JOURNAL OF CHEMICAL EDUCATION

Article

pubs.acs.org/jchemeduc

Uncovering Chemical Thinking in Students' Decision Making: A Fuel-Choice Scenario

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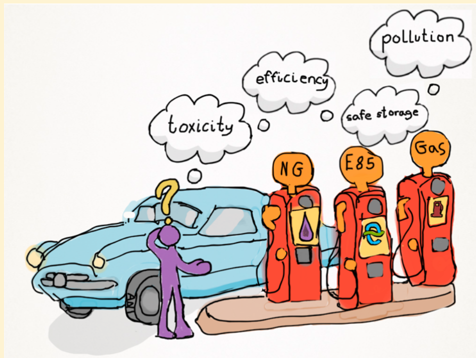
Supporting Information

ABSTRACT: Making decisions about the production and use of chemical substances is of central importance in many fields. In this study, a research team comprising teachers and educational researchers collaborated in collecting and analyzing cognitive interviews with students from 8th grade through first-year university general chemistry in an effort to map progression in students' ability to make decisions about the consequences of using and producing chemicals. Study participants were asked to explain their reasoning about which fuel would be best to power a small vehicle. Data were analyzed using a "chemical thinking" lens to characterize conceptual sophistication and complexity of reasoning. Results revealed that most reasoning was intuitive in conceptual sophistication and relational in argumentative nature, driven by the consequences of using the fuels based on their composition. Implications are discussed for the design of learning experiences and assessments that better support students' development of decision-making using chemical knowledge.



KEYWORDS: *Elementary/Middle School Science, High School/Introductory Chemistry, Chemical Education Research, Problem Solving/Decision-Making, Testing/Assessment*

FEATURE: Chemical Education Research

INTRODUCTION

The *Framework for K−12 Science Education*[1] and its translation into the *Next Generation Science Standards*[2] came about in large part because a lack of science literacy was widely recognized. In this context, we and others have argued that evaluating options and making informed decisions based on chemistry knowledge, as well as relevant factors beyond chemistry (economic, societal, environmental), must be practiced in chemistry classrooms at all educational levels.[3,4] Education reform efforts during the past few decades have resulted in instructional approaches that promote active engagement in authentic problems through science-technology-society approaches.[5−10] However, the use of chemistry to make judgments and decisions is seldom discussed in more conventional classrooms.[11] To support educational approaches that engage students in more authentic practices, we need to better understand how students actually use their knowledge to make judgments and decisions in realistic contexts.

We have formed a research team comprising middle and high school chemistry teachers and university chemistry education researchers focused on the analysis of progression of student understanding in chemistry.[12] In this contribution, we present the results of a study guided by the question: *How do middle school, high school, and first-year university students use chemistry knowledge to make decisions, such as what fuel to use to power a vehicle?* Decision making of undergraduate students, graduate students, and chemistry professors is reported in a separate paper.[13] In both studies, we were interested in characterizing the assumptions and modes of reasoning that individuals with different levels of preparation in chemistry use to evaluate choices and make decisions when facing a realistic problem that does not have a single best answer.

RESEARCH ON BENEFITS, COSTS, AND RISKS EVALUATIONS IN DECISION MAKING

Scant research exists on how students evaluate options, weigh consequences, and make decisions using chemistry knowledge in everyday life. The research that exists comes primarily from science education and risk psychology. Science education researchers have studied how students use chemistry models to interpret processes in the context of modern problems, such as carbon cycling.[14] Scientific argumentation has also been studied in the context of chemistry-related concerns, such as

DOI: 10.1021/acs.jchemed.5b00119
J. Chem. Educ. XXXX, XXX, XXX−XXX

biotechnology.[15] Risk psychology researchers have studied students' perceptions of risk in chemistry-related concerns, such as household hazardous wastes[16] and nuclear power.[17] They have also investigated expert-lay discrepancies and how the general public perceives risk in contexts that involve chemistry, such as health risks from chemical exposure[18] and food additives.[19] The results from these studies suggest that people usually hold strong preferences and biases when making decisions that involve weighing benefits, costs, and risks. What is "natural" is often considered preferable to what is perceived as "artificial" or containing "chemicals".[20] "Chemicals" are widely perceived by the public as being artificial or manmade, as well as dangerous or harmful to the environment instead of useful or innovative.[21]

