

# Crossing Levels and Representations: The Connected Chemistry (CC1) Curriculum

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**Abstract** Connected Chemistry (named CC1 to denote Connected Chemistry Chapter 1) is a computer-based environment for learning the topics of gas laws and kinetic molecular theory in chemistry. It views chemistry from an “emergent” perspective, how macroscopic phenomena result from the interaction of many submicroscopic particles. Connected Chemistry employs agent-based models built in NetLogo (Wilensky, NetLogo, Northwestern University, Evanston, 1999a), embedded in scripts that structure and log the students’ activities. A conceptual framework was developed to structure students’ experiences and learning through exploring the models. The framework describes three spheres of knowledge (conceptual, symbolic and physical) and four forms of access to understanding the system (submicro, macro, mathematical and experiential). Activities were designed to help students build an integrated view of the chemical system, by focusing on understanding within each form of access, and promoting transitions between the spheres of knowledge. The macro-level descriptions were used to bridge between the three spheres and support these shifts. The conceptual

framework for the Connected Chemistry curriculum is discussed and demonstrated. Further development directions are suggested.

**Keywords** Chemistry education · Computer models · Agent-based models · Complex systems · Gas laws · Kinetic molecular theory

## Introduction

Consider a single ball’s motion on a billiards table. The ball moves in a straight line, collides with the side and glances off. We can quite easily imagine this scenario and predict successive events. Perhaps surprisingly, so can infants. By the age of 6 months, infants reach their hand out to catch a moving object at an appropriate location and angle to coincide with its trajectory (von Hofsten et al. 1998) and show signs of surprise when colliding objects do not immediately move apart and continue along new paths (Leslie 1984). Thus, it seems we have a robust and early grasp, at least in action and perception regarding the motion of objects.

Now imagine and describe the motions of five, ten or one hundred such balls on a similar table. This task might make us feel confused and definitely out of our depth (or breadth). Relating between a single entity’s behavior and that of many is one of the central tasks and hurdles in learning chemistry (e.g., Dori and Hameiri 2003; Johnstone 1993; Talanquer 2007; Treagust et al. 2003). A deep understanding of many chemistry phenomena involves mentally simulating a population of bodies in motion, locally constrained in a solid and free-form in a gas. A significant proportion of most basic chemistry curriculum is devoted to a focus on individual entities (e.g., atoms and their bonding

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within molecules, symbolic and graphic descriptions of an individual reaction), a necessary and important condition to understanding more advanced topics. However, obtaining a deep understanding of chemical systems involves constructing a mental model that simulates the behaviors of many individual molecules, incorporating their diverse local behaviors as they emerge to global patterns. Such a mental model is fundamental to imagining and reasoning about the particulate nature of matter and is crucial to understanding central concepts, such as chemical equilibrium and chemical dynamics. Transitioning between submicroscopic and macroscopic levels while noticing the local interactions among individual entities is one of the main goals of the curriculum we describe. To this goal, the curriculum recruits this early and deep understanding of objects in motion to learning about the emergent phenomena at hand. Our claim is that it is in this very articulation of the submicroscopic behaviors, noticing and expressing in *specific* and *causal* terms what is well known about objects in motion that our view gradually expands to include local interactions and emergent behaviors.

Now, shifting from submicro- to macro-levels can be done with the math machine, e.g., differential equations that result in a good set of predictions. However, the use of such symbolic relations, while effective and important, removes the learner from reasoning about the actual physical system, thinking from-the-molecule-up which may have guided the construction of such equations. Once constructing these summary statements about the system in symbolic form, often the original molecular explanation that gave rise to them is forgotten, as seen in an abundance of research about the disconnect between students' abilities in solving quantitative chemistry problems and their lagging conceptual understanding (e.g., Nakhleh 1993; Russell et al. 1997; Niaz and Robinson 1992). Students may be adept at 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 conceptual reasoning. Thus, in addition to bridging the submicro- and macro-level behaviors of the system, the curriculum we describe engages with the transitions one makes in shifting between conceptual knowledge and its symbolic forms.

Johnstone (1993) in his insightful analysis of chemistry knowledge speaks of a triangle contained by three components of knowledge: the submicro (atoms, molecules and their kinetics), the macro (tangible, edible and visible phenomena) and representations (symbols of chemical entities, chemical equations and mathematical representations). He describes professional chemists as easily relating among these three components of knowledge and shifting among them flexibly in what he calls thinking "within the triangle". However, when turning to issues of *learning*

chemistry in school, he highlights the problematics of overloading the student's working memory with so many knowledge components and the linkages between them.

In our work with Connected Chemistry, we stand up to Johnstone's challenge of helping students "think within the triangle", understand and connect between these three components of knowledge. Moreover, we address the problematics of guiding such learning and present a conceptual framework to make such connections learnable and fluid. This paper describes the first chapter of the Connected Chemistry (CC1) curriculum, which we abbreviate herein as CC1. CC1 approaches the task of helping students construct a runnable mental model of many moving particles; increase their flexibility in shifting their focus between the individual interacting particles, a collective of many particles and their representation in mathematical terms; in the process deepen their understanding of the role of models in learning and doing science.

The Connected Chemistry (CC1) curriculum is anchored at the experienced macro-level that serves to ground students' reasoning and help them construct flexible linkages with other forms of description and explanation. It is based on a conceptual framework that makes the following claim: activities furthering an understanding of each separate form of access to understanding the chemical system (intra-level experiences), coupled with multiple bidirectional transitions along the three bridges connecting the macroscopic anchor level to the (a) submicroscopic; (b) experiences in the physical world; and (c) symbolic forms (inter-level experiences); constitute a rich and fertile learning environment that supports a deep understanding of the chemical system at hand.

The article has two main foci. First, a general discussion of students' learning about chemical systems with computer models is presented. This is followed by an introduction of the Connected Chemistry framework and its implementation in the curriculum. In the same issue, a separate paper (Levy and Wilensky 2009) reports on students' learning with the curriculum.

## Literature Review

This paper describes the design related to the first chapter in the Connected Chemistry curriculum. This chapter focuses on the gaseous phase, engaging with the concepts of pressure, kinetic molecular theory (KMT) and the gas laws. We review how learning with models can advance students' understanding in chemistry and the potential role of a complexity lens in furthering students' understanding. The paired paper (Levy and Wilensky 2009) reviews students' understanding of the gaseous phase, the focal content in the chapter.

## Multiple Representations in Learning Chemistry

Gabel (1998) attributes students' difficulties in understanding chemistry as due to one or more causes: (1) stress on the symbolic level at the expense of the submicro-level; (2) insufficient linkages between the three components of knowledge described by Johnstone (1993); and (3) the fact that much of the learning does not make explicit connections to everyday life. Treagust et al. (2003) have shown that effective learning in chemistry is related to the simultaneous use of the submicroscopic and the symbolic components of knowledge in chemical explanations. Similarly, Wu and Shah (2004) in their investigation of the role of visuospatial reasoning in learning chemistry proposed the use of multiple representations with explicit connections. Moreover, Ardac and Akaygun's (2004) study points to the privileged status of molecular representations in furthering students' learning. Dori and Hameiri (2003) have formed a framework for analyzing and constructing quantitative problems in chemistry based on two dimensions: the problem's complexity and the transformations between components of knowledge (symbolic-macroscopic, symbolic-submicroscopic, symbolic-process). Their research demonstrates the benefits to learning with a curriculum based upon this framework.

The Connected Chemistry curriculum addresses the problems posed by Gabel (1998) and builds upon the above-described research as the submicro-level is made visible and the framework accents the links and connections between the described components of knowledge.

## Model-Based Learning in Chemistry

A fruitful way of approaching the problem of bridging between levels and forms of representation is through exploring models, external and manipulable representations of the system under study (Gilbert and Boutler 2000). Computer modeling in chemistry education has been a focus of much development and research (e.g., Ardac and Akaygun 2004; Barnea and Dori 2000; Kozma 2000; Pallant and Tinker 2004; Wu et al. 2001).

