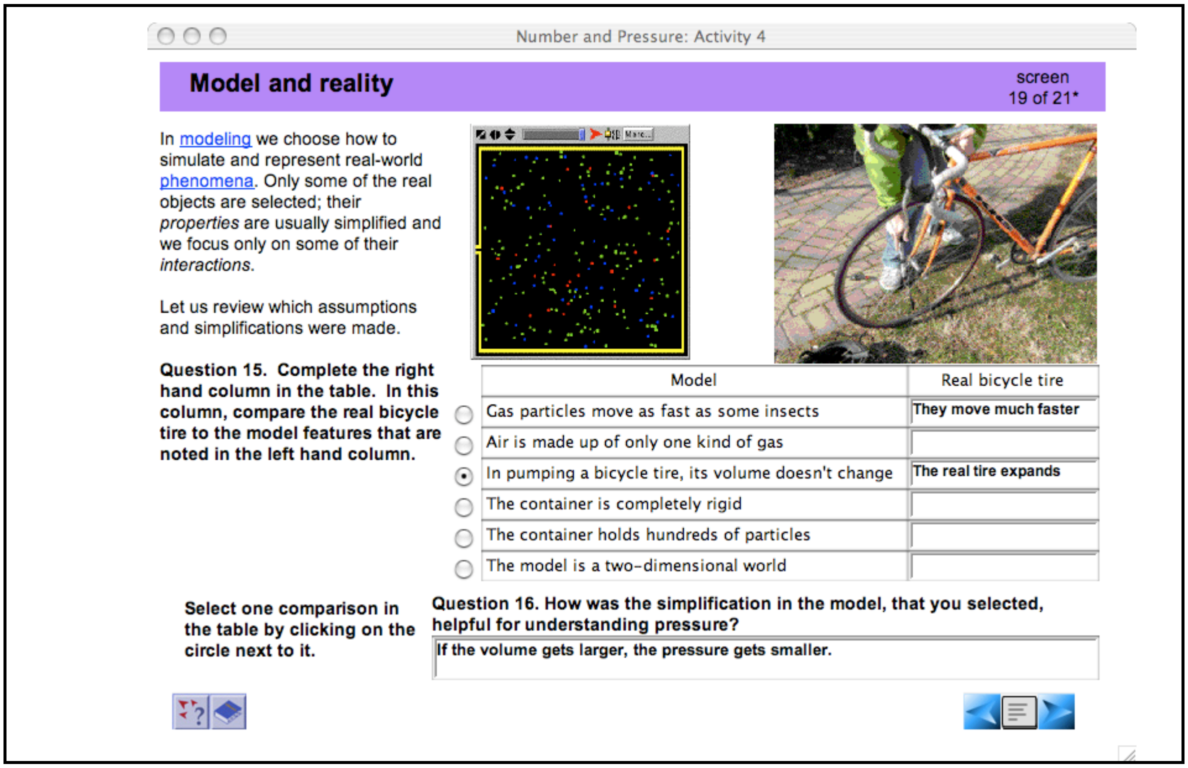
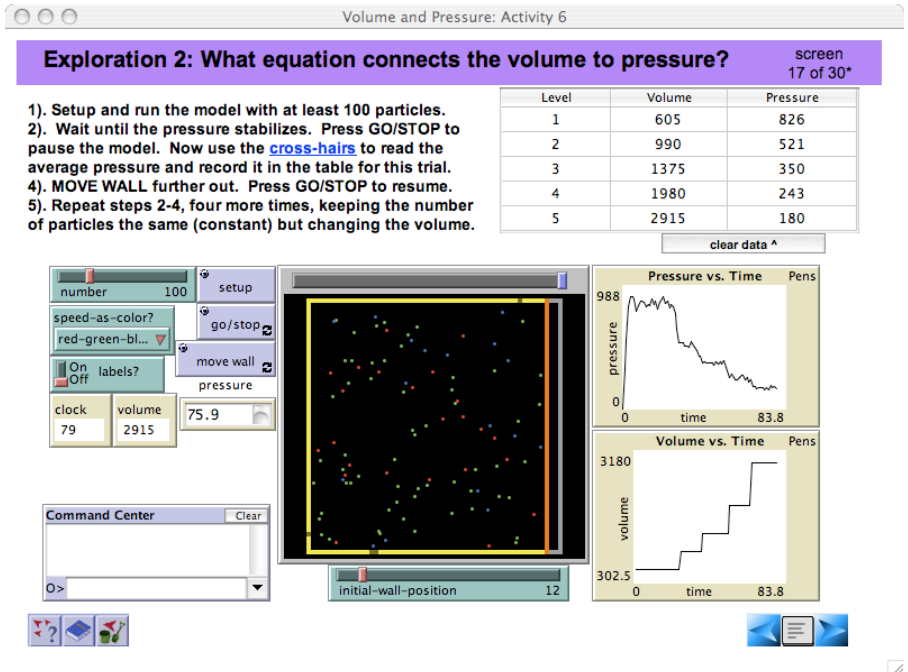
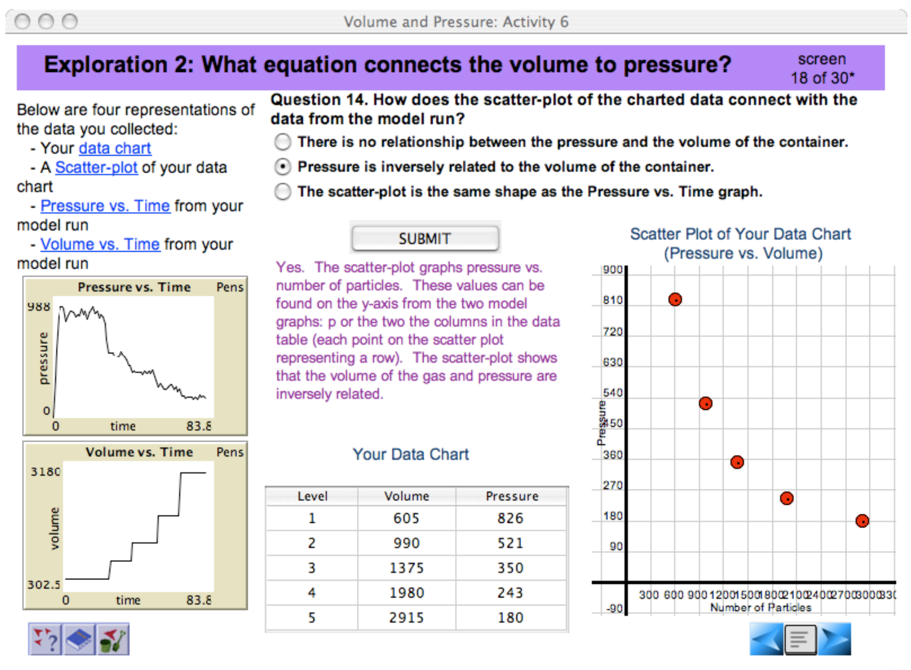


Figure 2: Model and reality in the Connected Chemistry curriculum

Coming full circle, in the very last activity, a new model is presented: the Atmosphere model. Before its introduction, the students are asked to construct a model (in theory) that would explain weather phenomena (Figure 3). Several questions are introduced, eliciting the students' more sophisticated understanding of models, including their predictive and explanatory power, as well as their limitations.

Mathematical modeling is prominent in the later activities, where the students are guided in constructing the equations relating the various properties of gases, such as Boyle's Law (the inverse relationship between volume and pressure, when other variables are held constant). They explore the models, construct scatter plots and compare these to canonical relationships. From these, the symbolic relationships are derived and then used to make and evaluate further predictions. Figure 3 presents a sequence of screens depicting one such activity. Further down the line, the students are asked to predict the equations relating the explored relationships, ending up with a construction of the Ideal Gas Law.


