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Chapter 6
MODELS AND MODELING

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DEFINITIONS OF MODEL AND MODELING

The Oxford English Dictionary notes that the term *model* can be used as a noun or adjective that means: "A simplified or idealized description or conception of a particular system, situation, or process, often in mathematical terms, that is put forward as a basis for theoretical or empirical understanding, or for calculations, predictions, etc.; a conceptual or mental representation of something." The kinetic molecular theory would be an example of such a model.

The OED also notes, however, that the term *model* can be used as a verb in the following sense: "To devise a (usually mathematical) model or simplified description of (a phenomenon, system, etc.)." For our purposes, we will use the term *modeling* to describe attempts to construct a model of a system.

Various attempts have been made to describe characteristics of a model within the context of science education, including.

- A model is a representation of an idea, object, event, process, or system [1], which concentrates attention on certain aspects of the system — thus facilitating scientific inquiry [2]
- Mental models represent significant aspects of our physical and social world, and we manipulate elements of these models when we think, plan, and try to explain events in that world [3].
- A model relates to a target system or phenomenon with which we have a common experience or set of experiences [4].
- Models are mental entities that people construct with which they reason; all of our knowledge of the world therefore depends on our ability to construct models of it [5].
- Scientific models are conceptual systems mapped onto a specific pattern in the structure/behavior of a physical system within certain limits of reliability [6].

Harrison and Treagust [7] argued that "modeling is the essence of thinking and working scientifically" and differentiated between analogical models, such as scaled or exaggerated objects, symbols, equations, graphs, diagrams and maps, on the one hand, and simulations used in model-based thinking, on the other hand. Greca and Moreira [8] tried to distinguish between *mental models* that exist within the mind of an individual and *physical models* that are shared among members of a community as follows: "... whereas mental models are internal, personal, idiosyncratic, incomplete, unstable and essentially functional, conceptual models are external representations that are shared by a given community, and have their coherence with the scientific knowledge of that community."

Gilbert [1] clarified the use of the term *model* by differentiating between four closely related ideas. A *mental model* is the product of an individual's cognitive activity; an *expressed model* is produced when a mental model is placed in the public domain through action, speech, or writing; a *consensus model* is an expressed model that has been accepted among a community of scientists; and a *teaching model* is an expressed model that was specifically developed to help understand an historical or conceptual model.

An important aspect of teaching models was revealed in interviews conducted by Grosslight, et al., [9] that probed students' understanding of the role of models. They noted that 7th-grade students often view models as "little copies of real-world objects." Even 11th-grade students "... still fundamentally see models as representations of real-world objects or events and not as representations of ideas about real-world objects or events." Readers interested in additional information on the research literature on the use of models and modeling in chemical education should refer to the recent review by Justi and Gilbert [10].

MODELS AND MODELING IN MATHEMATICS EDUCATION

Particular attention has been paid to the use of models and modeling in mathematics by Lesh and co-workers [11, 12]. Lesh argues that models can be used to describe a system, to think about it, to make sense of it, to explain it, or to make predictions about it. Thus, models can be predictive, interpretative, and/or analytic, not just examples of the system to which they refer. Models are tools that embody characteristics of phenomena that theory defines as important [13]. The theory can be as simple as "naive" conceptions held by a beginner or as complex as carefully studied scientific hypotheses. Because models provide the basis for drawing inferences, they enable new knowledge to be created from former knowledge.

MODEL-BASED LEARNING

If Harrison and Treagust [7] are right — that the construction and evaluation of models is the essence of scientific thinking — one might conclude that model-based learning should be an explicit part of science courses. Lesh [11, 12] has provided a basis for model-based learning in the form of "model-eliciting activities." The products that students produce as a result of a model-eliciting activity go beyond the short answers to narrowly defined questions that have dominated our classrooms for so many years. These products involve "sharable, manipulatable, modifiable, and reusable conceptual tools (e.g., models) for constructing, describing, explaining, manipulating, predicting or controlling ... significant systems" [13].

Lesh and co-workers argue that traditional textbook word problems are difficult for many students because they require the students to make sense of symbolically described situations. Model-eliciting activities, they argue, are different because they are based on real-life situations for which students have to construct symbolic descriptions. Within the context of mathematics, where model-eliciting activities were first developed, the activity usually involves "mathematizing" a real-world situation — quantifying, dimensionalizing, coordinatizing, categorizing, algebratizing, and systematizing relevant objects, relationships between objects, actions, patterns, and regularities. Lesh and co-workers note that students given model-eliciting activities often invent, extend, refine, or revise constructs that are more powerful than anybody has dared to try to teach them using traditional methods [14].