The complexity of understanding and relating multiple representations presents a serious challenge in designing learning environments. Scaffolding students' learning with models is a central issue since the earlier days of free-form exploration (Horwitz 1999; White 1993) highlighting the necessity of providing supports and partial direction for effective learning to take place within self-directed inquiry environments (Ardac and Sezen 2002; de Jong and van Joolingen 1998; Linn and Eylon 2000). Gobert and Buckley (2000) focus our attention on the interaction between a student's mental model and the external model and its accompanying learning supports, describing how a mental

model forms and changes based on prior knowledge or new information, reinforced, revised or rejected. They describe several pedagogical elements for teaching with models, such as advance organizers, puzzles, representational assistance and several kinds of questions. Veermans et al. (2006) have demonstrated how providing explicit heuristic support (e.g., "simplify the problem" or "explore in equal increments") facilitated students' learning in the domain of collisions. Lee et al. (2006) have shown how manipulating the visual information in the model to reduce cognitive load increased students' learning of the gas laws. Demonstration of surprising phenomena that run counter to students' expectations has been used creatively to launch a model-based curriculum (Snir et al. 2003).

Computer models that make use of multiple representations to support learning of the three components of chemistry knowledge (submicroscopic, macroscopic, symbolic) have been shown to be effective in helping students gain a deeper understanding of chemical phenomena (Ardac and Akaygun 2004; Kozma 2000; Russell et al. 1997; Snir et al. 2003). Creating dynamic, synchronized and simultaneous links between different representations is related to greater learning gains (Kozma 2000; van der Meij and de Jong 2006; Snir et al. 2003). Prompting students to attend to the correspondence between different representations of the same chemical phenomena is related to greater long-term learning (Ardac and Akaygun 2004). Most of the above-described store of design principles for scaffolding students' learning of chemistry with models has been incorporated into the Connected Chemistry curriculum; we also hope to add to this wealth.

An important aspect of learning with models is helping students realize the distinction between models and the physical world they depict, understanding a model's scope and limitations, mapping between the represented and its representation. Gilbert and Boulter (1998) raise a cautioning flag regarding the use of computer models in an exploratory rather than construction mode: "Students usually do not know what the program does with the input figures and often they do not know what the model actually is. In these circumstances, students cannot appreciate the scope and limitations of the model, are not led to a clearer appreciation that any model is an idealized representation and confuse the model with reality" (p. 61). Connected Chemistry approaches this issue in a variety of ways, as we will show.

## A Complexity Lens

This curriculum has grown out of previous work in the domain of physics and chemistry (Stieff and Wilensky 2003; Wilensky 1999b, 2003), in which agent-based models are used to explore scientific phenomena through a "complexity" lens.

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. Complex systems are made up of many elements (often referred to as “agents”), 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). The properties of a system’s patterns cannot be reduced to just the properties of its individual elements (e.g., Bar-Yam 1997, p. 10; Holland 1998). These patterns are often counter-intuitive and unexpected (Casti 1994; Strogatz 2003; Wilensky and Resnick 1999).

The Connected Chemistry curriculum is implemented with the NetLogo modeling environment (Wilensky 1999a). Agent-based modeling is a relatively new computational modeling paradigm, which simulates complex dynamic systems by simulating each of their many autonomous and interacting elements. By observing and experimenting with agent behaviors and interactions, we demonstrate and understand the collective behavior that results from the aggregation of the individual behaviors and interactions. NetLogo (Wilensky 1999a) is a widely used general-purpose agent-based modeling language that enables exploring and constructing models of complex systems. The NetLogo modeling environment is used to program the rules and behaviors of many individual entities, such as people voting at an election, grains of sand pouring down and trees in a forest with a spreading fire. These entities or “agents” operate independently and can interact among themselves. For example, a particular tree will set fire only if there is another tree nearby that is burning. Creating a system from its individuals removes the need for making assumptions at the level of the population, such as the density of trees in the forest. System-wide phenomena emerge through the parallel behaviors and interactions of many such individuals. Phenomena are thus related not only to global characteristics of the system, but to its local attributes as well. For example, a large clearing in a forest may prevent the spread of fire, even if, on average, the density of trees would predict its continuing spread.

Chemistry is a natural domain for such an agent-based approach, as all chemical phenomena emerge from local interactions among a multitude of interacting molecules. Moreover, this topic is gradually becoming more important in the science of chemistry, as nonlinear processes take a more central stage (Epstein and Pojman 1998; Whitesides and Ismagilov 1999). For example, one can construct a model in which each entity is a molecule. The molecule’s motion, interactions with walls and reactions with other molecules are modeled at the individual level. Concurrent

running of many such molecules results in collective behaviors such as reaction rates or containment.

Wilensky’s previous work on learning chemistry and physics with agent-based models (Wilensky 1999b, 2003) engaged students in *constructing* models, a powerful form of learning leading to deep understandings of the domain. Learning through model *exploration* was researched by Stieff and Wilensky (2003). They conducted a study of an earlier development of the Connected Chemistry curriculum on the topic of chemical equilibrium with six undergraduate students. Their findings show that students’ explorations of the NetLogo agent-based models were associated with a shift in the way they explained various phenomena related to the topic and their strategies in solving related problems. This shift involved a move away from rote memory and rigid procedures to problem-solving based on conceptual understanding and logical reasoning.

Our contention is that in the articulation of the submicroscopic behaviors, noticing and expressing in *specific* and *causal* terms what is well known about objects in motion our view gradually expands to include local interactions and emergent behaviors. We have seen this kind of reasoning arise spontaneously among sixth-grade students as they explained a social emergent phenomenon—the scattering of classmates in gym class as they prepare for calisthenics (Levy and Wilensky 2008). Some of the students well described how local interactions and negotiations (e.g., making sure you do not hit each other, move away if there is someone there) emerged into patterns in small groups (e.g., clustering). These very same students also had a deeper understanding of the system as complex, expressing ideas regarding the stochastic nature of the individuals’ behaviors and equilibration processes in the system. Having found this spontaneous strategy among some students and realizing its advantage to reasoning, we have incorporated it into the curriculum.

To summarize the review we have highlighted the importance of helping students make connections between molecular behaviors and tangible macroscopic phenomena, reviewed the use of computer models to advance such learning and presented the complexity view that backgrounds our approach of learning about systems, and more specifically, chemical systems.

## The Connected Chemistry Curriculum

The Connected Chemistry CC1 curriculum (Levy et al. 2006; you are invited to download the curriculum through the provided website link) goals are described, followed by a conceptual framework we have developed to support students’ learning and flexibility in (a) transitioning

between submicroscopic and macroscopic levels; (b) linking conceptual and symbolic descriptions and explanations; and (c) understanding models as powerful yet partial and limited representations of the physical world. We then demonstrate several categories of experience that make up this framework.

Under the umbrella of Connected Chemistry, the Center for Connected Learning and Computer-based Modeling (CCL) has created several curricular units. These Connected Chemistry units focus on topics in chemistry and employ multi-agent NetLogo models (Wilensky 1999a) to enable students' inquiry: creating, manipulating and observing interactions between objects at the molecular level in order to gain insight into emergent patterns and macroscopic phenomena. The diversity of these units reflects the breadth of topics in chemistry that have been approached. More than that, research with these units engages in experimentation with several forms of delivery, distinct in at least two ways. One central distinction is that between *model exploration* and *model construction*. The models used in the herein reported project serve the students in exploring models. They are a modified version of those originally created for the GasLab curriculum, in which students constructed and explored their own models (Wilensky et al. 1999; Wilensky 1997, 1999b, 2003). A second distinction is in the *degree* to which the students' *activities are structured*. An earlier unit involving relatively free-form explorations (CCFF) was created by Stieff and Wilensky (2003) on the topic of chemical equilibrium. This paper focuses on Connected Chemistry chapter one (CC1) that was originally developed as part of the Modeling Across the Curriculum (MAC) project (Gobert et al. 2003), in which high-school students explore computer models in science that are embedded in a supporting script (Levy et al. 2006; Wilensky 2004a, b, c; 2005a, b, c, d; 2006). In the project referred to herein the models are embedded within web-delivered Pedagogica scripts (Horwitz and Christie 1999) that sequence and structure the interaction of the students with the models and record every mouse and keystroke entered by the student. This curricular package could be placed on the more structured side of the above-described continuum. The CCL is still expanding the Connected Chemistry envelope and is generating more semi-structured units, one an adaptation of the CC1 curriculum to a less structured version (CC1F) and their creation of a new chapter (CC2F) on the topic of reactions.