Volume and Pressure: Activity 6
Exploration 2: What equation connects the volume to pressure?
screen
17 of 30*
1). Setup and run the model with at least 100 particles.
2). Wait until the pressure stabilizes. Press GO/STOP to pause the model. Now use the cross-hairs to read the average pressure and record it in the table for this trial.
4). MOVE WALL further out. Press GO/STOP to resume.
5). Repeat steps 2-4, four more times, keeping the number of particles the same (constant) but changing the volume.
Level Volume Pressure
1 605 826
2 990 521
3 1375 350
4 1980 243
5 2915 180
clear data
number 100
setup
speed-as-color?
red-green-bl...
go/stop
On Off labels?
move wall
pressure
clock 79
volume 2915
75.9
Command Center
Clear
O>
initial-wall-position 12
Pressure vs. Time
Pens
988
pressure
0
time
83.8
Volume vs. Time
3180
volume
302.5


Volume and Pressure: Activity 6
Exploration 2: What equation connects the volume to pressure?
screen
18 of 30*
Below are four representations of the data you collected:
- Your data chart
- A Scatter-plot of your data chart
- Pressure vs. Time from your model run
- Volume vs. Time from your model run
Question 14. How does the scatter-plot of the charted data connect with the data from the model run?
There is no relationship between the pressure and the volume of the container.
Pressure is inversely related to the volume of the container.
The scatter-plot is the same shape as the Pressure vs. Time graph.
SUBMIT
Yes. The scatter-plot graphs pressure vs. number of particles. These values can be found on the y-axis from the two model graphs: p or the two the columns in the data table (each point on the scatter plot representing a row). The scatter-plot shows that the volume of the gas and pressure are inversely related.
Your Data Chart
Level Volume Pressure
1 605 826
2 990 521
3 1375 350
4 1980 243
5 2915 180
Scatter Plot of Your Data Chart
(Pressure vs. Volume)
Pressure
Number of Particles
Pressure vs. Time
Volume vs. Time

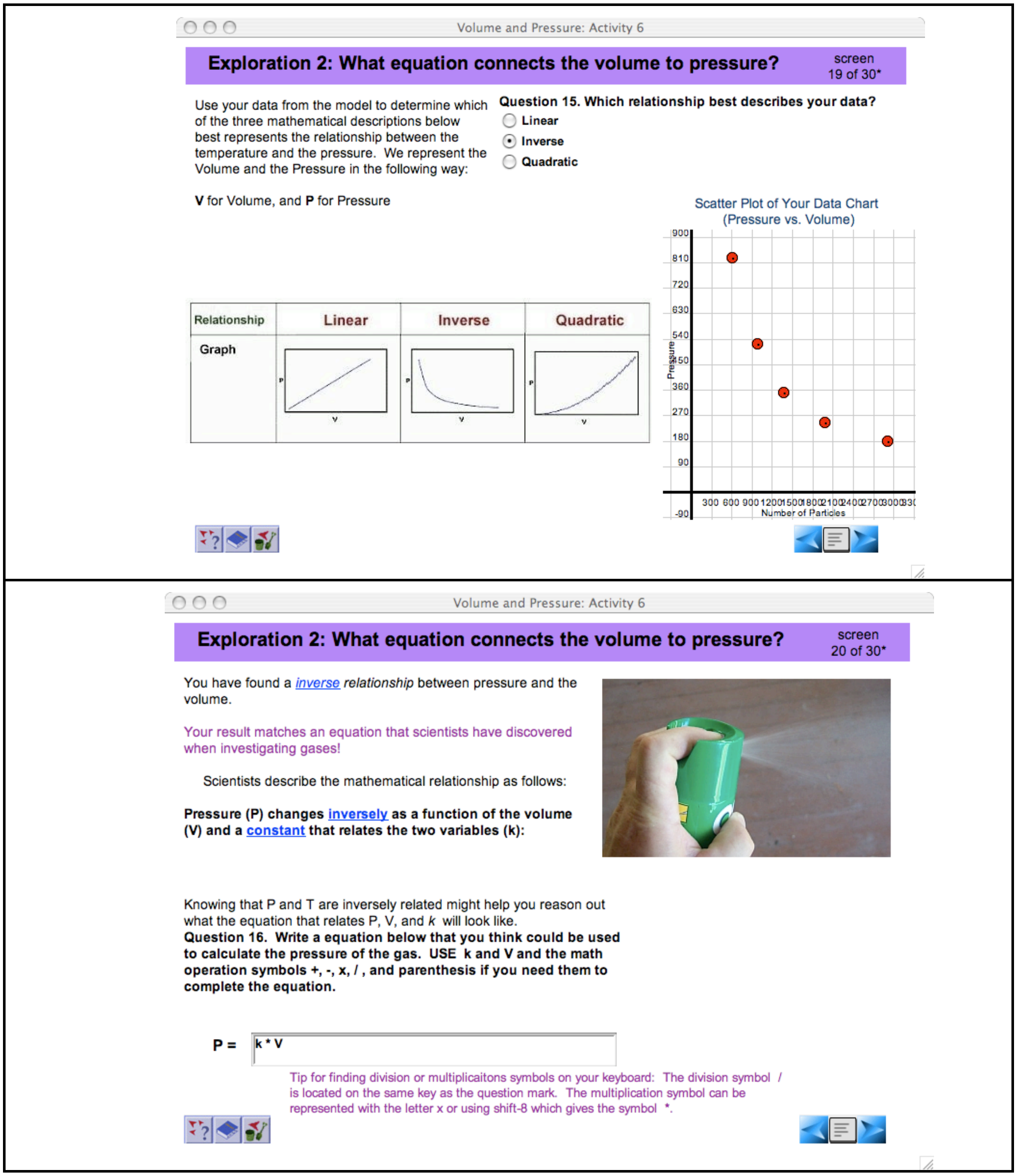


Figure 3: Mathematical modeling

Microscopic-to-Macroscopic Connections

Within an agent-based perspective of systems in general, as well as in chemistry, at least two distinct levels of description are necessary to make sense of phenomena. There is a two-way interaction between these two levels. Moving from the molecules upwards, a causal explanation of observed phenomena is made through their molecular descriptions. Molecules can be described via their behaviors and interactions. Through modeling of the multiple interacting molecules, these local behaviors emerge into coherent patterns of system-wide phenomena. However, the impetus for exploration is in the observed phenomena, when real-world events and situations beg for explanation. Thus, the curriculum moves both ways: from the phenomenon to its particles' behaviors, and vice versa.

To depict the curriculum as a whole, we have coded each question addressed to the students as one of four, with respect to the following:

(1) *Microscopic level*: Only molecular rules and behaviors are referenced. Examples: deriving gas particle rules, such as "moving in straight lines, unless they collide with something"; Describing changes in particle behaviors when they are allowed to collide with each other.

(2) *Macroscopic level*: Only group-wide patterns and variables are addressed. Examples: when the students are learning about the gas laws, relating any two macroscopic variables, qualitatively or quantitatively; relating symbolic representations and qualitative changes in the system.

(3) *Micro-to-Macro*: Involves reasoning "up" from the molecular behaviors to the system's patterns and variables. Examples: relating changes to all the particles when the particles are "instructed" to bounce of the container's walls, or including gravity in the model; Connecting the changes in particle behavior due to gravity, to macroscopic phenomena, such as differences of pressure at different altitudes.

(4) *Macro-to-Micro*: Requires reasoning "down" from change at the level of the system to local molecular behaviors. Examples: relating pumping up a bicycle tire to the air particles' behavior; relating average speed to energy transfer among the particles in their collisions.

Figure 4 (below) describes the seven activities in the curriculum with respect to the Levels dimension.

From this figure, we conclude:

(1) The curriculum shifts from a more microscopic perspective in the earlier activities to a more macroscopic perspective in the later activities, culminating with a combined perspective in the last activity.

(2) Transitions between levels are more dominant in the earlier activities, which involve a qualitative exploration of the models, targeting the agent-based causal reasoning in the system. They are less dominant in the later activities, as these focus on the gas laws and their deviation via quantitative reasoning.

(3) We can see a large proportion of questions that address the transitions among levels, both micro-to-macro and macro-to-micro.