Lesh and Doerr [12] describe the traditional view of problem solving as the process of getting from givens to goals when the path is not obvious. They note, however, that problem solving in the traditional classroom is constrained to answering questions using facts and rules that are restricted in ways that are artificial and unrealistic. Our favorite example of this phenomenon is a question from one of the National Assessment of Educational Progress exams that asked 8th-grade mathematics students: If a piece of wood 7' 3" long is cut into three equal pieces, how long is each piece?

The accepted answer was: 2' 5".[1] Unfortunately, the only place in which this answer could be achieved is the traditional mathematics classroom. In the real world, each piece would be 2' 4¾" or, if the saw blade was thin enough, perhaps 2' $4^7/_8$".

Lesh and Doerr [2] argue that bringing a models and modeling approach to problem solving would emphasize "important aspects of real-life problem solving, which involves developing useful ways to *interpret* the nature of givens, goals, possible solution paths, and patterns and regularities beneath the surface of things." They note that the process of getting the answer to real-life problems involves "... 'modeling cycles' in which descriptions, explanations, and predictions are gradually refined and elaborated."

Let's look at a model-eliciting activity developed for use in a middle-school math class.

- John is constructing a recreation room in his basement. He has put up the walls and put down a floor. He needs to buy baseboard to put along the walls. The room is 21 feet by 28 feet. The baseboards come in 10-foot and 16-foot lengths. How many of each kind should be buy?
- If John wants to have as few seams as possible, how many of each size baseboards should he buy?

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[1]Purists might note that one could obtain three equal pieces that are all 7' 3" long inasmuch as the problem does not specify the direction in which the cut was made. But this answer is never accepted.

- If John wants to have as little waste as possible, how many of each size should he buy?
- If the 16-foot boards cost $1.25 per foot and the 10-foot baseboards cost $1.10 per foot, how many of each kind should he buy if he wants to spend the least amount of money?
- There is a sale on the 16-foot baseboards. They now cost $0.85 per foot whereas the 10-foot baseboards still cost $1.10 per foot. How many of each should he buy if he wants to spend the least amount of money?

Like so many others, this model-eliciting activity is based on a “real-world” problem that takes the activity to the student, rather than trying to construct a virtual world in which the student has to come to the instructor. Model-eliciting activities differ from traditional problem solving activities because they are designed to help students adapt, refine, and modify many of the concepts they already have, and find new ideas to apply to a problem.

Lesh and co-workers [11] have enunciated six principles upon which the design of model-eliciting activities should be based. These principles involve the following guiding questions.

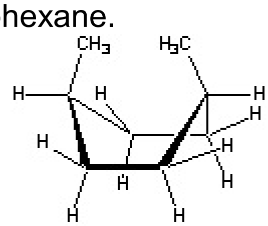
- The model construction principle: Does the task put the students in a situation where they recognize the need to develop a model for interpreting the givens, goals, and possible solution processes in a complex, problem solving situation?
- The reality or meaningfulness principle: Could this happen in a real life situation?
- The self-assessment principle: Does the problem statement clearly indicate appropriate criteria for assessing the usefulness of alternative solutions? Will the students know when they are finished with the problem? Is the purpose clear?
- The construct documentation principle: Will responding to the question require students to reveal explicitly how they are thinking about the situation by revealing how they took into account the givens, goals, and possible solution paths?
- The construct shareability/reusability principle: Is the model that is developed useful only to the person who developed it and applicable only to the particular situation presented in the problem, or does it provide a way of thinking that is shareable, transportable, easily modifiable, and reusable?
- The effective prototype principle: Does the solution provide a useful prototype, metaphor, or “tool” for interpreting other situations?

The fact that model-eliciting activities were first developed in mathematics education does not mean that they are not useful or applicable to chemistry, only that less explicit attention has been paid to the models and modeling perspective by chemists. We have begun the construction of model-eliciting activities for use in chemistry, the first of which deals with the mental rotation of the structure of molecules for use in a sophomore-level organic chemistry course [15].

INTRODUCING A MODELS AND MODELING PERSPECTIVE

The first step toward bringing a “models and modeling” perspective to your course is relatively easy. If you are teaching general chemistry you could start by helping your students understand the meaning of the term “law” when it is used in the context of Boyle’s law, or Charles’ law, or Dalton’s Law of Partial Pressures. Our experience has shown that many students in introductory courses believe that a “law” is “something that must be obeyed.” In fact, this term is used in the sense of a mathematic equation — or “model” — that fits experimental data, more or less, under certain conditions and within certain limitations [16]. At various points during the course you might build on this idea to convey the notion that one of the ways scientists think is in terms of constructing, evaluating, refining, adapting, modifying, and extending models that are based on the experiences with the world in which they live and work.