The first set of seven activities in chapter one of the Connected Chemistry curriculum (CC1) is on the topic of gases: gas laws, and kinetic molecular theory (KMT). We begin with these topics rather than with systems involving reactions, as several of the core ideas, e.g., dynamic equilibrium, perturbation and re-equilibration and diffusion may be more learnable when first approached with this

simpler system, in which a particle's identity does not change. KMT describes the rules underlying 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 in symbolic-algebraic form (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).

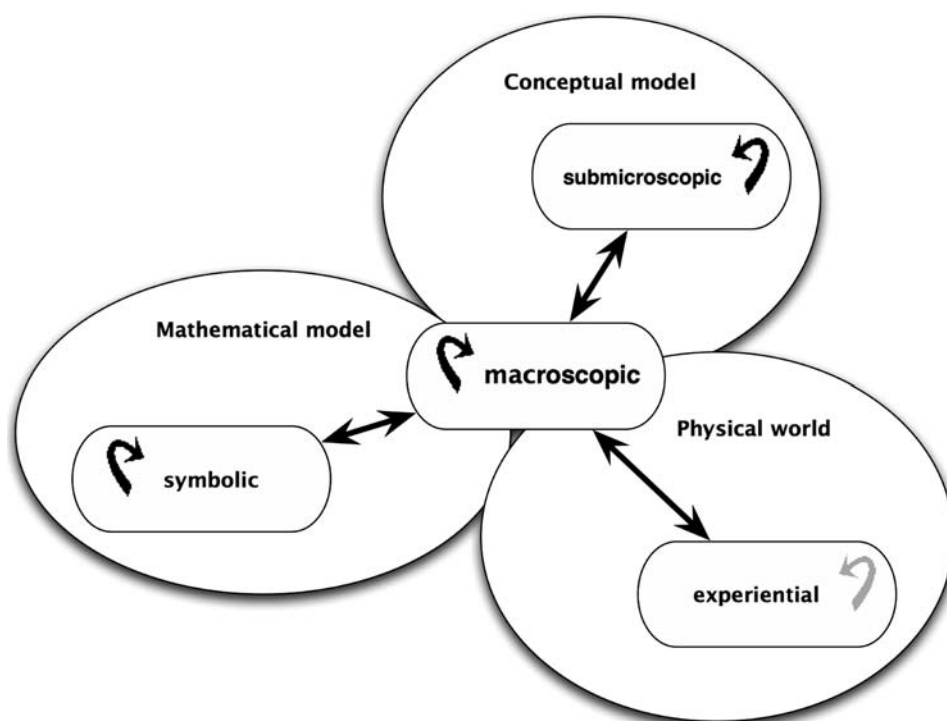
### Connected Chemistry Goals

With Connected Chemistry, our goal is to help students understand the invisible particulate world and connect it to its tangible emergent properties in real-world phenomena as a basis for deep conceptual understanding. The general framework we employ is a complex systems lens (Holland 1995; Kauffman 1995; Jacobson and Wilensky 2006). We find that this lens is particularly suited for understanding chemistry, as it supports focusing on an individual molecule's characteristics and interactions and letting the system's behavior emerge bottom-up. One can observe and come to explain the system's behavior as it evolves, rather than imposing extraneous assumptions regarding the system.

In order to gain a deeper understanding of this complex system's dynamics, Connected Chemistry focuses not only on equilibrium states, but also on *perturbations* and *transitional processes*. These topics are not usually incorporated into normal high school curriculum. Yet we claim that noticing, following and explaining such transitions necessitates more precise explanations, leading to a deeper causal understanding of the system at hand. Thus, the curriculum emphasizes careful observation by calling students' attention to the subtle local interactions and discrepant events, key phenomena in forming a causal understanding of the complex phenomenon at hand. Discrepant events are called in to problematize, promote curiosity and self-directed exploration. Thus, a double-focus on change and equilibrium are unique in viewing the system as complex.

Connected Chemistry addresses the above-described divide between conceptual and algorithmic understanding. Traditionally, students are given the equations that describe the gas laws in their final form. In Connected Chemistry, the students are supported in forging links between symbolic representations and the system's macroscopic behaviors: the curriculum structures the generation of data from the models which is then used to construct the gas laws. Connected Chemistry supports students in forming these equations from the models' behaviors, gradually building up to the Ideal Gas Law; once construction is

Fig. 1 Conceptual framework for supporting learning through model-exploration in the Connected Chemistry curriculum (CC1). *Larger circles* signify spheres of knowledge; *smaller ones* are forms of access to understanding the system; *arrows* signify the activities' learning goals—understanding of each form of access in itself and bridging among them. The experiential level *arrow* is gray because this version of the curriculum does not include physical world activities



completed, the students use these equations to predict the model's behaviors and set out to test them, revising them as needed. Nevertheless, practice in quantitative problem solving is not part of the curriculum and the teachers' guide encourages the use of external sources.

Finally, a central focus in the curriculum is not only on using and exploring models, but understanding how models are made and used, their limitations and affordances for science. To this goal, the students engage in designing theoretical models, make small changes to computational code underlying computer models, evaluate given models, construct mathematical models, critique modeling assumptions, and predict and test the outcome of changing a model's assumptions.

A more detailed description of the curriculum's structure and some of its more pragmatic design principles are provided at the following link: <http://ccl.northwestern.edu/mac>.

#### The Connected Chemistry Conceptual Framework

A conceptual framework was created to guide the curriculum's design and research (Fig. 1), addressing the learning of chemical systems through model exploration. It focuses on three spheres of knowledge: *conceptual understanding* of how molecular interactions emerge into the system's global behavior in a variety of conditions and under various constraints, *symbolic* expressions of the system's behavior and *physical experiences* of the explored

phenomenon. The system is described through its four forms of access: submicro, macro, mathematical<sup>1</sup> and experiential. The framework is *anchored at the experienced macroscopic level* that is common to the three spheres of knowledge and serves as a hub for bidirectional transitions among these forms of access.

The three spheres of knowledge or ways of understanding the chemical system are described and demonstrated. A *conceptual model* of chemical systems engages with both the molecular and the collective level, the submicro- and macro-levels of the system. Explaining how the system's properties and behaviors arise from its components' interactions is central to complex systems in general, and chemical systems as such. Macro-level behaviors such as containment, properties such as pressure and temperature emerge from the behaviors and interactions between submicro-level molecules. In Connected Chemistry, agent-based NetLogo models that compute the system's behaviors from its components support students' manipulation of a variety of constraints (e.g., creating containers) or setting and changing conditions (e.g., changing the temperature of the walls containing a gas). The *symbolic world* includes expressions, in the case of the gas laws, of the system's macro-level properties in mathematical-algebraic form. Interactions with the *physical world* provide for sensorimotor and experiential learning and take place in everyday

<sup>1</sup> When we use the term mathematical here, we refer to aggregate mathematical descriptions such as equations or graphs.

life or in more structured laboratory activities. In Connected Chemistry, everyday experiences are used to ground and frame the learning sequence.

The macro-level form of access anchors Connected Chemistry, as it is common to the three spheres of knowledge and serves to connect between them. The macroscopic level describes the collective behavior of a population of particles in the computer model, such as the rate at which particles hit the walls of a container. The very same level is described through quantifiable characteristics (e.g., temperature, pressure) and is expressed in algebraic representations of the gas laws, the mathematical model. Finally, experience in the physical world takes place at the macroscopic level and serves to ground students' understanding.

Each sphere includes a form of access that is not included in the other spheres: the submicro-level in the conceptual model, the mathematical equations within the symbolic world, and the actual experiences and interactions with the physical world. The macro-level operates as a hub to help connect and form linkages between them.