Intuitive decision making seems to rely on an *affect heuristic*[22,23] whereby positive or negative emotions triggered by words, images, objects, or events bias people's preferences. Two triggers for affective impressions concerning risks have been identified:[23] (1) dread risk, which is how much a person perceives there to be a lack of control, catastrophic potential, or inequitable distribution of risks and benefits; and (2) unknown risk, which is characterized in terms of a person's assessment of how unobservable, new, or delayed the risk is in its manifestation of harm. Laypeople tend to perceive risks as inversely proportional to assumed benefits, while experts tend to evaluate probability of damage.[23] Laypeople often also credit or dismiss evidence of benefits, costs, and risks based on personal values that they share with others rather than on scientific knowledge.[24] Students and experts have also been found to make decisions in measurably different ways. Students' decisions tend to focus on narrowly identified themes and to be less integrated than experts' decisions.[25]

CHEMICAL THINKING AS A LENS

We have proposed the concept of ***chemical thinking*** to capture the knowledge, reasoning, and practices that characterize the chemical enterprise.[26] The Chemical Thinking framework[4] characterizes chemical thinking as the development and application of chemical knowledge and practices with the main intent of analyzing, synthesizing, and transforming matter for practical purposes. The framework organizes chemical thinking into six disciplinary crosscutting concepts which are related to essential questions that chemistry allows us to answer:

- *Chemical identity* (What is this substance?)
- *Structure–properties relationships* (What properties does this substance have?)
- *Chemical causality* (What causes this substance to change?)
- *Chemical mechanism* (How does this substance change?)
- *Chemical control* (How can we control change?), and
- *Benefits-costs-risks* (What are the consequences of changing matter?).

Answering these essential questions requires asking more specific questions that define variables along which student learning is expected to progress. The 11 progress variables (summarized in Table 1) are core questions that chemical scientists seek to answer when practicing chemistry. The crosscutting disciplinary concepts run through all of the progress variables and depend on the problem at hand. For example, a chemist may face the challenge of removing a pollutant from contaminated soil. Doing so may require classifying what type of matter this compound is (chemical identity in PV1 and PV2), why and how it is likely to bind to soil (chemical causality and mechanism in PV4 and PV7), what kinds of processes may work best to undo the binding (chemical control in PV8, PV9, and PV10), and how components may be altered during the process (structure-properties and benefits-costs-risks in PV11).

Table 1. Progress Variables (PVs) in the Chemical Thinking Learning Progression

PV	Specific Question of Chemistry Practice
1	What types of matter are there?
2	What cues are used to differentiate matter types?
3	How do properties of matter types emerge?
4	How does structure influence reactivity?
5	What drives chemical changes?
6	What determines the outcomes of chemical changes?
7	What interaction patterns are established?
8	What affects chemical changes?
9	How can chemical changes be controlled?
10	How can the effects be controlled?
11	What are the effects of using and producing different matter types?

In each progress variable of the Chemical Thinking framework, progress in learning is measured along two major dimensions: (a) conceptual sophistication, and (b) modes of reasoning.[4] Conceptual sophistication is measured in terms of the evolution of underlying assumptions about the nature of chemical entities and processes that support, but also constrain, student reasoning in the domain.[27,28] On the other hand, modes of reasoning measure how students use the information available and their prior knowledge to connect ideas, build justifications, make decisions, and generate explanations.[29,30] Modes of reasoning, while domain-general, are not generic; they can differ depending on the question (progress variable) being answered.

