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Undergraduate Chemistry Students' Conceptualization of Models in General Chemistry

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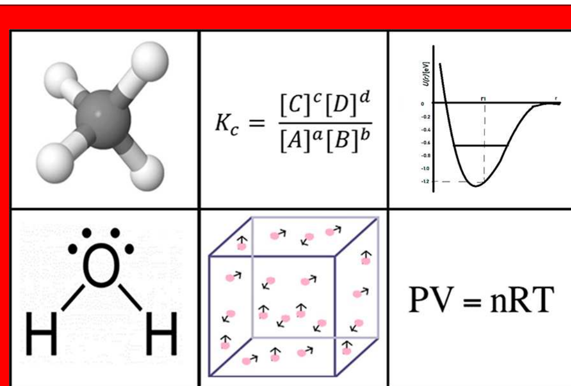
Supporting Information

Understanding the nature and purpose of models, including mathematical models, is critical to enabling undergraduate chemistry students to use models to predict and explain phenomena. However, students often do not have systematic conceptions about different kinds of models. To gain a sense of how students understand different models in the general chemistry curriculum, we developed a survey to examine students' reasoning about models generally and in some specific contexts within the general chemistry curriculum. The findings suggest that students have some productive ideas about what kinds of representations are scientific models and the characteristics of those models; however, students may not recognize these characteristics in models which are mathematical or graphical in nature.



Chemical Education Research, First-Year Undergraduate/General
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■ INTRODUCTION

The development and use of scientific models is a critical aspect of scientific inquiry and is especially central to chemistry, a discipline grounded in predicting chemical behavior at the macroscopic scale by considering processes and interactions at the molecular level.[1] In this study, we define models as tools which can take many forms, including diagrams, words, equations, and graphs,[2] and which serve as explanatory or predictive tools for making sense of real-world phenomena.[3] Undergraduate-level chemistry students encounter several types of models, including models of atomic-molecular structure (e.g., the historical Bohr model) and models of particulate-level behavior and interaction (e.g., kinetic molecular theory as embedded in the ideal gas law), which highlight the causal mechanisms that drive macroscopic chemical phenomena.[4] Students also encounter mathematical models, such as the well-known Boltzmann formula, $S = k_B \log W$, which serve as important bridges between the molecular and macroscopic scales.

The National Research Council's *A Framework for K-12 Science Education* (The Framework) identified the development and use of scientific models as one of eight practices that scientists engage in as they seek to understand the natural world.[5] Prior research has shown that engaging students in realistic scientific practices such as modeling promotes the development of deeper understanding of both content knowledge and the nature of the scientific endeavor.[5−10]

While several studies have focused on students' abilities to engage in constructing and using models,[8−12] fewer have examined students' ideas about the nature and purpose of scientific models and modeling.[7] This type of knowledge, which includes ideas about the nature of models, the purpose of models, evaluation and testing of models, and model multiplicity, has been referred to as *metamodeling knowledge*.[7,8,13,14] Scholars have argued that the development of epistemological knowledge, including metamodeling ideas, is required to fully understand both the nature and purpose of scientific inquiry[15] and content knowledge.[16−18] Indeed, research has shown that students who hold more sophisticated epistemological views tend to approach learning more actively and develop better conceptual understandings of science content.[16−18] With respect to metamodeling knowledge specifically, previous studies have found that integrating explicit scaffolds for the development of metamodeling knowledge within the context of model-based instruction supports students' content learning and their understanding of the nature of scientific inquiry.[7]

While most students are exposed to a number of scientific models in introductory chemistry courses,[19,20] these courses do not usually address metamodeling knowledge explicitly. Although some researchers have examined students' ideas

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about scientific models,[7,8,21−27] this work is domain-general. The study presented here examines students' epistemological ideas about the nature and purpose of models in chemistry contexts. Understanding students' epistemological ideas within the context of a traditional general chemistry course will provide an important baseline for curricular development aimed at improving students' knowledge of models and their ability to construct and use models. The research questions guiding the study include the following:

1. What types of representations do undergraduates consider to be scientific models?
2. What characteristics do undergraduates assign to scientific models?

In the following section, we briefly review the relevant literature on the assessment of students' ideas about models and modeling in chemistry and K−12 science contexts and discuss the theoretical perspectives that inform the study. We then report the results of a qualitative analysis of students' responses to open-ended questions about which types of representations common to the chemistry curriculum they consider to be scientific models and why.

Literature Background

Prior characterizations of students' ideas about models and modeling in chemistry contexts have largely focused on domain-general assessments of students' metamodeling knowledge. For example, Treagust et al.[21] developed the SUMS (Students' Understanding of Models in Science) instrument, a Likert response format instrument designed to assess students' metamodeling knowledge. The SUMS instrument is based on prior research on students' ideas about models including the work of Grosslight et al.[25] and Treagust et al.[28] Using factor analysis, the authors identified five subscales: models as multiple representations (MR), models as exact replicas (ER), models as explanatory tools (ET), uses of scientific models (USM), and the changing nature of models (CNM).[21]

Researchers have used SUMS to assess the efficacy of model-focused curricula[29−32] and to characterize the metamodeling knowledge of various student populations including students in high school and middle school biology, physics, and chemistry.[8,21,29−32] Gobert et al.[30] administered SUMS to high school students in biology, physics, and chemistry contexts and demonstrated that students' metamodeling knowledge is discipline-dependent. Biology students exhibited the most naïve ideas (according to mean differences in the MR, ET, and USM subscales) while physics students exhibited the most sophisticated ideas.

In addition to this evidence of discipline specificity, there is also evidence that students' ideas about different aspects of modeling, such as their ideas about how models are used and evaluated, develop independently. German researchers Upmeier zu Belzen and Krüger[33] and Grunkorn et al.[34] developed a "model of model competence" based on open-ended survey responses of seventh through tenth graders to questions about the five dimensions of metamodeling knowledge: nature, purpose, testing, changing, and multiplicity of models. Krell et al.[13] later used latent class analysis to show that students can have differing levels of understanding about each aspect of metamodeling knowledge, which supports the idea that students do not obtain such knowledge in a single, global process, but rather must develop knowledge related to each unique aspect.

The same authors also demonstrated the discipline-specificity of students' metamodeling knowledge in a later study. They asked secondary students to rank a series of statements about each of the five dimensions of metamodeling knowledge; statements were framed with either general or discipline-specific (biology, chemistry, and physics) contexts.[14] Across disciplinary contexts, they found that students tended to think of biological models in descriptive ways (Level 1), but chemical and physical models more often in explanatory and predictive ways (Level 2−3), perhaps owing to differences in how models are used in the disciplines.

Krell and Krüger[22] also found differences between undergraduate and graduate students' thinking when asked about models in general versus in specific disciplinary contexts. They used an open-ended survey to elicit students' ideas about both models in general and the models used in their declared discipline of study. The authors reported that university students expressed less "prospective", or expert-like, ideas about specific models than about models in general.

While several studies have investigated students' general metamodeling ideas, fewer have focused on metamodeling knowledge in the context of chemistry.[14,30,31] To date, no studies have focused on metamodeling knowledge specific to certain types of models such as mathematical and graphical models. Our own previous work addressing general chemistry students' reasoning about rate laws (in the context of method of initial rates tasks) suggests that students may not recognize the empirical basis of rate laws and that this lack of recognition may be related to a tendency to engage with mathematical models algorithmically.[35,36] Because previous studies have established that students' metamodeling knowledge is context-dependent,[13,14,30] understanding how undergraduate students think about specific types of models, including the mathematical models used in introductory chemistry, is important for the development of curricular resources that support students' development of epistemological knowledge.