Our central claim is that *activities furthering an understanding of each separate form and mode of access about the chemical system (intra-level experiences), coupled with multiple bidirectional transitions along the three bridges connecting the macroscopic anchor level to the (a) submicroscopic; (b) experiences in the physical world; and (c) symbolic-algebraic forms (inter-level experiences); constitute a rich and fertile learning environment that supports a deep understanding of the chemical system at hand.*

Activities need to be planned for each level and form of access, so that they are well understood. Furthermore, multiple, varied and bidirectional transitions should be made between them, encouraging flexibility in reasoning and relating these components of knowledge. By direction, we mean the temporal order by which reasoning proceeds in the activity—e.g., starting with a particle, the system or an equation and reasoning from these as givens, connecting and surmising as to another form of access.

Intra-level observation, exploration and reasoning within each form of access are necessary so that non-superficial connections can later be made. In Connected Chemistry, several activities are devoted to understanding the particles' rules and resultant behaviors. Within the macro-level, the students test how changing global properties impact the system, e.g., how the pressure changes when a container's volume expands. Understanding the mathematical equations and how they relate to other symbolic representations such as time-graphs in the model is necessary for a deeper understanding and connection with the model's behavior. In this version of the curriculum, we have not included laboratory investigations, a central activity in deepening student's experiential learning. This results from the general project definition and does not reflect our educational view.

In earlier and later versions of the curriculum, laboratories play an important part.

In Connected Chemistry, bidirectional inter-level bridges between forms of access are constructed and traversed several times in a variety of activities. Within the conceptual model, along the submicro/macro bridge this means changing particle rules and observing the system's resultant behaviors; but also carefully observing how particles are impacted by global system-wide characteristics. Across the conceptual model/physical world bridge, while the models are first ground in experience, they are later used to predict and extrapolate to the physical world. Along the conceptual/mathematical models bridge, equations are constructed from the model's behaviors, but these same equations are then used to predict behaviors in the model.

This conceptual framework is part of a broader view we have developed that concerns multi-dimensional experiences with the submicroscopic world. Our experience of chemical systems is normally focused at the macro-level. However, understanding the molecular level and relating it to the macro-level stands at the heart of a deep understanding of the system. In fact, extending the above-described conceptual framework, so that the micro-level can be approached via all spheres of knowledge provides the substrate for a well-connected conceptual understanding of the system. When students construct agent-based models, they define the micro-level rules that are described through logical and mathematical structures, such as the precise definition of a particle's bounce off a wall. In previous work, we have found that providing access to the formal-symbolic definitions and descriptions of the micro-level entities extends students' understanding significantly (Wilensky 1999b; Wilensky et al. 1999). Experiences in the physical world may be complemented with experiences in the virtual world by having students manipulate and explore the objects and systems made up of such molecular objects. In this paper's framework we focus on understanding the submicroscopic particles through their connection with the system-wide behaviors; however, we view this as part of a more comprehensive map of the kinds of experiences that may be conducive to a well-connected understanding of matter in its several forms of access.

The conceptual framework is further detailed in Table 1 with a large toolbox of categories of experience and their examples. These categories of experience were used to implement the framework in the Connected Chemistry curriculum. In the next section we illustrate several such activities as they play out in the curriculum.

#### Opening the Connected Chemistry Toolbox

The Connected Chemistry toolbox is demonstrated through intra-level experiences focusing on the submicroscopic

Table 1 Connected Chemistry (CC1) toolbox—learning experiences within and between forms of access

Sphere	Form of access <sup>a</sup>	Intra-level experiences	Bridge	Inter-level experiences
Conceptual model	Submicro	<ul style="list-style-type: none"> <li>• Change particle rules and observe a particle's behavior.</li> </ul> <p><i>Ex/Include "bounce" interaction between a moving particle and a wall.</i></p> <ul style="list-style-type: none"> <li>• Program an individual particle with "special" behaviors and explore its local interactions.</li> </ul> <p><i>Make one very fast particle and freeze the rest in place.</i></p> <ul style="list-style-type: none"> <li>• Observe a single particle's history of behavior in space.</li> </ul> <p><i>Make a particle leave a path colored by its speed.</i></p> <ul style="list-style-type: none"> <li>• Focus on individual particles and their immediate environment.</li> </ul> <p><i>Set a spotlight on a particle and follow its interactions.</i></p> <ul style="list-style-type: none"> <li>• Analyze a graph describing a single particle over time.</li> </ul> <p><i>Follow a single particle's speed over time while observing the particle's collisions with other particles and with the wall.</i></p>	Submicro → Macro	<ul style="list-style-type: none"> <li>• Set or change a particle rule and observe the system's behavior.</li> </ul> <p><i>Discover how including an interaction between a particle and a wall emerges into "containment" relationship.</i></p> <ul style="list-style-type: none"> <li>• Manipulate mid-level<sup>c</sup> models that include a small number of particles so that the multiple parallel and interacting character of the system can be observed and analyzed.</li> </ul> <ul style="list-style-type: none"> <li>• Change computational code for particles' behavior and observe resulting patterns and transformations for the system as a whole.</li> </ul> <p><i>Make one very fast particle and freeze the rest; observe how the energy re-distributes; relate to fluctuations in pressure.</i></p> <ul style="list-style-type: none"> <li>• Compare and coordinate a time-plot of an individual particle variable and a related global variable.</li> </ul> <p><i>Compare a single particle's speed with the system's pressure.</i></p>
	Macro	<ul style="list-style-type: none"> <li>• Manipulate global values and observe the system's resultant behavior.</li> </ul> <p><i>Change the container's volume.</i></p> <ul style="list-style-type: none"> <li>• Search for spatial global patterns.</li> </ul> <p><i>Observe how suddenly increasing the volume of the container is followed by the gas flowing into the created vacuum.</i></p> <ul style="list-style-type: none"> <li>• Analyze a graph describing how a certain quantitative aspect of the system changes over time.</li> </ul> <p><i>Analyze fluctuations and changes in pressure and temperature.</i></p> <ul style="list-style-type: none"> <li>• Coordinate two graphs that describe how different quantitative aspects of the system change over time.</li> </ul> <p><i>Explore how increasing a container's temperature impacts the contained gas' pressure.</i></p>	Macro → Submicro	<ul style="list-style-type: none"> <li>• Change a global variable and observe how it impacts individual particles.</li> </ul> <p><i>Observe how suddenly increasing a container's volume is followed by global flow, characterized by faster particles moving into the vacuum earlier than the slower particles.</i></p> <ul style="list-style-type: none"> <li>• Search for local particle behaviors and interactions that can explain macroscopic phenomena.</li> </ul> <p><i>Explain why pressure fluctuations increase and eventually reduce when new particles are added into a container; relate increasing randomness of the particles' direction of movement and the system's process of equilibration.</i></p>
Symbolic world	Mathematical-macro	<ul style="list-style-type: none"> <li>• Compare and relate symbolic representations.</li> </ul> <p><i>Relate between plots of data and canonical function plots to construct an equation.</i></p> <ul style="list-style-type: none"> <li>• Predict physical world situations by calculating with the constructed equations.</li> </ul> <p><i>Use gas laws to predict whether a bicycle tire will burst when heated.</i></p>	Macro → Mathematical	<ul style="list-style-type: none"> <li>• Construct functional and algebraic representations relating global variables.</li> </ul> <p><i>Construct the gas laws via mathematical modeling: run the model at several settings, record data, generate graphs and construct gas laws (e.g. Boyle's Law).</i></p>



Table 1 continued

Sphere	Form of access <sup>a</sup>	Intra-level experiences	Bridge	Inter-level experiences
			Mathematical → Macro	<ul style="list-style-type: none"> <li>Assess constructed equations by predicting values and testing them in the model.</li> </ul> <p><i>Use Boyle's Law to predict the pressure for a specific volume and then test the prediction with the model.</i></p>
Physical world	Experiential-macro	<sup>b</sup>	Physical world → Conceptual model	<ul style="list-style-type: none"> <li>Ground models in physical world objects and phenomena.</li> </ul> <p><i>Consider and reason about pumping up a bicycle tire before a model relating the number of particles to pressure is presented.</i></p> <ul style="list-style-type: none"> <li>Invent a theoretical model.</li> </ul> <p><i>Construct a theoretical model of pumping up a bicycle tire before interacting with the computer model: parts, their features and predicted evolution.</i></p> <ul style="list-style-type: none"> <li>Explore and assess alternative representations in the model.</li> </ul> <p><i>Explore three representations for a particle's speed: None, color-coded by regimes (slow-blue, medium-green, fast-red) and by graduated levels (dark to light purple represents slow to fast); discuss the model's affordances and limitations.</i></p>
			Conceptual model → Physical world	<ul style="list-style-type: none"> <li>Compare model parts, properties and rules with their physical world correlates.</li> <li>Extend the model to the physical world by asking "what-if" questions.</li> </ul> <p><i>Extrapolate how the stability of pressure would compare with the model if the number of particles increased from hundreds to several billions.</i></p> <ul style="list-style-type: none"> <li>Contrast and compare model and physical world in terms of the model's limitations and affordances for understanding.</li> </ul> <p><i>Compare the three-dimensional physical world and the two-dimensional model world and discuss the model's limitations and affordances.</i></p>