RESEARCH QUESTION

In this study, we focused on the knowledge and reasoning that middle school, high school, and first-year university students bring to bear on making decisions about which fuel is best for powering a small vehicle. The study was guided by the following research question: *What assumptions and modes of reasoning characterize less and more sophistication in students' thinking as they evaluate fuels to use to power a vehicle?*

METHODS

The research team was composed of two middle school teachers, four high school teachers, three graduate students, one postdoctoral researcher, and two university professors. The study followed a qualitative research design.[31] The primary tool for data collection was the GoKart interview protocol, whose development has been previously reported.[12] This instrument presents an evaluation scenario in which students must make a decision and explain why they select one fuel over other available options to power a GoKart for an amusement park. The options presented are gasoline derived from petroleum, gasoline derived from wood pellets, E85, and natural gas. Participants are told that gasoline from either source is comprised primarily of octane, E85 of ethanol, and natural gas of methane. They are also told to assume, for simplicity, that the cost per gallon is the same for each fuel. Following an initial question that explores fuel choice before providing more

DOI: 10.1021/acs.jchemed.5b00119
J. Chem. Educ. XXXX, XXX, XXX−XXX

information, participants are then gradually introduced to additional information about the fuels (e.g., state of matter, chemical composition and structure). At each stage, participants are asked whether the information is relevant to the decision and if their choice would now change, and they are asked to justify their statements.

The participants were middle and high school students from public schools in an urban school district, and undergraduate students enrolled in first-year general chemistry at a public university in the same city in the Northeastern United States. Prior to collecting the data for the study, all members of the research team (author set) trained in cognitive interview methods and engaged in a norming process to ensure the interview techniques and approaches were consistent.[12] The middle and high school students were interviewed by their teachers, and the university students were interviewed by research team members at the university. To obtain a representative sample of students, each of the six teachers on the research team tried to interview one student who they judged 'gets it', one student who 'earnestly tries but struggles', and, if possible, one student in between. This determination was made based on the teachers' observations of their students' attention and effort in learning chemistry rather than on students' grades. The university students who participated in the study were volunteers contacted in class, with their instructor's consent. The racial/ethnicity distribution of all student participants was a typical sampling of the diversity of their institutions. The lack of balance between male and female participants at the middle school and university levels was not a deliberate action by the researchers, however, could constitute a limitation of the study. All data collection received the necessary IRB approvals from the school district and from the university. For reference and privacy purposes, a label was assigned to each participant according to the educational level/course in which the student was enrolled: M (middle school), HS (high school regular and honors chemistry, primarily 10th graders), HSAP (high school Advanced Placement chemistry), and U (university first-year general chemistry).

Table 2 summarizes demographic information about the participants.

Table 2. Demographic Information about Study Participants

	Gender		Perceived Performance Level According to Teacher			
Educational Level/Course[a]	Female	Male	Tries but Struggles	Medium Performer	Gets It	Total *N*
M	4	1	0	1	4	5
HS	5	3	3	1	4	8
HSAP	2	3	1	2	2	5
U	9	2	N/A	N/A	N/A	11

[a]M = middle school science, HS = high school regular or honors chemistry, HSAP = high school Advanced Placement chemistry, U = university first-year general chemistry.

Interviews lasted between 10 and 30 min; they were audio recorded and transcribed verbatim. Qualitative analysis software (Dedoose) was collaboratively used to code the transcripts and facilitate the process of analysis. Interview transcripts were initially parsed into episodes, which usually comprised the reasoning associated with answering one of the questions. These excerpts were initially tagged as potentially associated with one or more disciplinary crosscutting concepts, which were later revisited when grouping the axial codes. All six disciplinary crosscutting concepts were observed in the data, but two of them, structure–property relationships (SPR) and benefits-costs-risks (BCR), were most prevalent. Excerpts were also described by one or more themes. For example: "Different substances have different efficiencies due to different compositions, and therefore run for different lengths of time," or "More energy is released when more bonds are broken, so the largest molecule, octane, gives the most energy." After describing the themes of each excerpt, attention was expanded to the entire interview to look for the presence of overarching arguments made by every student. Following a grounded theory approach,[31] themes were organized, using axial coding to refine the list of themes that appeared throughout all of the excerpts. This resulted in axial codes that described the interviews of middle school, high school, and university general chemistry students. All axial codes are provided in the Supporting Information, with examples of themes that fell into each axial code.

The groupings of themes within each axial category, and their associated excerpts, were then examined to (a) determine the progress variable and disciplinary crosscutting concept combinations under which the axial category fell, and (b) assign levels of conceptual sophistication and mode of reasoning to each excerpt. Where the same excerpt was associated with more than one theme, attention was focused on assigning conceptual sophistication to the theme under examination. Each argument or explanation presented in an excerpt was also assigned a mode of reasoning. The analysis considered the presence and frequency of each conceptual sophistication level and mode of reasoning to discern any patterns with increasing level of education.