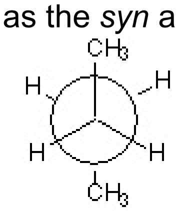
Instructors might bring a “models and modeling” approach to their organic chemistry courses if they recognize the limitations of discussions of steric effects in the boat conformer of *cis*-1,4-dimethylcyclohexane.



For at least 40 years, organic textbooks have noted the steric repulsion between the two methyl groups in this conformer, often talking about “bowsprit-bowsprit” repulsion [17]. It is almost 40 years, however, since the first author built a molecular model of this compound, only to find that the hydrogens on one methyl group didn’t seem to “touch” the hydrogens on the other.

He now knows that this is a “models and modeling” problem. The mechanical models of organic compounds we assemble from pieces of plastic or steel and the representations of these molecules we build on our personal computers are based on a “hard-sphere” approximation, in which it is assumed that hydrogen atoms are relatively small compared with carbon atoms. If you calculate the distance between the carbon atoms of the two methyl groups in the conformer shown above (3.38 Å), however, you’ll find that it is much larger than the sum of traditional estimates of the size of the relevant atoms (≈3Å).

A similar problem arises when one tries to build a model that would explain the steric repulsion in such common examples as the *syn* and *anti* conformers of *n*-butane.



The distance between the two methyl groups is simply too large to allow for interactions of the magnitude described in introductory organic textbooks.

The source of the problem, once again, is the hard-sphere approximation for the size of hydrogen atoms [18]. The steric effect in either *cis*-1,4-dimethylcyclohexane or *n*-butane can be understood more easily if one thinks about this interaction in terms of a model based on the van der Waals radius of hydrogen, which is more than three times as large as the covalent radius of this atom. Once this is done, the steric effect organic chemists talk about becomes immediately apparent. If one wants to quantitate this interaction, one can think about it in terms of the Lennard-Jones "6-12" potential:

$$\mu = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

where σ reflects the closest distance between the particles undergoing through-space attraction or repulsion and ϵ reflects the depth of the potential well. According to recently reported values of the Lennard-Jones parameters [19], repulsion between the two methyl groups in 1,4-dimethylcyclohexane would occur when the distance between the carbon atoms of these methyl groups is less than 0.373 nm and, as we have seen, the distance between these methyl groups is only 0.338 nm. According to the recently reported values of the LJ 6-12 potential, the magnitude of the repulsion between these methyl groups should be about 7 kJ/mol.

The instructor who brings a models and modeling perspective to the sophomore organic chemistry course would be likely to discuss the limitations of the model of the structures of organic molecules based on the traditional hard-sphere approximation that serves as the foundation for our model sets. But, regardless of whether this topic is addressed explicitly in the course, this individual would be ready to explain the apparent dichotomy between the information in the textbook and models of organic compounds when a student raises the question.

Perhaps the best example of a "models and modeling" approach to instruction might involve the first semester of the traditional physical chemistry course [20]. The first lecture typically looks at PVT relationships and reminds students of the ideal gas law:

$$PV = nRT$$

The second lecture introduces the van der Waals equation, which could be written as:

$$(P + \frac{n^2 a}{V^2})(V - nb) = nRT$$

but is often written as:

$$(P + \frac{a}{\bar{V}^2})(\bar{V} - b) = RT$$

where $\bar{V}$ is the volume per mole of gas in the sample.

As they discuss the van der Waals model of the behavior of a gas, some instructors compare the results of predictions based on the ideal gas law and the van der Waals equation for a given substance, at a given temperature and volume. Instructors who bring a “models and modeling” perspective to this class wouldn’t stop by noting that the predictions of the van der Waals equation are initially smaller and then inevitably larger than those of the ideal gas equation. They would go one step further. They would compare the predictions of these models with the pressure observed experimentally [20]. Consider the following results for one mole of CO_2 at 100°C as one gradually decreases the volume of the container.

	Ideal Gas Equation	*Van der Waals Equation*	*Experimental Value*
30.6 L:	1.00 atm	0.998 atm	0.998 atm
1 L:	30.6 atm	28.4 atm	28.5 atm
0.200 L:	153.1 atm	104.8 atm	110.5 atm
0.100 L:	306.2 atm	174.9 atm	182.6 atm
0.0500 L:	612.4 atm	2740.7 atm	629.7 atm

When the experimental data are included one finds that the van der Waals equation is not always a better model of the behavior of the real gas. It provides no advantage at pressures near one atmosphere and it “blows up” — as might be expected — when the volume of the gas starts to resemble the value of the “b” constant in the van der Waals equation.

Instructors who take that extra step in the beginning of their PChem class would set the stage for helping their students recognize that one of the goals of PChem is the construction *and testing* of models of the behavior of chemical systems; that one of the goals of the PChem class is to bring “modeling” to the forefront of our discussion of what chemists do [21].

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