*Note* Examples are provided in italic letters

<sup>a</sup> Based on Johnstone's (1993) classification

<sup>b</sup> In a later paper version of the Connected Chemistry curriculum, laboratories are included and provide students with physical-world experiences

<sup>c</sup> Mid-level is an intermediate level between the submicroscopic and the macroscopic, at which a limited number of entities interact, forming group patterns. In previous research (Levy and Wilensky 2008), using mid-level constructs was found to be a pervasive strategy in reasoning about systems

level; and through inter-level bridges between (a) submicroscopic and macroscopic levels in the conceptual model; (b) conceptual model and the physical world; and (c) the conceptual model and the mathematical model. For the sake of brevity, not all categories of experience are presented. Each of the demonstrated experiences references Table 1.

### *Taking a Particle's View*

Understanding how a single particle moves and interacts with other objects in its environment constitutes a significant component in Connected Chemistry. We recruit students' intuitions regarding individual objects in motion to further understand a system of particles. Focusing on a

single particle and keeping view of its behavior, interactions and history, while reasoning about a crowd of particles is a central characteristic of the mental model we wish to foster. To help students grasp this dual view, several enhanced visualization and analysis tools support observation of individuals in a multitude.

Leaving a trail, a history of an individual moving in space, is one such tool, long-used in Logo (Papert 1980) and NetLogo environments (Fig. 2). A particle's color denotes its speed and the path it leaves tells the history of its collisions and energy exchanges ([submicro], “*observe a single particle's history of behavior in space*”, intra-level). For example, one can observe that the rate at which a single particle reaches the wall of a container does not change when there are more particles inside it.

The activity depicted in Fig. 2 demonstrates two more submicro-level activity types. One involves programming particles and changing their behaviors, gaining greater control and understanding of the model's internal computational workings ([submicro], “*program an individual particle with “special” behaviors and explore its local*

*interactions*”, intra-level). In this case, the model run starts out with the particles frozen in place and one very fast particle. The graph on the right depicts the fast particle's speed over time, showing how it first becomes slower through collisions and energy exchange with other particles, but then gains energy in a collision, once the system is close to equilibrium ([submicro], “*analyze a graph describing a single particle over time*”, intra-level).

Expanding the view of an individual particle to include its local interactions is enabled by programming a spotlight that centers and moves with the particle. This helps focus on its local region ([submicro], “*set a spotlight on an individual particle and follow its local behavior and interactions*”, intra-level). The activity in Fig. 3 demonstrates the use of such a spotlight in a mid-level model, a model with a small number of particles that supports reasoning about the parallel processes of the particles' motion and interactions ([submicro → macro] “*manipulate mid-level models that include a small number of particles so that the multiple parallel and interacting character of the system can be observed and analyzed*”, inter-level bridge).

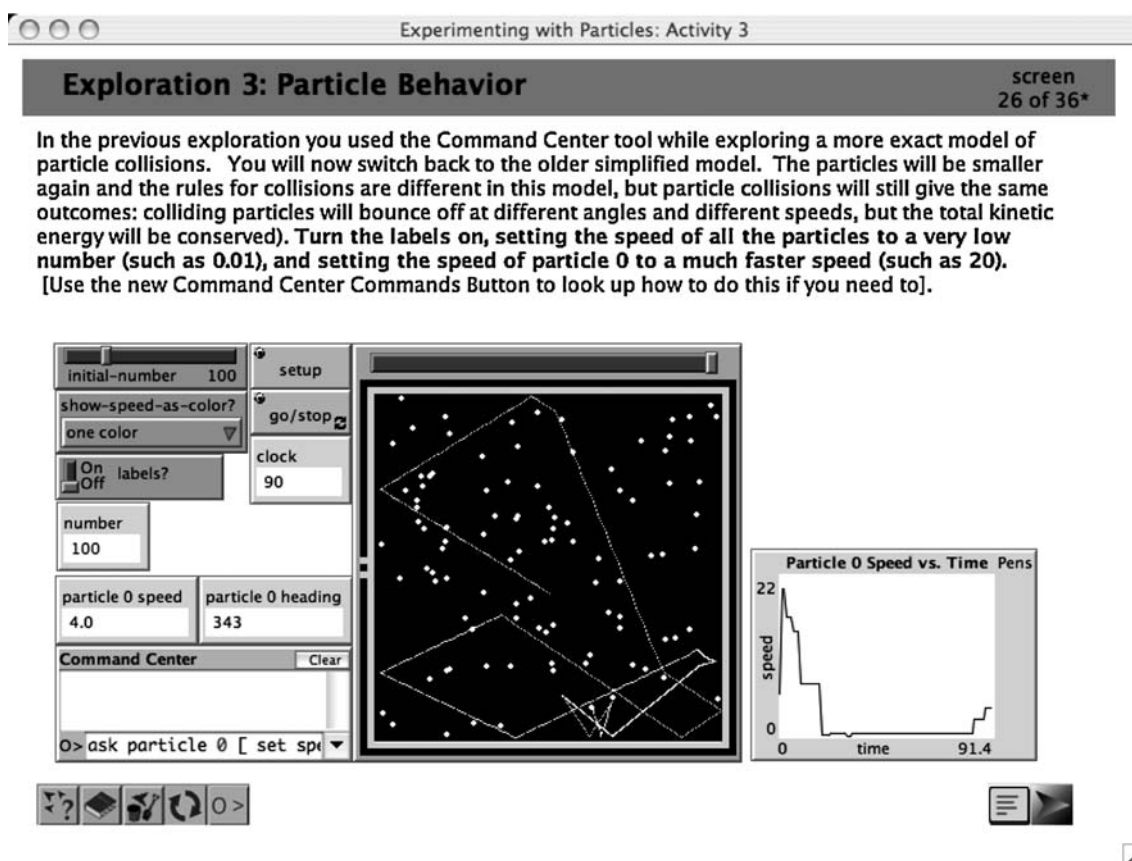


Fig. 2 Screenshot from the “Experimenting with particles” activity, in which the particles' speed is programmed into the model, freezing all the particles but one. This fast particle colors a path as it moves about, and a graph shows its speed over time

Experimenting with Particles: Activity 3

screen  
19 of 36\*

## Exploration 2: The Command Center Tool

Study the motion of one particle.

- 1). Set the INITIAL-NUMBER slider to 2.
- 2). Press SETUP and then GO/STOP.
- 3). Slow the model down using the slow motion slider.
- 4). Use the command center to enter:  
watch turtle 0

This view is helpful for focusing on one particle.

**Question 7. When a particle hits the wall:**

the particles change direction, but not speed

the particles change speed, but not direction

the particles change direction and speed

nothing changes

Yes, only direction changes.

Fig. 3 Screenshot from “Experimenting with particles” activity, showing how one can focus on one particle within the sphere of light, so that its local interactions are more easily viewed

### *Submicroscopic and Macroscopic*

One of the main goals of the curriculum is promoting reasoning “from the molecule up”, a conceptual understanding of how particle behaviors emerge into group patterns. There is a two-way interaction between these two levels. On one hand, explanations of observed phenomena start with causes at the molecular level. In modeling the molecules’ behaviors and interactions, local behaviors emerge into system-wide patterns and phenomena. However, the impetus for exploration may be an observed phenomenon, which takes place at the macroscopic level—physical-world events and situations. Moreover, some interesting observations involve the impact of changes in system-wide features on local events. Thus, the curriculum moves both ways: from the system to its particles’ behaviors, and vice versa.