Theoretical Perspectives

Our understanding of students' reasoning about models in chemistry is informed by the resources perspective, which was initially developed to describe the ways in which different types of knowledge elements or "epistemological resources" contribute to students' reasoning about physics.[37] Epistemological resources include knowledge about the various ways in which knowledge comes to be and the forms that knowledge takes, or more narrowly, knowledge about how models, one form of scientific knowledge, are developed and used.

Epistemological resources are described as intuitive ideas that arise through the generalization of experiences that inform students' ideas about the nature of knowledge.[37] Students' epistemological resources are neither stable nor inherently correct or incorrect; rather, they are dynamic and highly sensitive to context, and it is the context in which they are activated that determines whether students' ideas are productive or unproductive for making sense of the world.[37]

Students obtain and retain epistemological resources because they were at some point a productive tool for attaining knowledge. The following scenario illustrates the use of epistemological resources. When faced with an unfamiliar task, such as solving a novel physics problem, students may automatically activate a seemingly useful epistemological resource, for example, the understanding that knowledge can be acquired by memorizing the solutions from the textbook.[37]

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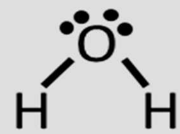
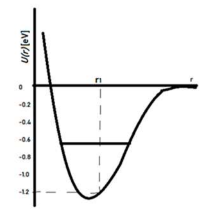
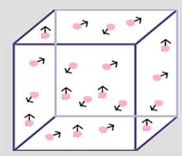
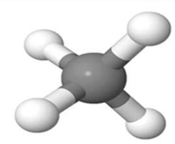
Table 1. Six Models Included in the Models in Chemistry Survey

Model	Description	Associated representation
Lewis structure	Lewis structures describe connectivity in molecules. They can be used to determine bonding and non bonding pairs of electrons in molecules and to predict connectivity and polarity in molecules.	
Potential energy diagram	Potential energy diagrams illustrate the relationship between potential energy of a system of interacting atoms and the distance between them. Such diagrams may be used to predict bond length and to explain why interactions at distances closer than the bond length are unfavorable.	
A diagram showing particulate-level motion and spacing	Particulate-level representations embody key aspects of kinetic-molecular theory and could be considered models when used by students to predict or explain chemical reactivity of macroscopic behavior.	
Physical model of a molecule	Physical models embody aspects of VSEPR theory and could be considered models when used to predict interactions with other molecules by considering geometry and polarity	
Equilibrium constant expression	Equilibrium constant expressions represent the ratio of products to reactants in a system at equilibrium. An equilibrium constant expression is used to predict how far a system will proceed towards completion.	$K = \frac{[NO_2]^3}{[N_2O_5][NO]}$
The Ideal Gas Law equation	The Ideal Gas Law equation represents relationships between factors influencing gas behavior in ideal systems. It can be used as a predictive tool, and when coordinated with Kinetic Molecular Theory, an explanatory tool.	$PV = nRT$

While memorizing is not a particularly practical strategy for learning science, it may have been a necessary and useful strategy in prior instances (e.g., memorizing vocabulary for a Spanish exam). A more appropriate epistemological resource for solving a novel physics problem, and one most students possess, is the understanding that they can "figure out new things from knowledge they already have".[37] Importantly, a student's use of nonproductive resources does not necessarily indicate that the student lacks productive resources, but rather that they fail to employ or "activate" a more productive resource. The aforementioned student, for example, likely knows that new knowledge can be attained by making connections to existing knowledge, but instead chose to gain knowledge by memorizing information in a textbook. From this perspective, the effectiveness of instructional practices is based on their ability to help students learn to identify and activate the most productive resources in novel contexts.[37]

This study draws on the idea that students approach the development and use of scientific models in chemistry contexts with certain epistemological resources related to the nature and purpose of models, which represent knowledge of the natural world. Some students possess and use productive and coherent epistemological resources related to models, but others fail to identify and employ productive resources when discussing scientific models in chemistry or do so only in certain contexts. In this study, we discuss the difficulties students face as they seek to employ productive epistemological resources in their discussion of various types of chemical models. In addition, we examine the context-dependence of students' metamodeling knowledge, which can be theoretically interpreted as a failure to activate resources in appropriate contexts rather than "incorrect" knowledge about models.

METHODS

Here, we report findings based on students' answers to questions about what types of representations they would consider as scientific models in chemistry; these questions were asked as part of an open-ended survey developed by our research group (Models in Chemistry Survey or MCS). Here, we report on our analysis of students' responses to questions 9−23 of the MCS, which address students' reasoning about items they listed as examples of scientific models, and about students' ideas about specific types of representations that are common to the general chemistry sequence; the first eight

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Table 2. Model Type Codes and Definitions[a]

Model Type	Definition
Scale	Models that highlight external structure or proportions
Pedagogical/analogical	Teacher-created models used to highlight other structural features such as the arrangement of atoms
Iconic and symbolic	Models that use discipline-specific written language or symbols
Mathematical	Models that quantitatively represent relationships between variables, for instance in the form of equations or graphs
Theoretical	Models that describe the unobservable entities believed to be responsible for natural occurrences
Maps, diagrams, and tables	Visual, often simplified, representations of natural phenomena
Concept-process	Patterns or rules that describe natural processes
Simulations	Computer models that allow users to visualize and interact with simplified versions of complex processes

[a]As adapted from Harrison and Treagust's[4] typology of school models.

questions of the MCS address students' ideas about the nature, purpose, changeability, and evaluation of scientific models. Findings from these questions will be discussed in another manuscript. The full survey is included as Supporting Information.

Modeling Survey Tasks

Model-Listing Tasks. We asked students to list two items they would consider to be scientific models and then explain why they would consider each to be a scientific model.

Representation-Classification Tasks. We asked students to indicate whether they considered six representations commonly used in the general chemistry sequence to be scientific models. To identify representations that, according to our definition, could also be considered scientific models when used to predict or explain chemical behavior, we surveyed documents such as the ACS Exams Institute's Anchoring Concepts Content Map (ACCM)[19,20] and common general chemistry texts (e.g., *Chemistry: The Central Science* by Brown et al. [2012][38]). The six representations we selected as well as a brief explanation of each are shown in Table 1. In the representation-classification tasks, students were asked to (1) indicate whether they considered the representation to be a scientific model and (2) explain their reasoning.

Participants and Data Collection

Participants and Setting. Participants were students enrolled in the first semester of a two-semester introductory chemistry sequence at a research-intensive university in the midwestern United States. Lectures were the predominant mode of instruction in the course. The course textbook was the 12th edition of *Chemistry: The Central Science* by Brown et al.[38] Students were concurrently enrolled in laboratory, case study, and discussion sections of the course. Case studies were intended to prepare students for the laboratories and help them apply chemistry to real-world scenarios, while discussion sections, which were led by teaching assistants, served as problem-solving sessions.

Development and Administration of the Models in Chemistry Survey. In the spring of 2017, we piloted the Models in Chemistry Survey (MCS) with first-semester general chemistry students. The pilot assessment included 23 forced-choice and open-ended questions. Question prompts were informed by the extant literature on metaknowledge about models and modeling[7,39] and the specific chemistry models discussed in the general chemistry course. At the end of the survey (administered via Qualtrics), we asked students to indicate whether they would be interested in participating in an interview outside of class time.

To examine the response-process validity of the survey items, we conducted interviews with eight students who had completed the pilot survey and had agreed to be contacted. We used a maximum variation sampling approach to select participants whose responses represented the range of responses to the pilot survey. Interviews were video recorded, and students used a Livescribe pen[40] for any written work. Participants received a $10 gift card as compensation for their time. During the interviews, students were asked to complete the tasks in the MCS again, this time describing their thought process aloud as they did so.