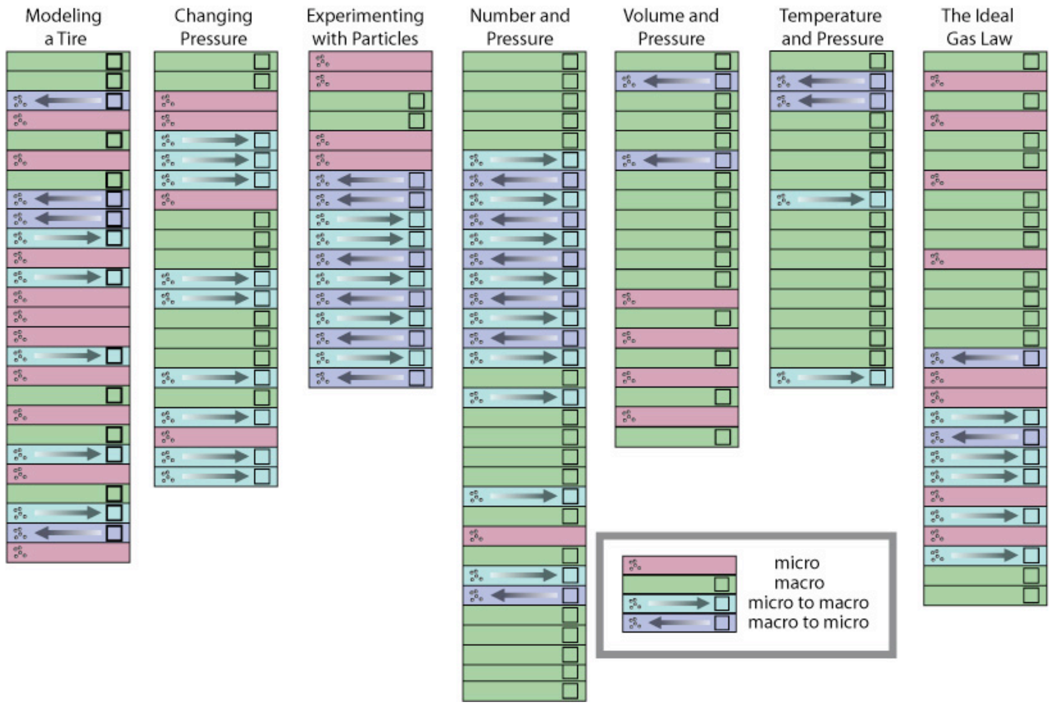


Figure 4: The "Levels" dimension in the Connected Chemistry curriculum. Each column is an activity. Each bar is a question addressed to the student. The bar is colored and illustrated via one of the four categories for levels: micro, macro, micro-to-macro, macro-to-micro.

Several explorations throughout the sequence call attention to microscopic particle behaviors and their relation to the system-wide variables. For example, in the "Experimenting with particles" activity, the students control the initial speeds of the gas particles, practically "freezing" them in place, creating a low pressure in the system. They then increase one particle's speed tremendously and observe its speed over time (see Figure 5). In the forthcoming run, the students observe how collisions between the particles re-distribute the speeds, with the system gradually coming to a new equilibrium at a higher pressure.

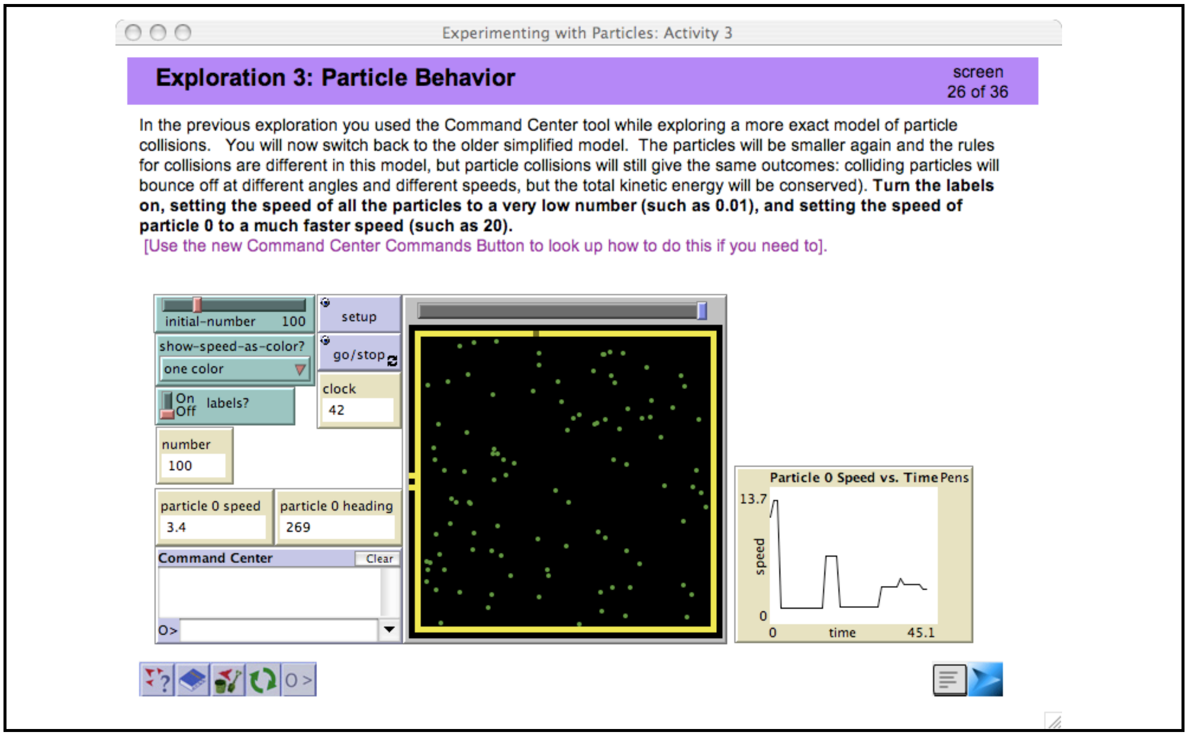


Figure 5: Micro-macro exploration in the system

Different observation tools are used to enhance students' attention to local behaviors and their connection to the system properties: following the path of a single particle among many, changing the particles' colors, and generally, calling attention to local events via guided explorations.

Dynamics of change in a complex system

Change and equilibrium

A central affordance of computer models is the possibility to speed up time (as in modeling evolutionary processes) or slowing it down. In the case, of gas particles, slowing them down supports an understanding of dynamic nature of such systems. To achieve a greater understanding of a gas system, we need to include more than just the equilibrium states, which are the focus in standard curriculum. By noting the effect of a local perturbation (e.g., increasing the speed of one particle to an extreme value), its propagation via collisions and energy transfer to the rest of the system and the eventual equilibration of the pressure, a greater understanding of the connection between local particle behaviors and system-wide changes can be made. By relating the effect of a system-wide change, such as heating a container's walls, and the local interactions, by which particles may speed up upon colliding with the walls, we afford a comprehensive understanding connecting the solid container and the gas via energy transfer, speed and temperature.

To describe the nature of the Connected Chemistry with respect to this dimension, each question, which is addressed to the student, is coded as either "equilibrium", "change" or both.

(1) "Equilibrium" denotes questions that focus only on stable states of the gas. Examples:

describing the differences between an inflated and deflated tire; relating the variables that describe the states of the gas system, such a Boyle's law.

(2) "Change" denotes questions that focus on the dynamics of the processes in the system. Examples: describing and relating the local changes in energy to an overall conservation of energy in the system; explaining why it takes time for the pressure to rise after particles are added into a container.

(3) "Equilibrium & Change" marks questions that address both equilibrium and change. Example: Relating changes in pressure to the changes in the particles' behaviors.

The following Figure 6 describes the Connected Chemistry curriculum with respect to this dimension.