The curriculum is described with respect to the submicroscopic and macroscopic levels and transitions (Fig. 4). Using Table 1, each question in the activities was coded as relating either to the submicroscopic or to the macroscopic levels, or to the transitions between levels: submicro-to-macro or macro-to-submicro. From this figure, we

conclude: (1) The curriculum shifts from a more submicroscopic 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 activities focus on the gas laws and their derivation via quantitative reasoning; (3) The curriculum includes a large proportion of questions that address the transitions among levels, both submicro-to-macro and macro-to-submicro transitions.

Transitions between levels are demonstrated. In moving from a macroscopic description of the system to the particles, students are asked to notice how the particles’ random motion is related to the stability of pressure (Fig. 5; [macro → submicro] “*search for local particle behaviors and interactions that can explain macroscopic phenomena*”, inter-level bridge).

In the last activity, Ideal Gas Law, the student is asked how adding gravity to the model would impact the system’s behavior. Following this, a model of the atmosphere

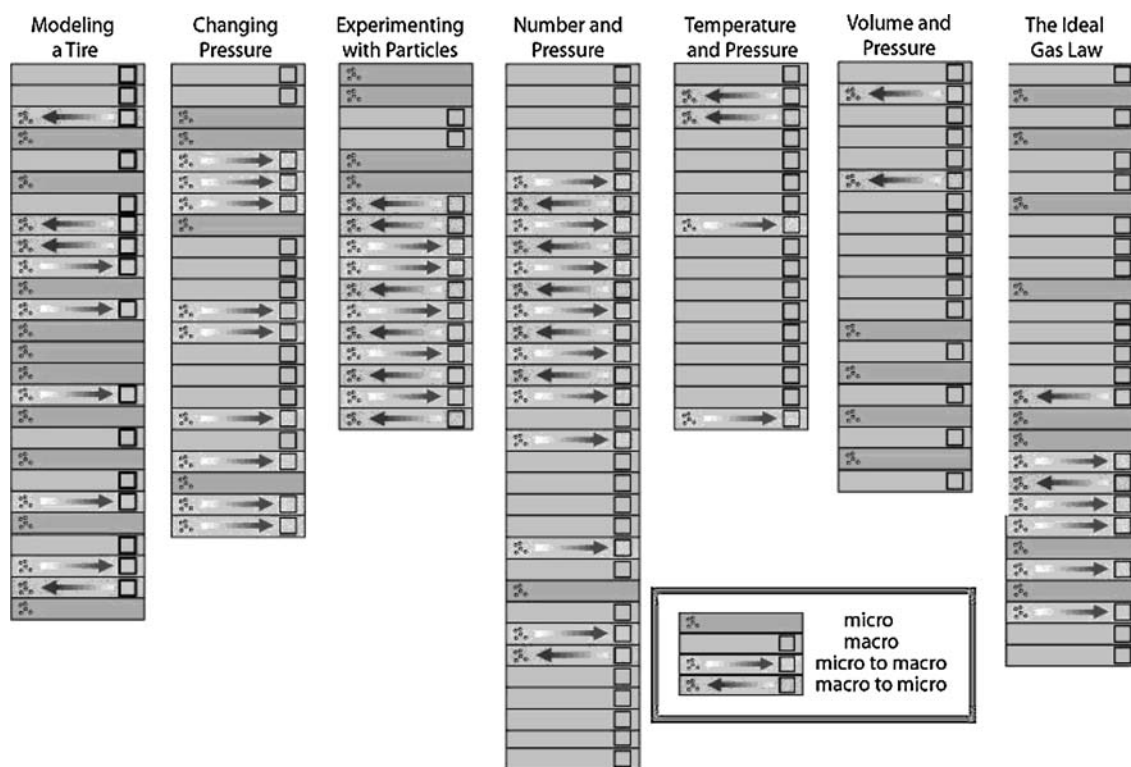


Fig. 4 The submicro/macro levels dimension in the Connected Chemistry (CC1) curriculum. Each bar represents a question addressed to the student

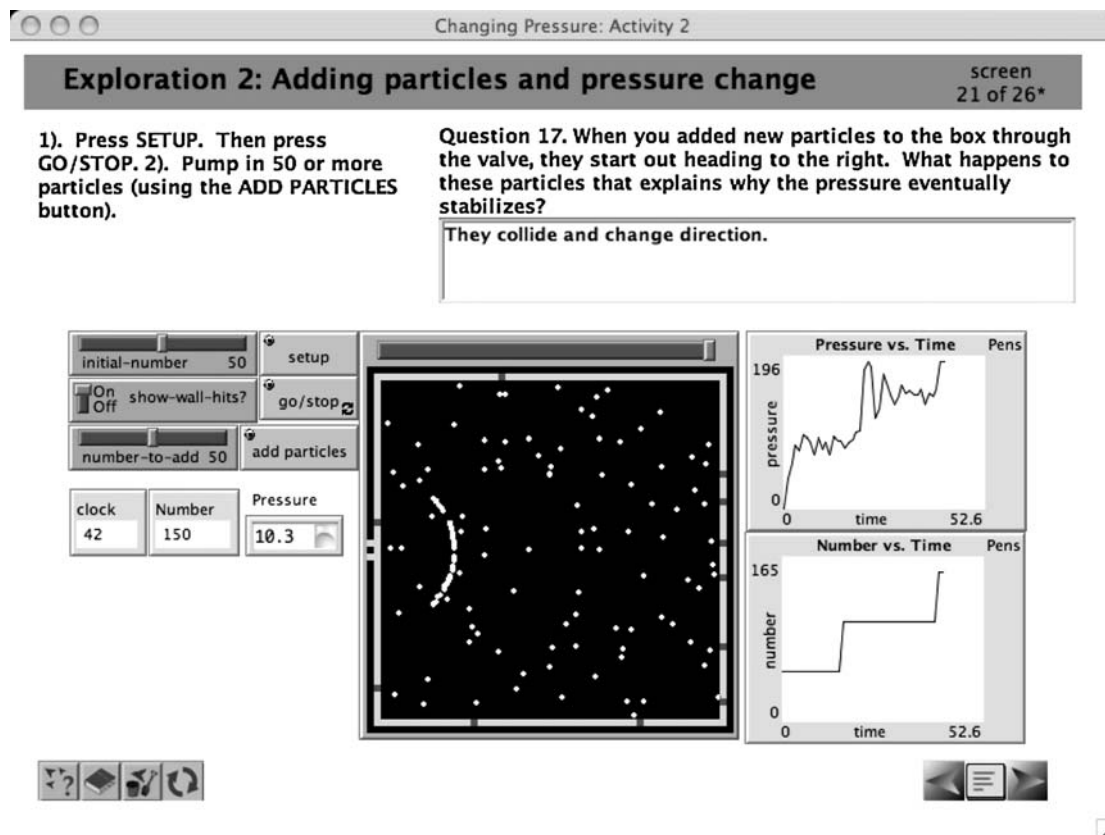


Fig. 5 Screenshot from the changing pressure activity focuses on the pressure fluctuations and how the system equilibrates once the particles' directions are randomized through collisions

is explored (Fig. 6), a model similar to the previous, with the addition of a gravity rule ([submicro  $\rightarrow$  macro] “set or change a particle rule and observe the system’s behavior”, inter-level bridge).

### Model and Reality

Addressing Gilbert and Boulter’s (1998) concern with students’ confusion between models and the physical world they represent, in Connected Chemistry we provoke and facilitate the distinction and connection between models and the physical world. Scientific modeling takes place from the very first activity, even before the first computer model is introduced. The activity is set within a physical-world context of pumping up a bicycle tire ([physical world  $\rightarrow$  conceptual model] “ground models in physical world objects and phenomena”, inter-level bridge). Several questions promote students’ noticing central features; both at a macroscopic and submicroscopic level, exemplifying the principle: [within  $\rightarrow$  between levels] “understand each form of access before bridging between them”. They are then asked to construct a theoretical model of this phenomenon: the students suggest components and their

properties, and mentally simulate the process ([physical world  $\rightarrow$  conceptual model] “invent a theoretical model”, inter-level bridge). Thus the macroscopic level serves as a bridge between the computer model and the physical world, as tangible experiences are represented in the students’ model.