We then analyzed the data from the pilot survey and the interviews, focusing on how well the students' responses addressed the target construct in each question. We were especially interested in construct-underrepresentation (i.e., not measuring the full range of the intended construct) and construct-irrelevance (i.e., measuring constructs outside the scope of the intended construct).[41] On the basis of this analysis, we modified, expanded, or eliminated several survey questions.

We administered the revised survey in Fall 2017. The final version of the MCS is composed of 23 forced-choice and open-response questions on models and modeling as well as a series of demographic questions (see Supporting Information [SI] for the full survey). We administered the survey online via Qualtrics the week before final exams in the fall of 2017. Therefore, the results of this study reflect students' metamodeling knowledge after completing nearly a full semester of undergraduate introductory chemistry.

Students who completed the survey received three extra credit points. Students were given the option to decline to have their survey data used for research purposes and received extra credit points regardless of research participation. Of the 1,017 students in the course, 864 participated in the assessment. Twenty students completed the survey twice; the second set of responses for each of these students was excluded. Twelve students were under the age of 18 and thus were excluded from the sample, and 79 students did not consent to have their data used for research purposes. Therefore, 773 students were included in the final sample, which translates to a response rate of 85.0%. Almost all the students were 18−21 years old (93.9%). With regard to gender identification, 52.7% identified as female, 45.7% identified as male, and <1% identified as nonbinary (1.0% did not respond). Most were in their first semester in college (79.6%). Institutional Review Board approval was obtained for all data collection.

Data Analysis

To analyze the data collected via the MCS, we developed deductive coding schemes based on literature accounts of students' knowledge about the nature and purpose of

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Table 3. Deductive Codes and Definitions[a]

Code	Definition
Accuracy	Student response indicates that a model should accurately reflect some aspect of a system's behavior or structure. Students in this category do not necessarily use the word accurate but may allude to the accurate nature of models via a discussion of validity, correctness, reliability, consistency, or other concepts related to the accuracy of models.
Coherence	Student response indicates that a model should fit with everything that is known about the domain. In particular, a model should cohere with other models to form an integrated theory of the domain.
Generality	Student response indicates that a model should account for as wide a variety of phenomena in the world as possible.
Parsimony	Student response indicates that a model should be as simple as possible, but no simpler.
Usefulness	Student response indicates that a model should have potential application to understanding and predicting the behavior of the modeled system.

[a]As adapted from White et al.[39]

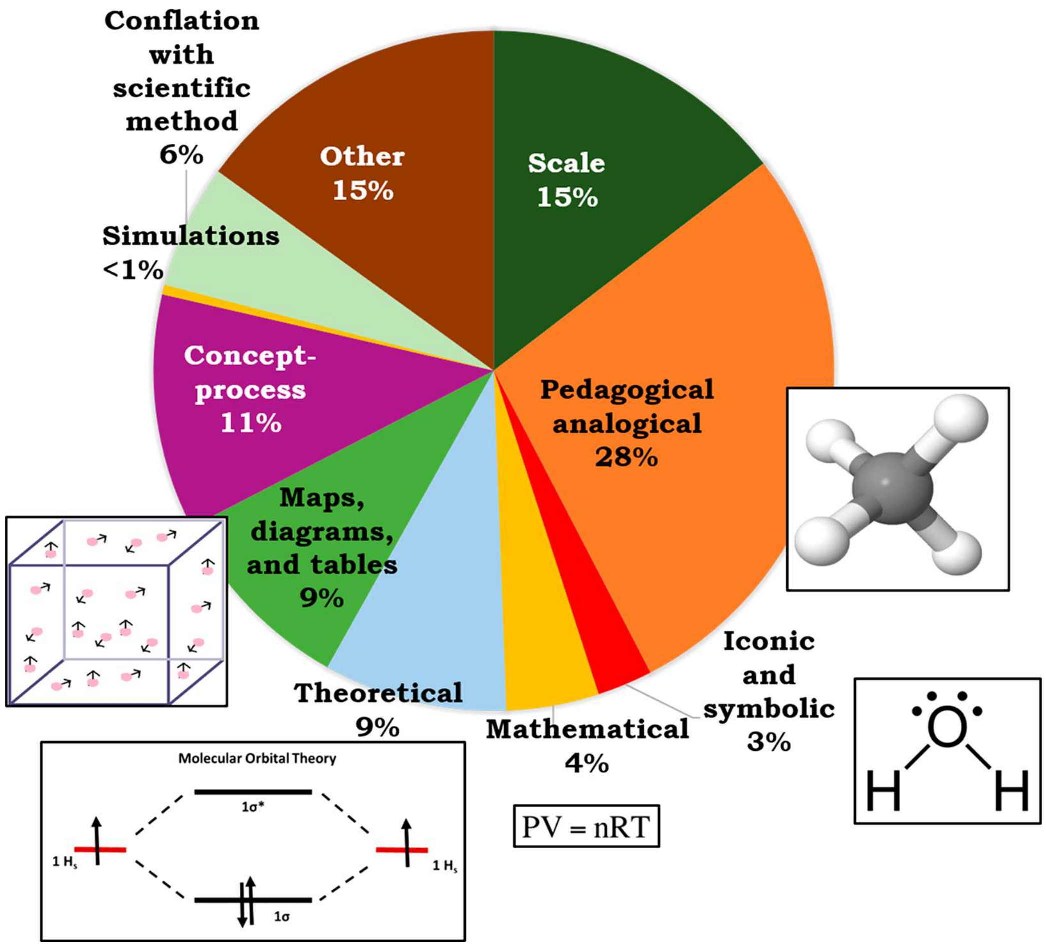

Figure 1. Student-listed models categorized according to Harrison and Treagust's[4] typology of school models and inductive analysis. Inductive categories include "conflation with scientific method" and "other" categories; n = 1,546.

models.[4,39] In addition, we used inductive coding to capture emergent themes that did not fit the deductive codes.[42]

Responses to the Model-Listing Tasks. For the analysis of the responses to the two model-listing tasks, we adapted Harrison and Treagust's[4] typology of school models. This typology includes eight types of models, as shown in Table 2.[4] We added two additional inductive codes based on emergent themes, which we discuss in detail below. (See SI for complete code definitions and examples.)

Analysis of Student Reasoning about Characteristics of Models. To analyze students' reasoning processes about why they would or would not consider a representation to be a model, we developed a deductive coding scheme based on White et al.'s[39] discussion of model characteristics. According to White et al., there are five key characteristics of scientific models: accuracy, coherence, generality, parsimony, and utility. Accuracy addresses how well a model reflects some aspect of the target phenomena and/or explains experimental observations. Coherence addresses how well the model fits with what is known about the target phenomena. Generality relates to a scientific model's ability to explain or predict a range of phenomena. Parsimony addresses the ways in which a model simplifies the elements of the target system and highlights others. Finally, Usefulness relates to the ways in which a model can be used to predict or explain aspects of the target phenomena. Our definitions for these codes are summarized in Table 3. For student ideas that did not fit the codes in Table 3, we used an inductive approach to capture emergent themes in students' reasoning.