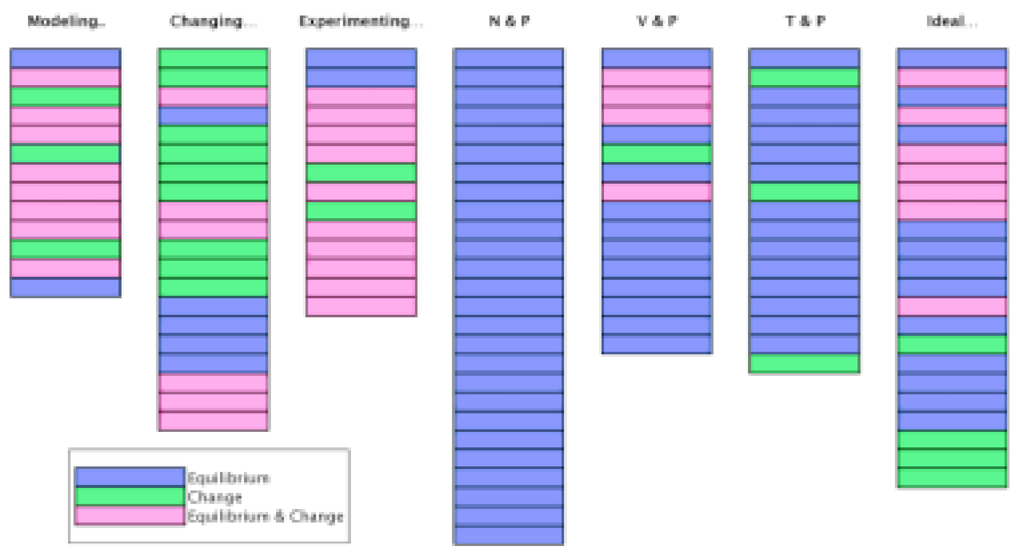


Figure 6: The "Change and equilibrium" dimension in the Connected Chemistry curriculum. Each column is an activity. Each bar is a question addressed to the student. The bar is colored and illustrated via one of the three categories: equilibrium, change, both.

From this figure, we conclude: The earlier activities focus upon all forms of change and stability, although a greater accent is placed upon "change" than on "stability". In the later activities, this perspective is switched to focus upon the equilibrium states, when the gas laws are explored. The final activity balances both perspectives.

In the following example, we demonstrate the way ideas regarding the dynamics of change are presented in the curriculum (Figure 7).

The activity concerns the introduction of new particles into a container, or pumping up a bicycle tire. Prior to this section, the students have been introduced to the idea of pressure and how it is measured in the model, when particles hit the wall. They have explored the qualitative relationship between the number of particles in the box and pressure. In these screens, the students are asked whether the pressure goes up immediately after particles are added. Noticing the time lag between pumping particles in and the rise of pressure is the target phenomenon. Thus, the focus is on the dynamics of the process of change between states, in which a change to the system is gradually propagated throughout. They are offered tools (the "cross-hairs") to quantify the values on the two graphs describing these variables over time. In the second screen, an explanation of the phenomenon is described in open form.

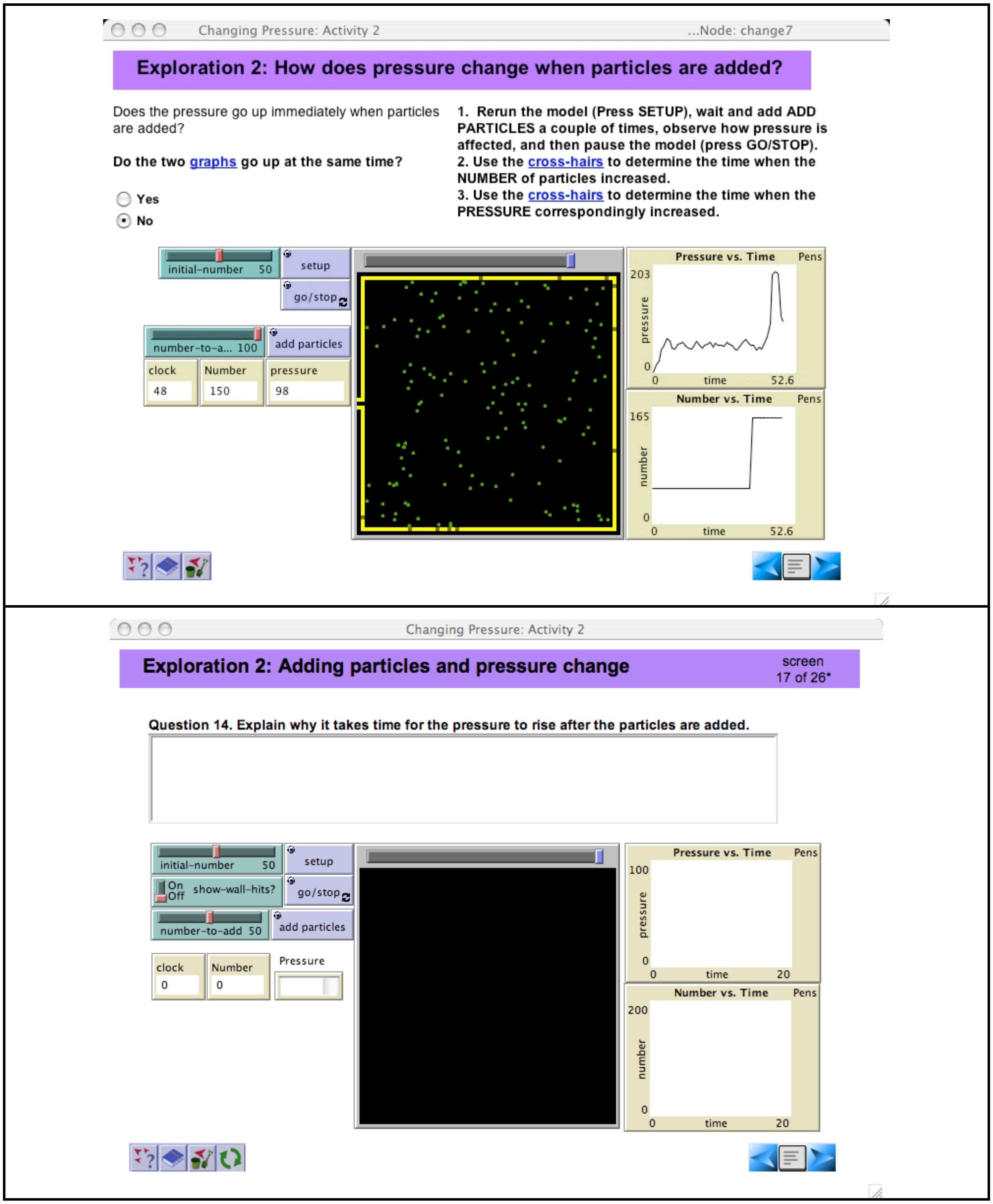


Figure 7: Change and equilibrium

Randomness and stability

A central idea of complex systems theory relates to the role of randomness in creating stability -- quite a counter-intuitive idea. In the curriculum, this is explored via noticing the fluctuations in pressure. When new particles are introduced in a particular direction, the pressure is destabilized, as a result of their directed motion. As the particles collide with each other, their direction of motion becomes randomized, thus stabilizing the pressure. This activity is demonstrated in the following screens (Figure 8):