Only later is the computer model introduced, part-by-part (Fig. 7), rule-by-rule; each object in the model is defined and compared with its real-world counterpart ([conceptual model  $\rightarrow$  physical world] “compare model parts, properties and rules with their real-world correlates”, inter-level bridge). This gradual introduction supports a careful contemplation of each component and feature and promotes a growing realization that the model is an artifact, a human-made creation that can be critiqued and changed. In the third “Experimenting with particles” activity, this understanding is enhanced as the students are supported in learning several programming commands, with which they alter the model ([submicro  $\rightarrow$  macro] “change computational code underlying model and observe resulting patterns and transformations”, inter-level bridge). By these experiences, the students participate in constructing the models, while coming to realize what

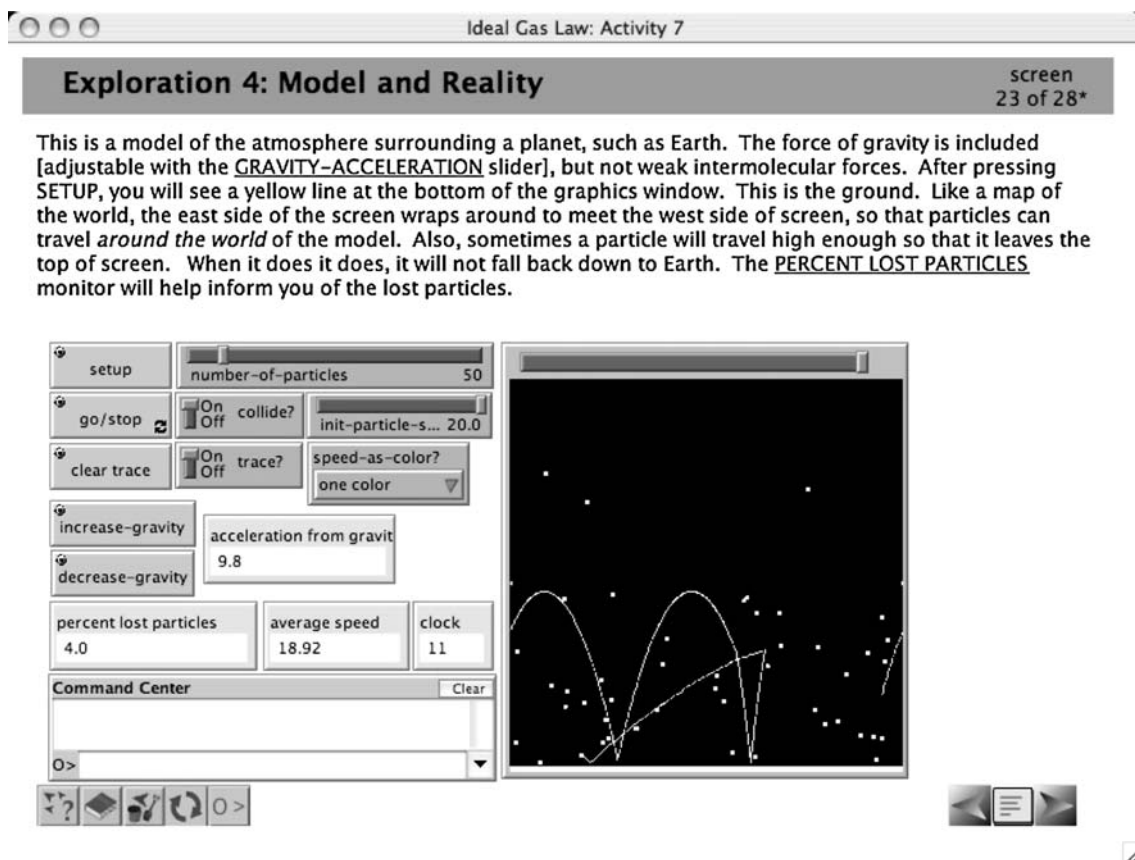


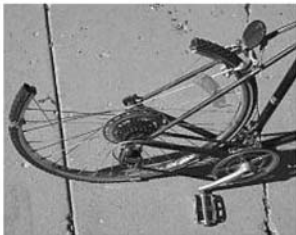
Fig. 6 Screenshot from Ideal Gas Law activity, in which gravity is added to the model

Modeling A Tire: Activity 1


## Exploration 1: Modeling a Bike Tire

screen 6 of 23\*

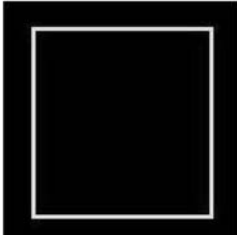
The model you will be using in the remainder of the activity will include only two types of objects: the walls of the tire and the air particles.



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 continuous 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.

Fig. 7 Screenshot from “Modeling a tire” activity, showing the transition and comparison between a real bicycle tire and its representation as a *yellow box* in the model

Modeling A Tire: Activity 1


## Exploration 1: Modeling a Bike Tire

screen 9 of 23\*

If the particles are allowed to move around, you predicted that: The particles will move inside the box.

Follow the directions below to test your prediction:

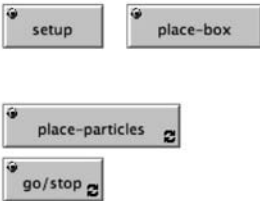
- Below the other buttons on the right is the GO/STOP button. Press this button.
- Try running the model again, while slowing it down by dragging the SLOW MOTION slider on top of the WORLD & VIEW a little bit to the left.



TIP: Careful. If you pull this slider all the way to the left, the model will stop.

Question 7: Did your prediction match what you saw in the model?

Yes  No



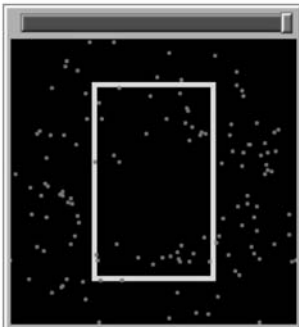


Fig. 8 Screenshot from “Modeling a tire” activity showing the introduction of a new rule into the model by using a discrepant event—at first, only the “move in a straight line” rule is activated and the gas particles are not contained in the box

models are made of and how these materials and human decisions impact their nature and structure.

Rules are introduced progressively as well. We demonstrate how a surprising event motivates the rules' distinction and definition. Figure 8 shows an early activity with the model: only one gas particle rule is activated "move in straight lines" starting with the particles at random headings. Placing a box in the model does not contain the gas particles, and they fly out. Upon adding another rule that defines the interaction between gas particles and the box a containment relationship emerges. This demonstrates the use of *discrepant events* to promote students' careful attention and probing. After the rules underlying the gas particles' behavior have been explored and outlined, KMT is presented and further investigated and tested with the model.

In the fourth activity "Number and Pressure", the construction and exploration of the basic model is revisited and integrated through an activity comparing between the real bicycle tire and the computer model (Fig. 9). The students are encouraged to discuss the impact of such differences upon the validity of the model, demonstrating the ([conceptual model → physical world] "*contrast and compare*

*model and physical world in terms of the model's limitations and affordances for understanding*", inter-level bridge).

In this section, some of the activity types bridging the conceptual model and the physical world it portrays were exhibited. Additional activities include changing a model's assumptions and predicting its behavior; extending a model to the physical world and exploring alternative representations and visualizations.