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Table 4. Subthemes Emerging from Inductive Analysis of Students' Discussion of Model Usefulness and Associated Frequencies (%)[a]

Inductive Codes Addressing Students' Ideas about Model Usefulness	Student Responses (%)
Usefulness-Other: Responses address the use of models for solving problems; alternately, students mention model usefulness without further discussion	9%
Usefulness-Show/Teach: Student response explicitly mentions the potential uses of models such as showing, displaying, describing, or representing a phenomenon; teaching about a phenomenon; or making the phenomenon easy to understand	36%
Usefulness-Explain: Student response refers to models as useful for explaining why or how a phenomenon occurs.	17%
Usefulness-Predict: Student response refers to the utility of models for predicting phenomena. This includes both responses that make a general reference to prediction and responses that explicitly refer to specific phenomena that models can be used to predict.	6%

[a]Frequencies here represent the percentage of all student responses (N = 773) which discuss utility of models for the specified purpose.

Analysis of Students' Ideas about Model Usefulness. We noted early on in our analysis that the theme of model Usefulness was the most prevalent in our data and that there was considerable variation in the ways students talked about model use. As such, we used an inductive analysis and the constant comparative approach[42] to document themes in the way students discussed the usefulness of models. Our final coding structures included both the deductive codes and codes capturing emergent themes. Refer to SI for the complete set of code definitions and examples.

In our analysis of student reasoning in both the model-listing and representation-classification tasks, we applied as many codes as necessary to capture students' ideas. For responses to the representation-classification tasks in which students indicated a representation was "not a model", we observed that students listed characteristics of models that the representations lacked. As such, we used the same coding scheme (Figures 3 and 4) to capture students' ideas about which model characteristic(s) the representation lacked.

Reliability. To assess the reliability of the coding process, we performed an inter-rater reliability study. For the model typology coding scheme, the first author acted as the primary coder and the second author independently coded approximately 20% of the data (150 randomly selected responses). The calculated values of inter-rater agreement (81.3%) and inter-rater reliability (0.78, Cohen's kappa) provide substantial evidence of reliability.[43]

For the model characteristics coding scheme, the second author acted as the primary coder and the first author independently coded approximately 20% of the data. Because multiple codes could be applied to each student response (a one-to-many coding scheme), we used the Fuzzy-kappa statistic, an inter-rater reliability statistic based on Cohen's kappa and modified for the application of multiple codes to a single response.[44] The calculated values of inter-rater agreement (88.1%) and inter-rater reliability (0.81, Fuzzy kappa) indicate "almost perfect" consistency for the application of the model characteristics coding scheme.[43,44]

■ FINDINGS

In this section, we present the results of qualitative and quantitative analyses of the data on the types of representations that undergraduate general chemistry students consider to be scientific models. We also discuss students' reasoning about what makes a representation a scientific model.

Student-Identified Models

For the task in which we asked students to list two items that they would consider scientific models, we used Harrison and Treagust's[4] typology of school models to classify student responses. Of the items listed by students, 28% fit Harrison and Treagust's[4] profile of pedagogical/analogical models (Figure 1). Models of this type included 3-D molecular modeling kits and Bohr's model of the atom. The high frequency of pedagogical/analogical models is perhaps not surprising given that the only time metamodeling ideas (e.g., multiplicity of models and the changing nature of models) were discussed explicitly in the focal course (a lecture-based general chemistry course) was in the early weeks when various historical models of the atom were presented. The second-most common category of student responses was scale models (15% of responses), which included responses such as "a model of the solar system" or "model airplanes".

Less commonly mentioned model types included iconic-symbolic models (e.g., Lewis structures, chemical equations; 3%), mathematical models (e.g., equations, graphs; 4%), and theoretical models (e.g., molecular orbital theory diagrams and VSEPR; 9%). This distribution of responses is noteworthy because these three types of models were used frequently in the course. The low frequency with which students listed these types of models suggests that representations such as Lewis structures and mathematical equations are not salient examples of scientific models.

Of the students who listed two items that could be classified according to Harrison and Treagust's[4] typology, 34% listed two of the same type of model. An additional 21% listed a pedagogical/analogical model and a scale model. No students included scale models pertaining to chemistry. This observation supports our earlier claim that although general chemistry students are exposed to a wide variety of model types in the general chemistry sequence, they may not recognize these representations as scientific models.

Some students listed items that did not fit into Harrison and Treagust's typology[4] (21% of responses). Using inductive analysis, we observed two main themes in these responses. First, 6% of responses referred to elements of the scientific method, for example, "observations", "hypotheses", and "results". This pattern suggests a possible conflation of the scientific method and scientific models. Second, 15% of responses referred to specific scientific phenomena (e.g., "water boils") or physical entities (e.g., "atoms", "the solar system") as examples of models (we classify these responses as "other"). On the basis of our definition of modeling, we consider these the target phenomena rather than the model and, thus, these responses reflect conflation between the model and the target system.

Reasoning for Model-Listing Tasks

After students listed things that they would consider as scientific models, we asked them to discuss *why* they would consider them to be models. The majority of student responses

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addressed characteristics of models and the ways in which models could be used. We characterized students' ideas about model characteristics using codes adapted from White and Fredrickson's[39] discussion of characteristics of scientific models (Table 3) and used an inductive analysis to capture emergent themes that did not fit these codes.

Model Usefulness. In students' explanations of why they classified certain items as scientific models, students mentioned model usefulness most frequently. The idea of model usefulness was mentioned in 48% of all responses. As noted earlier, we observed a range of ways which students discussed model usefulness and used inductive analysis to capture this variation (Table 4). Most commonly, students talked about models as tools for showing, representing, or describing some aspects of the target phenomenon. Some students also mentioned that this kind of showing may be useful for teaching others or helping people to understand a phenomenon (Usefulness-Show/Teach: 36% of student responses).

For example, one student who listed a ball-and-stick model of a molecule (a pedagogical/analogical model according to our analysis in Figure 1) noted that "[It] gives a visualization of an otherwise not observable object for ease of understanding" (Usefulness-Show/Teach). Our interpretation of this response is that this student considers models as supports for understanding something about unobservable processes.

A second theme in students' ideas about the usefulness of models related to the use of models in explaining experimental results and how or why a phenomenon occurs (Usefulness-Explain; 17%). For example, one student who listed J. J. Thomson's plum pudding model of the atom (a pedagogical/analogical model) explained that he would consider it a scientific model because "it was a proposed explanation of observed data. Even though it was later proved to be not true, it still represented a reasonable explanation of how and why the data was as it was" (Usefulness-Explain). Here, the student seems to suggest that the plum pudding model of the atom enabled explanations of experimental observations, and in doing so, this highlights explanatory power as a key feature of models.

A third theme in students' ideas about the usefulness of models related to the predictive power of scientific models. This was the least prevalent theme, with only 6% of student responses discussing the predictive power of models. For instance, a student who listed a model of weather systems reasoned that the model "helps us understand the way weather systems work and [helps us] predict them" (Usefulness-Predict). While it is unclear what, specifically, this student thinks can be predicted (i.e., weather behavior based on weather models), her response clearly suggests that an important and defining characteristic of some scientific models is their predictive power. Interestingly, most students who discussed the predictive power of models listed models from biology or geoscience, and few students mentioned models of chemical phenomena.

We also saw a small number of responses that discussed the usefulness of models generally, or for solving problems (9% of responses). For example, one student who listed "an equation" as an example of a scientific model noted that an equation "is a set rule and method that you follow to reach a conclusion" (Usefulness-Other). We interpreted the student's description of using rules and methods to reach a conclusion as a reference to solving quantitative problems algorithmically. The student did not reference the broader predictive utility of such mathematical models or the way in which a model provides insight into the target system.

Infrequently Discussed Model Characteristics. Students discussed the other four of White et al.'s[39] characteristics of a good scientific model quite infrequently compared to model usefulness: 3% of responses mentioned accuracy, 1% addressed generality, 3% discussed parsimony, and 1% addressed coherence.