All members of the research team were involved during all coding stages, with numerous instances of coding and recoding throughout several months. At each stage, small teams (usually one teacher and one university researcher) were organized, and each person coded individually and then compared the coding with the other person. Afterward, the whole team met to discuss, resolve differences, and reach consensus.

RESULTS

Participants in our study completed evaluations, made decisions, and provided explanations that fell primarily into the crosscutting concepts, progress variables, and axial codes summarized in Table 3. In general, participants' reasoning within these categories fell into three major levels of conceptual sophistication:

(a) *Intuitive*, involving judgments based on everyday experiences and intuition;
(b) *Mixed*, relying on a combination of intuitive judgments and academic knowledge often used inappropriately; and
(c) *Normative*, using appropriate and relevant knowledge to make judgments.

These three general levels of conceptual sophistication share similar characteristics with levels of knowledge integration identified by Clark and Linn.[32] On the other hand, participants exhibited the following major modes of reasoning:[4]

(a) *Descriptive*, in which explicit properties of recognized substances are verbalized and assigned based on experiences and knowledge from daily life;
(b) *Relational*, in which correlations between properties and behaviors are established but not explained or justified;

DOI: 10.1021/acs.jchemed.5b00119
J. Chem. Educ. XXXX, XXX, XXX–XXX

Table 3. Crosscutting Disciplinary Concepts and Progress Variables into Which Axial Codes Are Located

Crosscutting Disciplinary Concept	Progress Variable	Axial Code	Description of Axial Code
Benefits-costs-risks (BCR)	PV11. What are the effects of using and producing different matter types?	Source	Assessment of consequences is associated with the source of a fuel
		Process	Concern with consequences from the process of using the fuel
		Production	Arguments that the production of a fuel is relevant to consideration of the fuel
		Components	Reasoning about effects that depend on what the fuel is made of
		Purpose	Reasoning about benefit or lack of benefit deriving from the purpose of a fuel, usually based on familiarity with a fuel
		Practical Use/Storage	Arguments about attributes of a fuel (usually physical, e.g., phase) having bearing on what happens when a fuel is used or what could happen when it is stored or transported
Structure−property relationships (SPR)	PV3. How do properties of matter types emerge?	Composition-Properties	Consideration of relationships between the composition of fuels and fuel properties
		Size/Bonding/Shape	Arguments about fuel properties based on sizes or shapes of molecules and bonding within or among molecules
		Source-Properties	Arguments about properties based on the source of a fuel
	PV4. How does structure influence reactivity?	Composition-Products	Consideration of relationships between the composition of fuels and the products
		Phase-Rxn Processes	Consideration that phase of a fuel affects its reaction process
		Composition-Rxn Processes	Arguments about how the composition of fuels affects the reaction process