*Conceptual Model and Symbolic World*

A central goal of the curriculum is to foster an understanding of the symbolic/mathematical representations, which is tightly coupled with a deep conceptual understanding, attending to the frequent disconnect found between algorithmic and conceptual understanding (Russell et al. 1997; Niaz and Robinson 1992). 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. These activities bridge between the conceptual understandings the students develop earlier in the activities through exploring the model and the algebraic symbolic

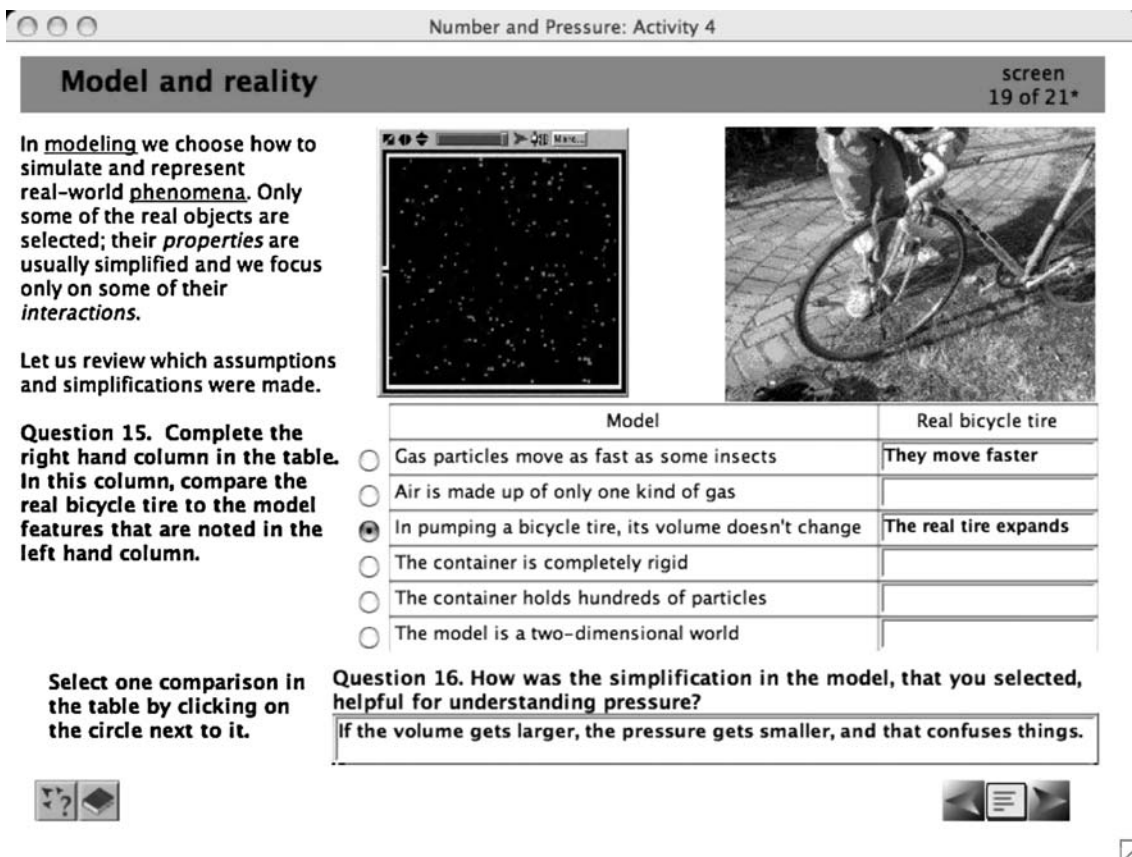


Fig. 9 Screenshot from "Number and Pressure" activity, in which students compare between the model and the physical world phenomenon represented by the model

representations, commonly exercised in traditional curriculum ([macro → symbolic] “construct functional and algebraic representations relating global variables”, inter-level bridge). The students explore the model, capture data regarding macroscopic variables into a table, obtain a scatter plot of the data and compare it to canonical relationships. From the canonical relationship, the students construct the algebraic equation (Fig. 10). This process is highly guided at first, with gradually fading scaffolds. In constructing the Ideal Gas Law (made up of four variables), the students can traverse an independent or a more guided path. Notice how different mathematical representations are presented and bridged in the second screenshot ([symbolic] “compare and relate symbolic representations”, intra-level).

This equation is later used to calculate values for new states, predict and then test this prediction with the model ([symbolic → macro] “assess constructed equations by

predicting values and testing them in the model”, inter-level bridge).

### Summary

In our depiction of Connected Chemistry we have focused on three bridges that connect to the common macroscopic form of access of the chemical system and serve to connect between the conceptual model, the symbolic world and the physical world. We have proposed that activities within forms of access need to precede such bridges, paving the way for a deeper and integrated conceptual understanding of the chemical system.

### Conclusion

The Connected Chemistry (CC1) curriculum was launched to help students construct an understanding of matter in the

**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.  
3). Repeat steps 2-4, four more times, keeping the number of particles the same (constant) but changing

Level	Volume	Pressure
1	600	654
2	935	431
3	1375	285
4		
5		

**Exploration 2: What equation connects the volume to pressure?** screen 18 of 30\*

Below are four representations of the data you collected:  
- 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.

**Your Data Chart**

Level	Volume	Pressure
1	600	654
2	935	431
3	1375	285
4	2090	174
5	2970	118

**Exploration 2: What equation connects the volume to pressure?** screen 19 of 30\*

Use your data from the model to determine which of the three mathematical descriptions below best represents the relationship between the temperature and the pressure. We represent the Volume and the Pressure in the following way:  
V for Volume, and P for Pressure

**Question 15. Which relationship best describes your data?**

Linear  
 Inverse  
 Quadratic

**Exploration 2: What equation connects the volume to pressure?** screen 20 of 30\*

You have found a **inverse** relationship between pressure and the volume.

Your result matches an equation that scientists have discovered when investigating gases!

Scientists describe the mathematical relationship as follows:  
Pressure (P) changes **inversely** as a function of the volume (V) and a **constant** that relates the two variables (k):

Knowing that P and T are inversely related might help you reason out what the equation that relates P, V, and k will look like.  
**Question 16. Write an equation below that you think could be used to calculate the pressure of the gas. USE k and V and the math operation symbols +, -, ×, /, and parenthesis if you need them to complete the equation.**

$$P = k / V$$

Tip for finding division or multiplication symbols on your keyboard: The division symbol / is located on the same key as the question mark. The multiplication symbol can be represented with the letter x or using shift-8 which gives the symbol \*.

Fig. 10 A sequence of four screenshots from the “Volume and Pressure” activity, portraying construction of Boyle’s Law through experimenting with the agent-based model



gaseous state, one that would help them reason with both the individual molecules and their emergent collective behaviors. Several guided activities and tools were developed to help them view, manipulate and reason about single particles and the system.

We return to the scenario introduced in the opening of this paper, that describing rolling balls and collisions on a billiards table. Connected Chemistry recruits our early and deep understanding of solitary bodies in motion to learning about the emergent phenomena at hand. The curriculum engages students in manipulating, observing, predicting and testing out various configurations for five, ten and a hundred such balls in the NetLogo simulations. Our claim is that it is in this very articulation of the submicroscopic behaviors, noticing and expressing in *specific* and *causal* terms what is well known about objects in motion that our view gradually expands to include local interactions and patterns, and finally relate the system's emergent behaviors.

The curriculum focuses on furthering conceptual understanding of the phenomena at hand but does not lose sight of the need to connect this understanding to the symbolic level. By guiding students in *constructing* such representations instead of only testing their veracity we hoped to help them form a strong linkage between conceptual and algorithmic understanding. This is also a specific advantage in using the models as a laboratory.

Finally, we have addressed the issue of students' understanding of models as a human-made artifact, a representation and not a depiction of their physical world. With the curriculum, the students form theoretical models, critique its representations, compare the model with reality and reason with "what-if" questions that involve changing the model's underlying rules. Moreover, they plunge their hands into the innards of the model, changing its computer code and effecting changes.

Approaching the multiple goals of supporting students' learning about models, learning with models and connecting among different kinds of models has urged us to form a unifying conceptual framework (Fig. 1). This framework is anchored at the macroscopic experienced level that serves to connect the conceptual model, the mathematical model and the physical world, understanding and then bridging between the submicroscopic, macroscopic, symbolic and experiential forms of access. Understanding each form and representation precedes bridging between these forms. Bridging takes place in two directions. We have demonstrated several activities that address each of the framework's components, some of these may serve as new design principles, which can be investigated individually in future research.

However, the value of this framework is its generalizability to the learning of any complex system. Students' experience relates to chemical systems at the macro-level,

which connects and anchors the curriculum. For other systems, it is possible that the submicro-level is the experienced level, such as individuals in ecosystems. Further research into learning about different types of systems, could further test and extend this framework.

In a second paper in this issue (Levy and Wilensky 2009), this framework is transformed into research questions and students' learning with Connected Chemistry is explored.

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