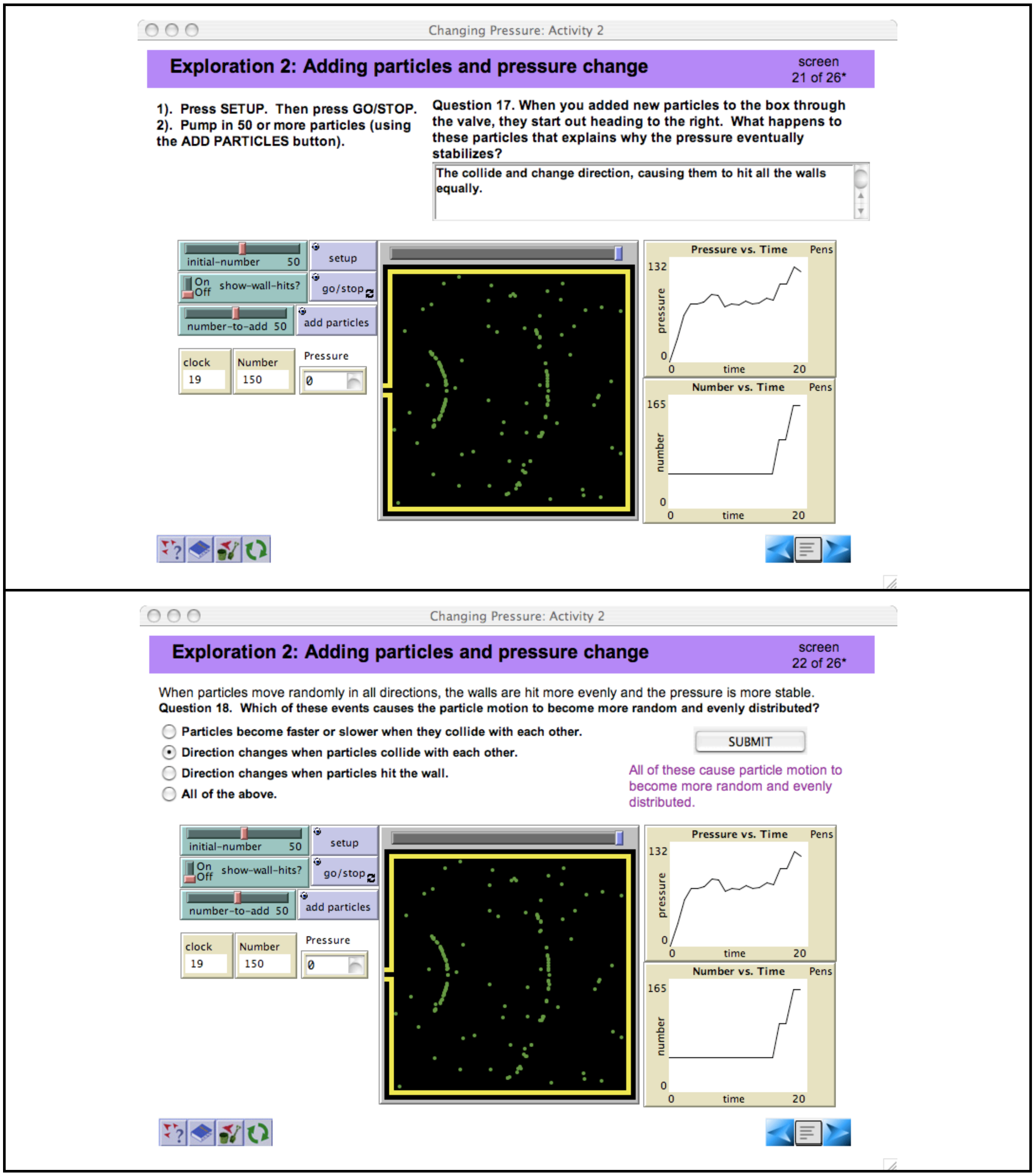


Figure 8: Randomness and stability

Visualization Tools

Students are introduced to new visualization tools through the first three activities. The first tool they are introduced to is a "slow motion slider". This tool allows students to slow the speed of the model down so that interactions between objects is easier to observe. Students are given a discrepant events to explore in the model that motivates the use of the "slow motion slider". (Figure 9)

In the second activity, students are introduced to a visualization tool for particle and container collisions (Figure 10) and the interpretation of the special structure of line graphs in NetLogo (which as the model runs provide a continual updating trace of various macroscopic values over time).

In the third activity, students are introduced to visualization tools to label particles, to represent particle speeds with color maps, and to record a trace of the motion of a particle through space with a virtual pen. (Figure 11)

Each of these visualization tools is introduced in a structured way at the start and herein remain accessible in the remainder of the curriculum for free exploration.

Fading Scaffolds

Throughout the curriculum, the students are guided in several structured inquiry activities. However, in many sections throughout, more open explorations complement the structured ones. The students construct and design their own experiments in a more open fashion in "sandbox" mode. As they gain fluency with manipulating the models, they conduct investigations with greater freedom.

In the first activity "Modeling a tire", they explore their first model gradually coming to understand its objects, rules and many interactions. Primarily students engage with the model in a "messing about" mode, repeating simple user interface actions to explore what the model is doing. In the latter part of the same activity, the Kinetic Molecular Theory (KMT) assumptions are presented and the students select two of these to explore in the model. In this activity what the tools that the students are given to explore are minimal and the assumptions to explore predefined.

In a later activity, "Experimenting with particles", students now learn to use simple code to impact the models. This simple code base opens the exploration of the model up to infinite variation and customization of model settings and visualization techniques. After exploring the use of these more sophisticated actions, students are then offered to select (out of a list) or invent a research question to investigate and then design their own experiment. This process is guided through several phases of: prediction, planning the experiment, observing and recording their data and drawing conclusions from their investigation.

To summarize this section, we have presented the rationale for the Connected Chemistry curriculum, its sequence of activities and how the main principles are exemplified in actual activities. Through the design, critique, exploration and manipulation of models, which enable dynamic views of both micro- and macro-level phenomena, we afford a deep causal understanding of the content of gas particle behavior and gas laws, while supporting the transition of student inquiry from guided to independent investigations.

EVALUATING DESIGN HEURISTICS – LEARNING FROM OUR STUDENTS

In this section, we describe some of many investigations we have conducted in order to explore the quality of the Connected Chemistry activities. We have implemented the CC activities in a variety of secondary school classrooms with about one thousand students. All student keystrokes were logged and analyzed. As students progressed through the activities and gained fluency with the tools of investigation and ways of thinking, the scaffolding in the activities was gradually faded. Our investigations include an analysis of "population-per-screen", which affords an examination of the more structural aspects of the curriculum and an analysis of the students' responses to questions. Other unreported activities include attitudes questionnaires and analysis of the pretest-posttest gains. Each of these resources has impacted our understanding of the students' interaction with the curriculum. We describe the activities and provide some examples, which have led us to change the curriculum in the later versions.

Population-per-screen

An analysis of the "populations-per-screen" affords our examination of the more structural aspects of the curriculum. When we "lose" students in the screens, we can assume that some problem has arisen or that (if they are later in the activity), the activity is too long.

The following Figure 9 shows the number of students that entered each of the screens within a single activity. This activity was part of one of the first versions and has since been changed. We later present a similar graph for one of the new activities.