Students who discussed accuracy most often focused on the ways in which models represent or depict a target phenomenon, in contrast to discussing the accuracy of explanations of or predictions about a target phenomenon. For example, one student who discussed a human anatomy model explained that the model "provides an accurate (or close to accurate) portrayal of the actual human body" (Accuracy). Here, the student's reference to "accurate (or close to accurate)" to us suggests attention to the exactness of the model's representation of the elements of human anatomy. The student also mentions that models may be only "close to accurate", which perhaps suggests some recognition of the role of parsimony in scientific modeling.

Students who discussed model generality most often mentioned that a particular model could be used to represent many different atomic-molecular species. For example, one student noted that Bohr's model of the atom "can be applied to atoms of all elements" (Generality). This response refers to the ability of Bohr's model to represent the structure of an atom regardless of its elemental identity.

Many students who discussed parsimony recognized that models are often simplified versions of reality that highlight specific, relevant features or variables of a system. Another student who listed Bohr's model of the atom noted: "It shows the nucleus and its electrons in a simplified but still fairly accurate way. It's not exactly how electrons behave, but it's pretty close and that's good because electrons are very complicated" (Parsimony).

The few students who discussed coherence noted that models should be consistent with previous research and findings in other fields.[39] For example, one student wrote about "the atomic model": "It demonstrates the atom to the best of our knowledge, based on all of the research humans have ever done" (Coherence).

Other Emergent Themes. In addition to coding the responses based on White et al.'s[39] five characteristics, we added inductive codes to account for student reasoning that did not fit these model characteristics.[8] We identified three additional types of justifications students offered for classifying an item as a scientific model: (1) the relationship between a model and experimental results, (2) the representational form of a model, and (3) the ontological status of the representation.

The first theme, that models are related to experimentation or empirical data, accounted for 20% of responses. Students in this group commented on the fact that models are built on or tested via empirical observations. Indeed, evolution based on emerging evidence from experiments is a key element of models—Krell and colleagues[13,14,22] highlight this evolution as a metamodeling idea distinct from the nature and purpose of models. One participant stated: "I would consider [a model of] climate change a scientific model because it is also based on decades worth of data" (Related to experimentation). Other students noted that models are tested empirically and evolve over time. For example, one student explained that "the

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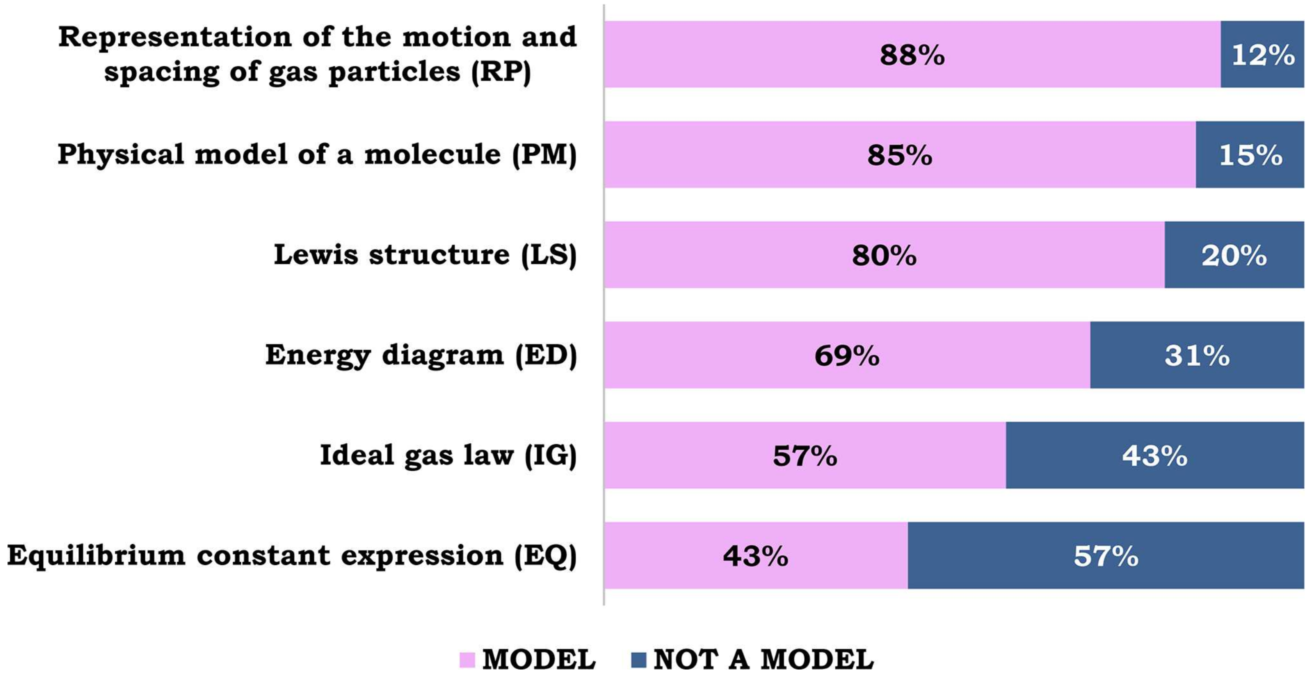

Figure 2. Participant responses to the chemistry-specific representation-classification tasks; N = 773.

Table 5. *p*-Values for Pairwise *t*-Tests between Proportions of Students Who Classified These Representations as Scientific Models[d]

	Physical model of a molecule (PM)	Lewis structure (LS)	Energy diagram (ED)	Ideal gas law (IG)	Equilibrium constant expression (EQ)
Representation of the motion and spacing of gas particles (RP)	ns (0.45)	ns (0.09)	sig (< 0.001)	sig (< 0.001)	sig (< 0.001)
Physical model of a molecule (PM)	-	ns (0.33)	sig (< 0.001)	sig (< 0.001)	sig (< 0.001)
Lewis structure (LS)		-	sig* (0.02)	sig (< 0.001)	sig (< 0.001)
Energy diagram (ED)			-	sig (0.0028)	sig (< 0.001)
Ideal gas law (IG)				-	sig (< 0.001)

[d]Significance indicated for α = 0.05 and Bonferroni-corrected α = 0.003, N = 773; *sig at α = 0.05, ns at α = 0.003.

periodic table was tested and tested over time which caused it to continually change over time" (Related to experimentation).

A second emergent theme was the use of heuristics pertaining to the representational form of a model (e.g., graph, equation, diagram) to identify items that could be considered a scientific model (Representational form, 3%). For instance, one student noted that "a diagram of a water cycle [could be considered a model] because there is a diagram with pictures and labels that are used to teach what the water cycle is" (Representational form). This participant's emphasis on pictures and labels appears to reflect a rule they use to determine whether a representation can be considered a model. In addition, the response contains a reference to the model's use (Usefulness-Show/Teach).

Lastly, some students referred to the ontological status of a listed item, most often referencing the fact that models must be "proven", "fact", or "true" (Ontological status, 7%). A student who listed the "Law of Gravity" as a model explained that "it has been proven by many people" (Ontological status). As in the previous group, students in this category seemingly used rules to determine whether to consider "laws", "theories", or other "proven knowledge" as scientific models. These responses may reflect a fundamental misunderstanding about the distinctions between models, laws, and theories.

Overall, the analysis of students' reasoning on model-listing tasks suggests that while students have some productive ideas about how scientists create and use scientific models, they

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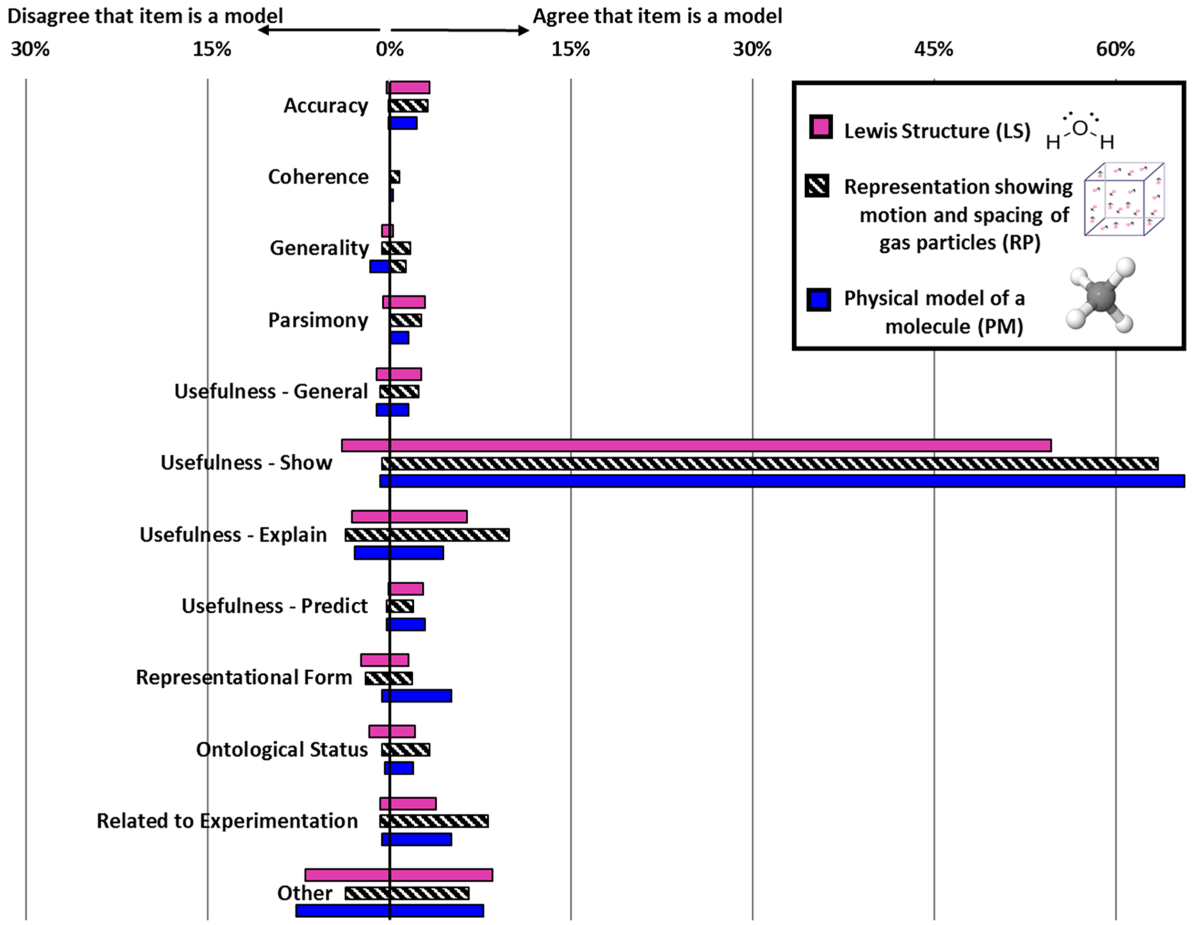

Figure 3. Code frequency (percentages) for students' reasoning about whether three visual models (LS, RP, PM) should be considered scientific models. The responses of students who disagreed that the items were models were coded for the model characteristic that students saw as lacking. These responses are indicated by the negative *x*-axis. We assigned as many codes as necessary to capture all ideas in the response; *N* = 773.

most often exhibit relatively naïve ideas about the uses of scientific models (Usefulness-Show/Teach).

Representation-Classification Tasks

In the representation-classification tasks, we asked students whether they would classify six different models they had encountered in their general chemistry course (Table 1) as scientific models. The six models were the following: a representation of the motion and spacing of gas particles (RP), a physical model of a molecule (PM), a Lewis structure (LS), an energy diagram (ED), the ideal gas law (IG), and the equilibrium constant expression (EQ). Each classification task was followed by an open-ended prompt asking students to explain their reasoning.

Classification Tasks. The percentage of students who categorized each item as a scientific model is shown in Figure 2.

We performed pairwise *t*-tests to identify differences in the proportions of students who categorized the six representations as scientific models. We used an initial alpha value (α) of 0.05, but to minimize the probability of family-wise error (Type I error), we applied a Bonferroni correction for a corrected alpha (α) of 0.003.

We observed no statistically significant differences in the proportions of students who classified RP, PM, and LS as scientific models (Table 5, purple box). Although Harrison and Treagust[4] argued that these three models differ in type, chemists commonly use each to represent or visualize particulate-level species responsible for chemical processes.[45] Thus, it is somewhat unsurprising that students classified them similarly.

There were significant differences in the proportions of students who classified the three models of particulate-level entities (RP, PM, and LS) as scientific models and the proportions who classified the representations that would be considered mathematical models in Harrison and Treagust's[4] classification system (ED, IG, and EQ) as scientific models (Table 5, green box). Thus, while students seem to recognize models of atomic-molecular structure and entities as scientific models, they are significantly less likely to recognize mathematical and graphical models as scientific models.

Interestingly, pairwise comparison of the proportions of students who categorized the three mathematical models (ED, IG, and EQ) as scientific models revealed statistically significant differences between each pair (ED and IG, p = 0.0028; ED and EQ, IG and EQ, $p < 0.001$; Table 5, orange box). This result suggests that students may not have stable, coherent conceptions[46,47] of mathematical equations and graphs as models.

Representation-Classification Reasoning. We then analyzed students' reasoning about their classification of the six representations in Table 1 as models (or not) using the model characteristics coding scheme that was adapted from White et al.'s[39] description of the characteristics of scientific models and later modified to include emergent themes, as