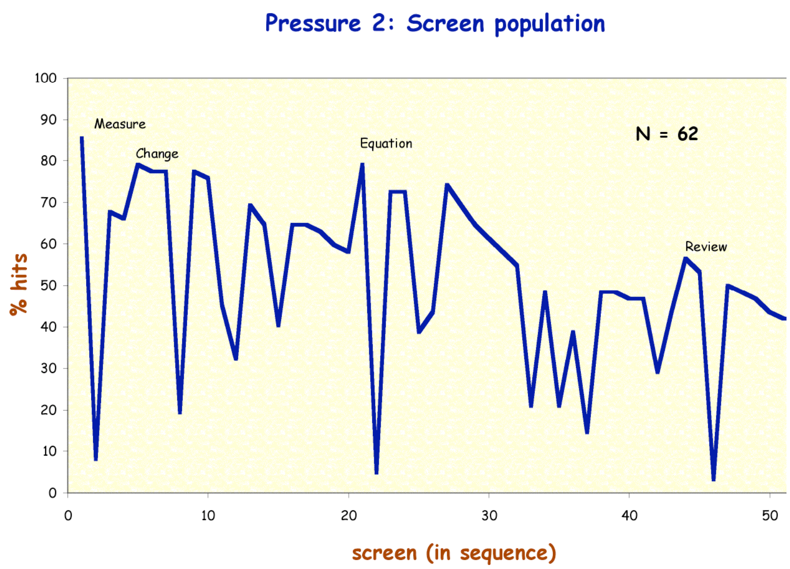


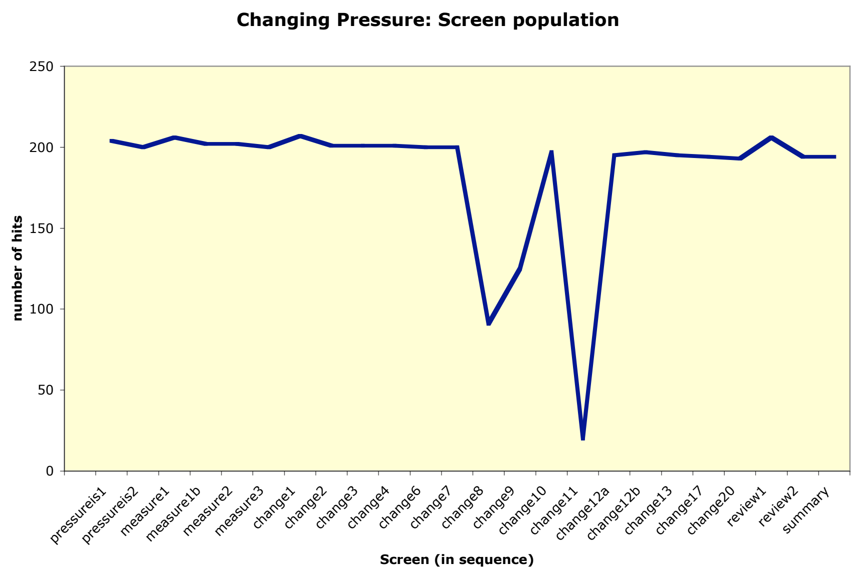
Figure 9: "Population per screen" for 62 students, who used the "Pressure 2" activity. The words on the graph denote the beginning of a new section in the activity.

In this graph, we can see a gradual decline from start to end in the number of students who reached a particular screen. More than that, within each section we can see such a decline, and then a rise when a new section is reached. About half the students reached the last screen[1].

Clearly, the structure of this activity was incorrectly timed. The activity was too long overall as were each of the sections.

This activity has since been cut back and converted into two activities. The sections are much shorter as well.

The following graph describes the screen population in one of the new activities. We can see that a horizontal level line is held throughout, there is no attrition.



Students' responses to questions

This part of the analysis targets a number of goals: (1) assessing students' understanding of the focus content; (2) identifying problems in the way the questions were worded (e.g. whether they encouraged explanation); (3) detecting problems in the sequencing of the activities; (4) locating problems, where more feedback is needed. In the earlier versions, the questions were posed in open form, so that we could access the students' understanding in their own words. One of our motives was to find out how the students understand the various concepts, so that some of them can be converted into multiple-choice questions, for ease of analysis in the large-scale research.

The students' answers in each activity were logged, parsed and arranged. All the responses were read. The categories arose from the data.

We provide a number of examples for such analyses, problems, and solutions.

[1] Some of the "deep dips" in the graph denote screens that were remedial – only some of the students reached them.

Modeling a Tire – the interaction between internal models regarding particles' speeds and computer models are a problem!

In our curriculum, we have been continually struggling with the students' mental models regarding the particles' speeds. In a gas, the particles' average speed changes only when the temperature changes, energy is removed or added to the system. This is explicit in the Kinetic Molecular Theory, which is examined at the end of the first activity. However, students' alternative ideas are much stronger. From several interviews with students, as well as class discussions, the following internal models are prominent:

Collisions release energy: When two particles collide, they both become *faster*. The collision releases an internal energy, which is converted into speed, or kinetic energy. Therefore, increasing the number of particles in a fixed container, increases the rate of collisions among particles, thus increasing their average speed.

The party model: When there are more particles in a container, they become *slower*. Since they have less room to move before they "run into" another particle, their speed goes down. Frequently, students explain this using a party analogy. When there are many people in the room, it's more difficult to move around, and you move from your location much less.

Frequently, the same student will express both models, at different times, in different contexts, an example of fragmented knowledge (diSessa, 1988).

We care about the students' understanding of speed for two main reasons: (1) the concept of pressure is prime in the curriculum. Changing the particles' speed changes the pressure – the students understand that walking in. When they are reasoning about speed changes, then their understanding of the separate effects of density (or number of particles within a fixed container), volume and temperature overlap and become ambiguous; (2) Conservation of energy is tightly linked into the underlying model assumptions and Kinetic Molecular Theory. When the speeds are changing in these two models, energy is not conserved.

Unfortunately, in the NetLogo model, this problem is exacerbated. When more particles are added into the model, more computation takes place for each time-step. Beyond a threshold, this slows the model down, so that each time-step takes a longer. Thus, the students can *see* that the party model is "true".

In the first year, we could see in the pre-test and post-test results that the students' party model is strengthened. At this point, the questionnaires were still essay questions. We asked the students what changes when a basketball is pumped up. From 39% that mentioned the particles' speed changing in the pre-test, in the post-test this went up to 67%.

In the second year, we provided an intervention. We dealt directly with the issue of computation speed, explaining the "internals" of the computer. In addition, we helped the students focus on the speed reading monitors in order to assess the speed, This alleviated the problem somewhat. In the pre-test, 22% thought that the speed would change, and in the post-test this went up to 28%.

During this second year, we observed the following interactions between the activity and the students' thinking about speed.

In the first activity "Modeling a Tire", the students are introduced to the gas model via its rules. At first, the particles move only in straight lines, oblivious of their surroundings, going through the walls of the container. When the students add the "bounce" rule, the particle bounces off the wall, changing direction, but not speed. When the students add the "collide" rule, energy transfer takes place between the pairs of colliding particles. Some become slower, and some become faster. Each particle frequently changes its speed. However, when “collide” is added to the computer model, one more thing happens: the “collide” code is very heavy computationally, as conservation of energy and momentum are calculated in every collision. This slows down the computer enormously. The particles now *look* slower.

In this activity, we gauge the students’ ideas via essay questions along five time points:

1. Prediction: Before the model is run
2. Observation: After running the model, when the “bounce” and “collide” rules are off.
3. Observation: After running the model, with the “bounce” rule on, and the “collide” rule off.
4. Prediction: Before adding in the “collide” rule
5. Observation: After running the model when both the “bounce” and “collide” rules are on

The sample included 59 students. The results are presented in the following figures.

Stage	Particles will be faster	Particles will be slower	Total
Predict: before the model is run	25%	5%	31%
Observe: when bounce and collide are off	29%	8%	37%
Observe: when bounce is on, collide is off	20%	8%	29%
Predict: before turning on collide	63%	20%	83%
Observe: when bounce and collide are on	25%	42%	67%

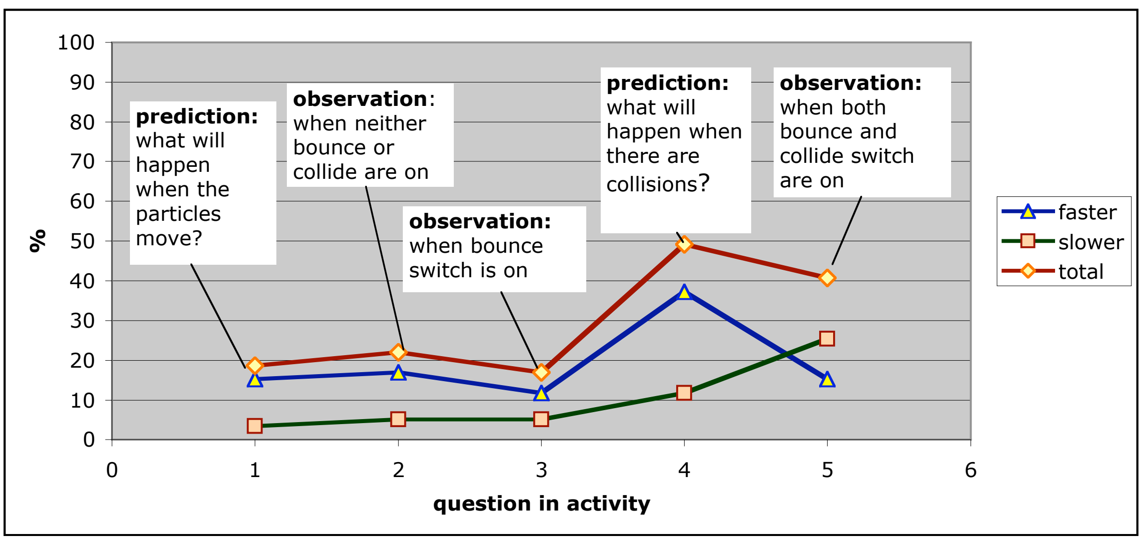


Figure 10: Number of students that predict or observe that the particles will be faster or slower. N=59.