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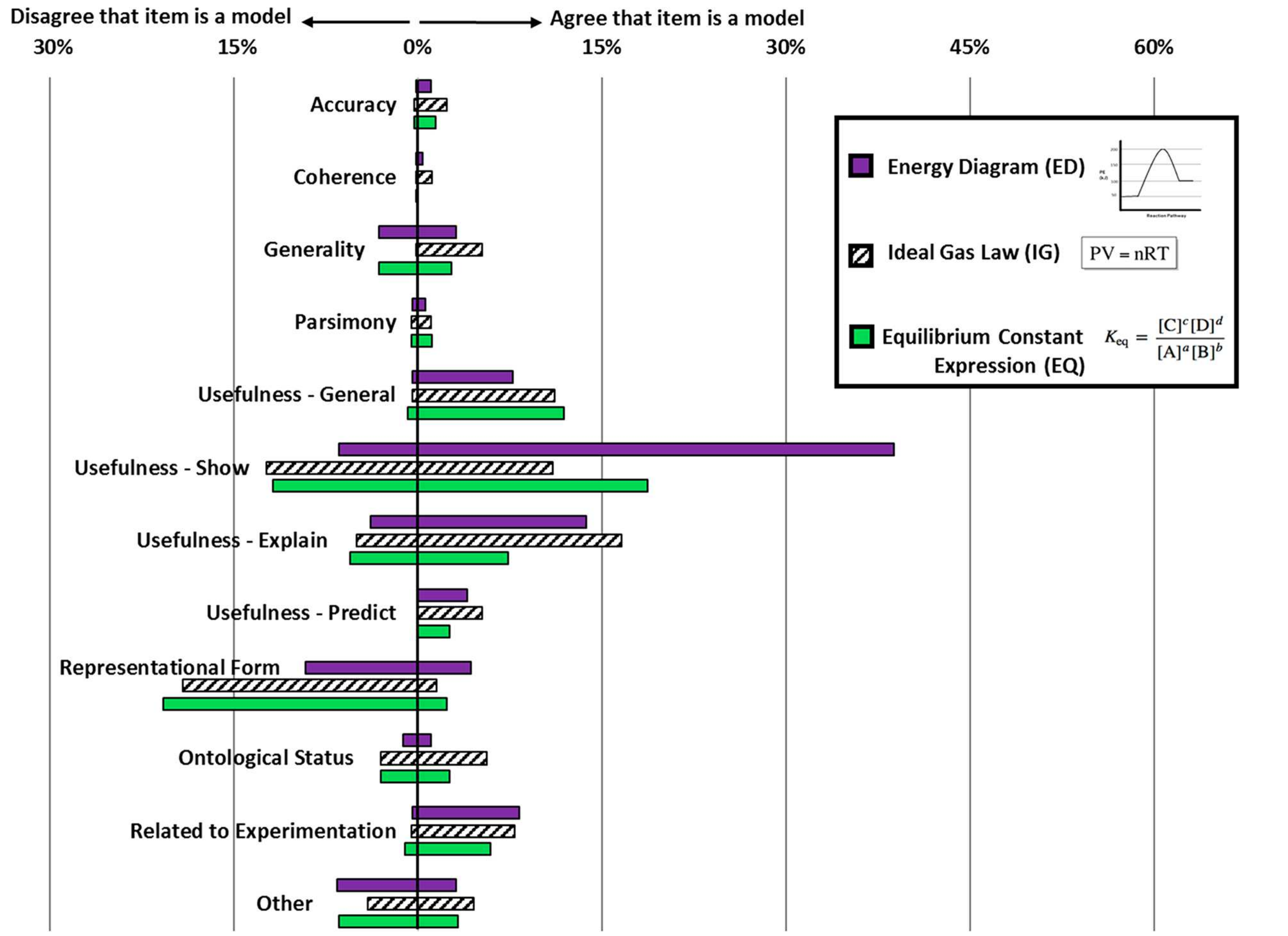

Figure 4. Code frequency (percentages) for students' reasoning about whether the three focal mathematical models (ED, IG, EQ) should be considered scientific models. The responses of students who disagreed that the items were models were coded for the model characteristic the items supposedly lack, indicated by the negative x-axis. We assigned as many codes as necessary to capture the essence of the response. $N = 773$.

discussed earlier. Overall, we found that the reasoning underlying students' classification of models as scientific models (or not) often included canonical ideas about models, for example, ideas about the utility of models or the way in which models simplify aspects of the target phenomena. However, the inductive analyses revealed that students also voiced several alternative conceptions about what counts as a model in science.

The reasoning students used to justify their classifications was similar within the two model types: the particulate-level models (RP, PM, and LS) and the mathematical models (ED, IG, and EQ). Therefore, we discuss the emergent qualitative themes in each of these two groups of models, rather than discussing each model type separately. Figures 3 and 4 show code frequencies as percentages. When students classified a representation as "not a model", their responses were coded for the characteristic they claimed the representation lacked; this is indicated in Figures 3 and 4 by the bar to the left (negative side) of the y-axis.

Models of Particulate-Level Entities. When discussing the three models of particulate-level entities (LS, RP, PM), students overwhelmingly referred to the models' utility for showing nondirectly observable phenomena such as bonding, molecular structure, and particulate motion (Usefulness-Show/Teach). A student who indicated that she would consider a Lewis structure to be a scientific model explained, "It's an illustration of what a molecule should look like, which is something we can't see and is only theorized by the scientific community" (Usefulness-Show/Teach). Another student, who was discussing a representation of the motion and spacing of gas particles, noted that "it represents something we cannot directly see (motion and spacing of gas particles) in a directly observable manner" (Usefulness-Show/Teach). While these students recognized the utility of models, they discussed models as tools for representing unobservable aspects of phenomena, which we consider a relatively naïve idea about model utility compared to recognition of models for explaining or predicting.

A few students offered justifications that addressed the explanatory (Usefulness-Explain) and predictive (Usefulness-Predict) power of scientific models, both higher-level ideas about the purpose. For example, one student said, "Molecular shape is used to explain various chemical properties and this [a physical model of a molecule] is a way to understand molecular shape" (Usefulness-Explain). Another student commented that "you can use it [a Lewis structure] to predict how the compound behaves" (Usefulness-Predict).

Students who classified representations of particulate-level entities as "not a scientific model" most often discussed the items' inability to explain phenomena (Usefulness-Explain). For example, one student explained that they would not consider a representation of the motion and spacing of gas particles to be a scientific model "because it does not provide an explanation for why the gas particles are moving and spaced

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as such" (Usefulness-Explain). Interestingly, quite a few students who indicated that they would not consider particulate-level representations as models gave little or no reasoning for their assertions (39% of total responses classifying particulate-level representations as "not a model": 50% [n = 59] for PM, 31% [n = 28] for RP, 35% [n = 35] for LS). To illustrate these types of "uncodeable" responses, consider the following explanations: "I don't think it [a Lewis structure] is a model, I just think it's a different way of writing H_2O" or "I don't have a definitive answer, I just believe that this isn't a model."

Mathematical Models. When deciding whether or not they considered mathematical representations (ED, IG, EQ) to be models, participants most often focused on usefulness and representational form as key characteristics, especially models' utility for solving math problems or homework sets (Usefulness-Other). Some students discussed the use of mathematical or graphical models for illustrating unobservable factors such as the energy of a reaction (Usefulness-Show/Teach). One student noted, "I consider this [an energy diagram] a scientific model because it is a visual representation of the changes in potential energy accompanying the formation of a chemical bond" (Usefulness-Show/Teach). Others discussed the ways which mathematical models can be used to explain or predict chemical behavior. In a response typical of those characterized as Usefulness-Explain, the following student stated that they would consider an equilibrium constant expression to be a scientific model "because it explains something that cannot be easily observed or experienced." While an equilibrium constant expression is useful for predicting the extent to which a reaction will progress or calculating concentrations at equilibrium, Le Chatelier's principle is the explanatory model for chemical equilibrium. This student, and others in our sample, seemed to miss this distinction.

Interestingly, students who indicated that they would not classify mathematical models as scientific models often used reasoning similar to the justifications of those who did classify these representations as scientific models, claiming instead that the items did not show or explain phenomena. The frequency (in percent) of these types of responses is indicated left of the y-axis in Figure 4. For example, when discussing an energy diagram, one student claimed, "There is no imagery, it is just numbers in graph form, there is no representation of what is physically happening" (Usefulness-Show/Teach). For this student, a defining characteristic of scientific models is that they are visual in nature and depict what is physically occurring in a scientific phenomenon. For her, graphical models did not meet this criterion. Another participant echoed this sentiment when discussing the ideal gas law, stating, "It's an equation, a way to calculate a quantitative amount of something. Not an explanation of how/why that thing is" (Usefulness-Explain).

Relative to reasoning given for not classifying the particulate-level models as scientific models, students' justifications for not classifying mathematical models as scientific models more commonly referred to representational form or ontological status. Typical responses were "Equations are not scientific models" and "This is a graph not a model" (Representational form). Similarly, students referred to mathematical models' status as "laws" or "proven" to justify their categorizations. One student indicated that the ideal gas law would not be considered a model because it is a law: "It [the ideal gas law] has law in the name... It goes something like model, theory, law" (Ontological status). This type of response may reflect naïve perceptions of mathematical models that prompt students to rely on rules about the kinds of things that might be models rather than considering whether mathematical equations and graphs possess model characteristics.