In the beginning, only 20% predict that the speeds will change overall, tending mainly towards “faster”. This does not change too much when the model is observed in the first two explorations. However, this figure jumps up to 50% when predicting what will happen when collisions are added: students are mainly predicting that the particles will become faster when they collide with each other! However – what they see is the exact OPPOSITE: the particles become slower, because of the increased computation. And so, when describing their observation of the model: about 40% see the particles changing their speeds overall – with "slower" overcoming the "faster" tendency.

The questions were relatively non-directive. The features the students chose to mention in their answers are the ones that came to mind at first when thinking about the topic. However, when they were asked about collisions, this triggered the "collisions releases energy" model, which predicts that the particles will become faster. Looking at our NetLogo model caused some of them shift to the "party" model. We see this in their explanations in later activities.

Clearly, our curriculum was very confusing at this point, triggering their dormant fragmented models, which produced opposing outcomes.

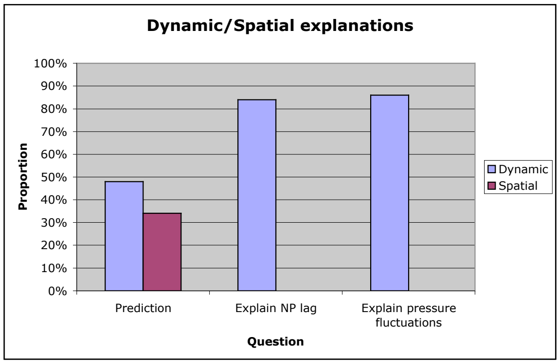
We had tried to intervene via "explaining the machine" and addressing the issue of "limitations of models". This helped, but not enough.

We tried one solution – slowing down all the models to a regular "beat". This produced an even speed, but was very slow, jagged and annoying to use. A new team member came up with a compelling idea. Let's add invisible particles into the model. The total number of particles the computer computes will be constant. These invisible particles will collide among themselves, to create the computation load that would slow down the model, even when there are no collisions among the visible particles. We have implemented the solution, and now await the results from the schools that are currently using the activities.

Changing Pressure – the evolution of a dynamic and dual-level perspective

The "Changing Pressure" activity is quite challenging for the students. It targets the patterns of change in the system, noticing fluctuations and their cause, going back and forth several times between the micro- and macro-perspective. In one section, when a container is pumped up with particles, the students are asked to notice and explain a time lag between the particles entering the container and the rise of pressure. In another section, they are asked to explain the fluctuations of pressure in the model, which arise from the stochastic nature of the particles' behaviors, and result from their small number, when compared with a real-world sample. This activity has been revised several times. However, even one of the earlier versions shows the following characteristics.

When explaining these two phenomena, the students' answers were coded along two dimensions: whether the explanation included dynamic aspects of the system behavior, and the micro/macro levels of description. The same was done for their predictions of these phenomena before exploring the model. The following figures show the evolution of the students' understanding.



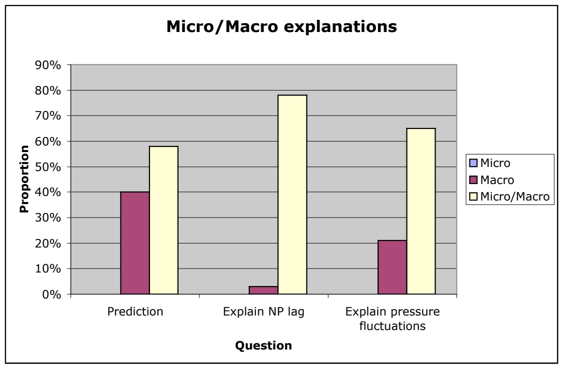


Figure 11: Changing Pressure predictions, explanations of the time lag between the particles entering a container and the pressure rises, and explanations of the pressure fluctuations. N=107.

In these graphs, we can see a strong shift from the beginning of the activity until the end. When predicting the system's behavior, as a group, the students are balanced between dynamic and static descriptions. The students all shift to dynamic descriptions in the activities. For example, when explaining the number-pressure time lag, we can see a dynamic view: "It takes time because there is an interval between when the particles are added and when they are bouncing off the walls." When predicting the system's behavior, 40% are using only macroscopic descriptions. After exploring the models, close to 80% employ micro-macro descriptions when explaining the time lag. Close to 70% use this dual-level perspective in explaining the pressure fluctuations. For example, in explaining the pressure fluctuations, we can see a clear connection between the levels: "The pressure changes more frequently, because it depends on how many particles bounce off of the wall, and these particles are constantly in motion, so the number of particles that bounce off of the wall [a] changes very rapidly and all of the time."

After many struggles, we realized that at this point we had succeeded in creating an activity that encourages reasoning about the system as dynamic and through two levels of description.

Overall learning of content, pre-post results

We have analyzed the results from the students' answers to the pre-test and post-test questionnaires. We compare the scores in the following way:

(1) Overall

(2) Items that focus on micro-level understanding

(3) Items that focus on macro-level understanding

(4) Items that focus on connecting micro and macro levels

In addition, we provide results from an early analysis of first version of the questionnaire. One question targeted the students' understanding of models, via their construction of a theoretical model. Currently, this item has been shifted into the activities, for reasons of brevity.

In the earlier part of the year, we analyzed the results of the implementation in a lab-school we worked with in Chicago. The school is an inner-city high-school, with a high 91% rate of reduced or free lunch. 2.5% of the students were white, 15% were AA, 82.5% were Hispanic. The sample (including only students who completed both pre-test and post-test questionnaires) included 44 11^{th} grade students. Of these, 27% were in an "honors" chemistry class, and 73% were in a "regular" chemistry class. During the implementation, the students employed earlier versions of our activities, which are equivalent to activities 1, 2 and 4, in the curriculum today: Modeling a Tire, Changing Pressure and Number & Pressure.

The results are presented in Table 1. These results show an overall gain, however only in one dimension: that relating to the microscopic viewpoint. These results were leveraged in the later revisions of the activities, which now encompass a more comprehensive treatment of the macroscopic viewpoint, as well as sections that target transitions among the levels.

	Pre-test Mean (SD)	Post-test Mean (SD)	t-statistic (paired)
Overall	40 (12)	51 (10)	5.26**
Dimensions			
Micro	34 (16)	55 (13)	7.14**
Macro	47 (21)	41 (21)	-1.40
Micro-Macro	37 (34)	46 (28)	1.27

N = 44; **: $p < 0.01$

Table 1: Pre-test Post-test results, 2004 Chicago High-school implementation.

In a later implementation, the following results were obtained.

	Pre-test Mean (SD)	Post-test Mean (SD)	t-statistic (paired)
Overall	45 (13)	60 (14)	10.8**
Dimensions			
Micro	45 (19)	76 (15)	11.7**
Macro	49 (25)	59 (26)	6.2**
Micro-Macro	34 (16)	45 (21)	4.8**

N = 94; **: p<0.01

Table 2: Pre-test Post-test results, April, 2005 implementation.

We can see a large improvement in the students' gains between the previous year and the current year. The gains in understanding of all aspects of the curriculum have all improved: the macroscopic, the microscopic and the combined emergent perspective.

Understanding of models

One of the questions that was included in an earlier version of the pre-test and post-test provides some insight into student changed understanding of models.

The sample was taken from a lab-school we worked with in Chicago. The school is an inner-city high-school, with a high 91% rate of reduced or free lunch. 2.5% of the students were white, 15% were AA, 82.5% were Hispanic. The sample (including only students who completed the question in both pre-test and post-test questionnaires) included 47 11th grade students. Of these, 27% were in an "honors" chemistry class, and 73% were in a "regular" chemistry class. During the implementation, the students employed earlier versions of our activities, which are equivalent to activities 1, 2 and 4, in the curriculum today: Modeling a Tire, Changing Pressure and Number & Pressure.