Comparison of Student Reasoning across the Model-Listing and Model-Characterization Tasks

A comparison of the model characteristics discussed by participants in the model-listing and representation-characterization tasks revealed several trends in the ways students think about different types of models in the chemistry curriculum. The inductive analyses of students' reasoning in these two tasks revealed that students have some potentially productive ideas (productive epistemological resources) about scientific models. For example, both the derivation of models from experimental data and the usefulness of scientific models, the fifth characteristic identified by White et al.,[39] were common themes in students' responses. In their discussions of the utility of models, however, participants focused mainly on the idea that models can serve as visual aids (Usefulness-Show/Teach), which suggests the students had relatively unsophisticated ideas about the purpose of models in science, and, more specifically, in chemistry.

Participants expressed more sophisticated ideas about the usefulness of models in the model-listing task than in the chemistry-specific model-characterization tasks. Specifically, in the model-listing tasks, 17% of participants mentioned the utility of scientific models for generating explanations of macroscopic phenomena while in the model-characterization tasks only 9% of students referred to this type of utility (Usefulness-Explain). The pattern was similar for discussions of using models to generate predictions about a target system; 6% of participants referenced this use in the model-listing task, compared to 3% in the chemistry-specific model-classification tasks. In addition, fewer responses employed broad heuristics such as "mathematical equations are never scientific models" or "models must be visual representations" in the model-listing tasks (3%) than in the representation-classification tasks (12%). Students also referenced the empirical nature of scientific models far more often in the model-listing tasks (20%) than in the representation-classification tasks (7%).

The students' responses suggest that they have a particularly difficult time recognizing appropriate model characteristics with respect to mathematical models. For example, for mathematical models, students were more likely to incorrectly list explanatory power and the ability to serve as a visual aid as the characteristics of a model than predictive power, thus failing to recognize the models' intended purpose, predicting chemical phenomena. In addition, students were most likely to rely on rules about representational form and ontological status when reasoning about mathematical models and rarely relied on such rules when discussing the items they listed themselves. We argue that this pattern indicates that students have the appropriate "resources" to identify scientific models and that, with appropriate instruction, they will be able to utilize these "resources" to form expert-like understandings of a variety of types of scientific models.

■ LIMITATIONS

A potential limitation of the study may be our assumption that students' responses comprehensively reflected their epistemological understanding associated with the models in the survey.

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We recognize that students may have had additional ideas that were not articulated, perhaps due to the written response format. However, themes from our analysis of MCS mirror themes that emerged in the think-aloud interviews used to establish evidence of the response-process validity of the survey. Thus, we have reason to believe that our interpretations of the data are valid for this population of students.

A second potential limitation relates to the fact that we asked students to classify the representations in Table 1 as models (or not) without specifying a use for the representation. Recall that we defined scientific models as tools developed and used by scientists in making explanations and predictions about natural phenomena. In part, this suggests that models are defined by their use. Our assumption in designing the MCS was that students would make classifications based on their prior knowledge of the representations and their uses as discussed in their chemistry coursework. This assumption seems to fit our data since students often made reference to ways in which representations had been used in their classes (e.g., in problem solving). In summary, we acknowledge that students' classifications and reasoning here are highly reflective of their curricular experiences in chemistry.

■ DISCUSSION AND CONCLUSIONS

This study is a qualitative analysis of how undergraduate general chemistry students understand scientific models and assign characteristics to scientific models. In both the model-listing and representation-classification tasks, participants rarely discussed accuracy, generality, coherence, or parsimony, four of the five characteristics of a good scientific model identified by White et al.[39] This pattern suggests that students may not have well-developed ideas about what a scientific model is or how such models are developed and tested and may not recognize some important characteristics of scientific models, for example, that they involve simplifications aimed at highlighting the causal or predictive features of a system (Parsimony) or that they can be used to explain or predict a range of related phenomena (Generality).

This is, however, not surprising, as students in traditional general chemistry courses are rarely, if ever, asked to consider characteristics of chemical models such as the assumptions and limitations (Parsimony) or the range of phenomena for which a model is appropriate (Generality). Students are, however, asked to use chemical models to solve problems;[20,38] therefore, it seems reasonable that students discussed the Usefulness of models more frequently than White et al.'s other four characteristics.[39] A key implication of this work is thus that, to develop deeper epistemological understandings, students need opportunities to engage in the practice of modeling by constructing and evaluating models, in addition to using models as predictive and explanatory tools.[7,10]

With respect to the variation in students' ideas about model usefulness, we identified three main ways in which participants discussed the usefulness of models: to show or teach, to explain, and to make predictions. Some students also discussed models as useful for solving homework problems (Other category). Similar themes have been identified in the literature. For instance, Upmeier zu Belzen and colleagues propose a three-level hierarchical progression of biology students' ideas about the purpose of models. Lower-level ideas in this progression include the use of models in describing the target phenomenon. Midlevel ideas include developing explanations, and the most sophisticated ideas address predictions related to the target phenomena.[33] Though Upmeir zu Belzen et al.'s progression considers recognition of predictive power of scientific models as more sophisticated than recognizing models' utility for crafting explanations, we do not see this distinction in our data. In part, this may be because the six representations used in the MCS do not all possess both explanatory and predictive power. For instance, mathematical models, such as the ideal gas law, are more predictive in nature than explanatory. We do, however, agree that recognizing the explanatory and predictive power of models is more expert-like and aligned with the realistic use of models by scientists than using models only to represent phenomena.

When we asked students to classify specific types of models in the chemistry curriculum as models (or not models), we saw significant quantitative differences between the proportions who classified mathematical models as scientific models and the proportions who classified models that visually illustrate chemical phenomena at the particulate level as scientific models. Further, we saw qualitative differences in the model characteristics that students discussed for mathematical and particulate-level models. While students commonly discussed particulate-level models as useful for making nonobservable phenomena more accessible (Usefulness-Show/Teach), they struggled to (correctly) recognize the utility of mathematical models beyond solving quantitative problems.

In addition, when students were prompted to list items they believed to be scientific models, they rarely listed mathematical models, indicating that most students do not immediately think of mathematical equations and graphs when they think of scientific models. The analysis of students' reasoning across tasks revealed that students were more likely to rely on ideas about representational form or ontological status (e.g., status as a "law") when reasoning about mathematical models compared to particulate-level models or student-listed models. Our observation that students tend to think of mathematical models as related to algorithmic problem solving is consistent with our earlier work on students' reasoning about rate laws and method of initial rates tasks.[35,36]

When viewed through the lens of the resources perspective, these results suggest that students have some productive "resources" for understanding the characteristics of scientific models but fail to utilize these resources when reasoning about mathematical models.[37] Therefore, both modeling-focused curricula and traditional chemistry curricula, which often use a multitude of established models, should consider that students may not have coherent, general ideas about what counts as a scientific model and may not recognize the variety of forms that scientific models can take. Instructors and researchers alike should consider ways to help students develop a coherent understanding of models and modeling, allowing students to apply their existing ideas about models and modeling to all forms of scientific models.

An important implication of this study is that domain-general assessments of students' ideas about models and modeling (e.g., the Students Understanding of Models in Science Instrument[21]) may be of little use in gauging the development of students' ideas about different types of models. Open-ended assessments, such as the survey used here, may serve as better indicators of student thinking about specific types of models.

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■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.8b00813.

Coding structures, definitions, and exemplar quotes (PDF, DOCX)

Survey instrument (PDF)

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Notes

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