The item is the following:

A basketball starts losing air since it has a small hole in its wall.
How would you make a model to describe this process?

1. What objects would you include in the model? Describe these objects in detail.
2. What are the properties of these objects?
   Properties are the attributes or features of the objects.
3. What are the rules by which these objects operate?
   A rule describes what the object does under different conditions. For example: "If a ball is let go, then it falls down until it hits a solid surface"; "If the ball hits the ground, then it bounces upwards."
4. Describe the process by which the air leaves the basketball.

The students replied to the questions in open form. Their responses were coded in the following way, addressing the following two questions: (1) Are the students constructing a theoretical model? Or are they performing a different activity? (2) What levels of description do they employ in constructing their model?

The following examples describe our categories.

Question 1: Are the students constructing a theoretical model? Or are they performing a different activity?

Through reading the students' responses, we could see that they did one of three activities: (1) Describe or explain the phenomenon they were asked to model; (2) Propose an experiment to test or demonstrate the phenomenon; (3) Propose a model of the phenomenon.

Activity	Example
Describing / Explaining	A basketball a hoop and a wall… Big, round, hard, solid, brick and others… It filters out.
Proposing an experiment	Fill up a basketball and show how air gets out in water and bubbles come out… A pump to give air and a ball w/out a hole to show how air stays in and one w/a wall hole to show how it escapes…
Modeling	I would include a basketball built out of a container. And cut out little ball shaped paper for the air particles.. If there is a [w]hole in the ball, air would be released and the ball would deflate… The air leaves the basketball because since the air particles are moving randomly when the ball has a hole in it the particles start leaving the ball. I would make a model of the basketball walls with a [w]hole in it and less or fewer particles moving slowly.

Table 3. Categories and examples for students course of action when asked to construct a theoretical model of a phenomenon.

The results for the pre-test and post-test are presented in the following Figure 12.

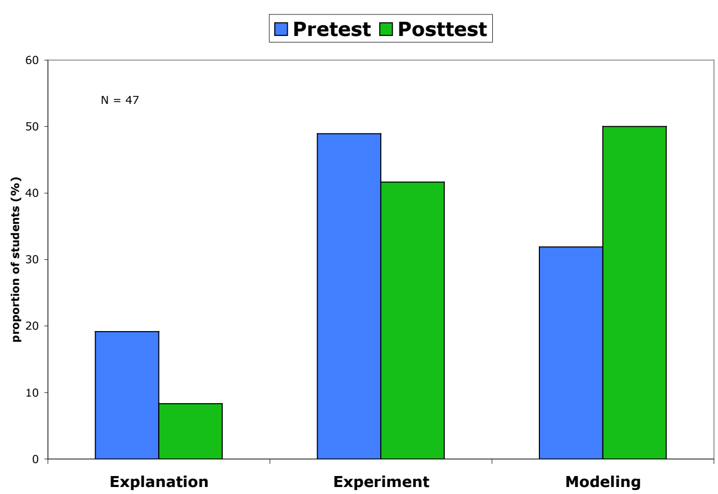


Figure 12: Students' activity when asked to propose a model of a phenomenon. The results are presented for both pre-test and post-test.

In the pre-test, the majority proposed an experiment, and only 33% suggested a model. In the post-test, the majority (about 50%) proposed models. Thus, we can see a rise in the students' understanding and distinction between the scientific activities of modeling, experimenting and explaining phenomena.

To summarize, we have seen that when asked to construct a theoretical model of a phenomenon, some of the students increased their understanding of what it means to construct a model, distinguishing it from an experiment in the laboratory or an explanation. The micro-level was introduced more frequently in the post-test, exemplifying a shift from a focus on the observed level macro-level alone.

CONCLUSION

We have described three primary and two subsidiary design principles that guided the design of the Connected Chemistry curriculum. These design principles emerged from previous research conducted with free exploration of agent-based models and were adapted for the Modeling Across the Curriculum project so as to be useful in a structured interaction between students and agent-based chemistry models. After testing this curriculum in year 1 in Chicago high schools, we saw significant gains in student understanding of the micro-level of Chemistry phenomena. But, we did not see significant gains in the micro-to-macro transition as we had hoped. Reexamining the curriculum in this light, we saw that in the effort to compensate for the lack of micro-level focus in traditional high school, we neglected to make explicit connections between the micro-level and the macro-level phenomena Based on these findings, we redesigned the curriculum interleaving observation and experiments with macro-level phenomena with experiments at the micro-level that generate the macro-level phenomena. After this redesign, we retested the curriculum in Chicago high schools and this time saw significant gains in all our measured dimensions.

REFERENCES

Bowen, C.W. & Bunce, D.M. (1997). Testing for conceptual learning in general chemistry. *The Chemical Educator*, 2(2), 1-17.

DiSessa, A. A. (1988). Knowledge in pieces. In G. Forman & P. Purfall (Eds.), *Constructivism in the computer age* (pp 49070).

Gobert, J., Horwitz, P., Tinker, B., Buckley, B., Wilensky, U., Levy, S.T., Dede, C. (2003). Modeling across the curriculum: Scaling up modeling using technology. Paper presented at the 25th Annual Meeting of the Cognitive Science Society, CogSci 2003, Boston, Massachusetts, USA, July 31-August 2, 2003.

Holland, J. (1995). *Hidden Order: How Adaptation Builds Complexity*. Helix Books/Addison-Wesley, Reading, MA.

Kauffman, S. (1995). *At home in the Universe: The Search for the Laws of Self-Organization and Complexity*. Oxford University Press, Oxford.

Kozma, R., Russell, J., Jones, T., Marx, N., & Davis, J. (1996). The use of multiple, linked representations to facilitate science understanding. In Vosniadou, S., Glaser, R., DeCorte, E., and Mandl, H. (Eds), *International Perspectives on the Psychological Foundations of Technology-Based Learning Environments,* Erlbaum, Hillsdale, NJ, 41-60.

Kozma, Russell, J., Johnston, J. and Dershimer, C. (1990). *College students' understanding of chemical equilibrium.* A paper presented at the Annual Meeting of the American Educational Researcher Association, Boston, MA.

Levy, S.T., Novak, M., Wilensky, U. (2005). Connected Chemistry Curriculum 1.3 Evanston, IL. Center for Connected Learning and Computer Based Modeling, Northwestern University. ccl.northwestern.edu /curriculum/chemistry/.

Lin, H., Cheng, H. & Lawrence, F. (2000). The assessment of students' and teachers' understanding of gas laws. *Journal of Chemical Education*, 77(2), 235-238.

Marbach-Ad, G., Stavy, R. (2000). Students' cellular and molecular explanations of genetic phenomena. *Journal of Biological Education*, 34(4), 200-205.

Mas, C.J.F. & Perez, J.H. (1987). Parallels between adolescents' conceptions of gases and the history of chemistry. *Journal of Chemical Education*, 64(7), 616-618.

Niaz, M., Robinson, W.R. (1992). From 'algorithmic mode' to 'conceptual gestalt' in understanding the behavior of gases: An epistemological perspective. *Research in Science and Technological Education*, 10(1), 53-65.

Resnick, M. & Wilensky, U. (1993). Beyond the Deterministic, Centralized Mindsets: New Thinking for New Sciences. American Educational Research Association, Atlanta, Ga.

Stieff, M. & Wilensky, U. (2003). Connected Chemistry – Incorporating interactive simulations into the chemistry classroom. *Journal of Science Education and Teaching*, 12(3), 285-302.

Wilensky, U. (1999). *NetLogo*, Center for Connected Learning and Computer-Based Modeling, Northwestern University. Evanston, IL. http://ccl.northwestern.edu/netlogo

Wilensky, U., Hazzard, E & Froemke, R. (1999). An Extensible Modeling Toolkit for Exploring Statistical Mechanics. Proceedings of the Seventh European Logo Conference - EUROLOGO '99, Sofia, Bulgaria.