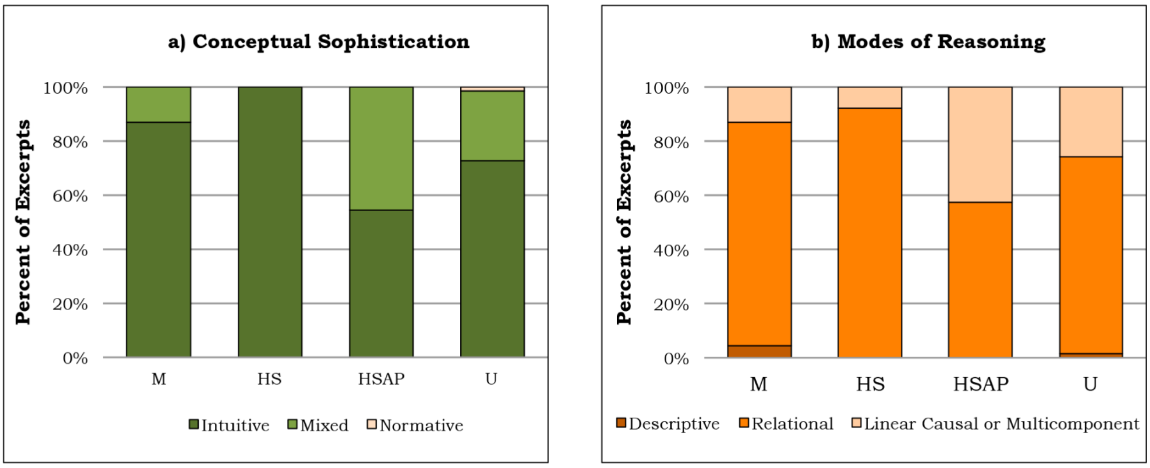


Figure 1. Percent of excerpts coded within each of the major (a) levels of conceptual sophistication and (b) modes of reasoning for participants at different educational levels.

(c) *Linear Causal*, in which phenomena tend to be reduced to the result of the actions of a single agent on other entities, and proposed mechanisms involve linear cause-effect relations and sequential chains of events; and

(d) *Multicomponent*, in which effects of several variables are considered and weighed, and relevant interactions between multiple entities are invoked to build explanations.

Figure 1 depicts the percent of excerpts coded within each of the major levels of conceptual sophistication (Figure 1a) and modes of reasoning (Figure 1b) for study participants at different educational levels. In general, high school AP and university students expressed higher levels of conceptual sophistication and more complex modes of reasoning than other students. However, the most common co-occurrence within all educational levels was the intuitive level of conceptual sophistication and the relational mode of reasoning (hereafter called the *intuitive-relational* co-occurrence).

In what follows, we summarize the main results of our study organized by crosscutting concept and associated progress variables, first characterizing the *intuitive-relational* approach to decision making, and afterward describing major differences in the responses of participants who exhibited more advanced ways of thinking, either as greater conceptual sophistication or as more complex modes of reasoning.

Benefits-Costs-Risks: What Are the Effects of Using and Producing Different Matter Types?

Consideration of benefits, costs, or risks (BCR) was the most predominant form of reasoning during decision making, with 57% of all excerpts falling within a pattern in which participants expressed concern about the environmental, health, or safety consequences of the products of fuel consumption. As shown in Figure 2, where we depict the number of excerpts coded within the BCR category distributed by level of conceptual sophistication and mode of reasoning, the intuitive-relational co-occurrence was dominant among our study participants.

Intuitive-Relational Judgments about BCR. Intuitive-relational judgments about potential consequences of using a fuel involved a variety of considerations, from affective impressions to intuitive inferences of the properties of materials based on their chemical composition and structure. At this level, student reasoning was primarily characterized by the use of familiarity, surface characteristics, or dread risk as the basis for forming an affective impression of "goodness" or "badness" of a fuel, usually termed an *affect heuristic*.[22] For example, M3 relied on familiarity to form affective impressions: *"I think I'm*

DOI: 10.1021/acs.jchemed.5b00119
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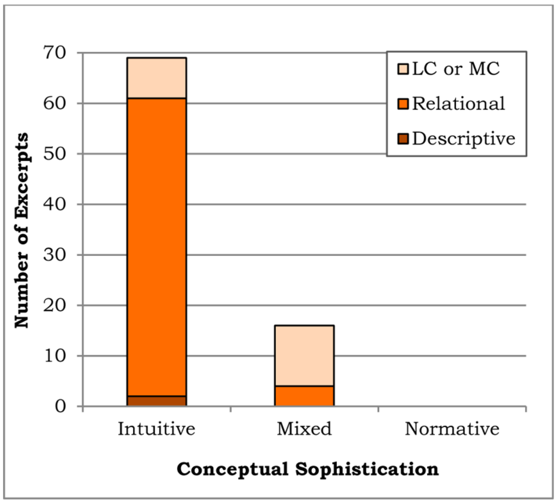

Figure 2. Number of excerpts coded within the Benefits-Costs-Risks (BCR) category distributed by level of conceptual sophistication (intuitive, mixed, normative) and mode of reasoning (descriptive, relational, linear causal or multicomponent).

underestimating the ethanol, I don't think I'm trusting it because I kinda know what is petroleum and what is wood pellets, I've heard of them, I've seen people talk about them, and then so as for methane but I, the word ethanol doesn't come into my mind as often as these two come in so I don't think I'm taking this one too seriously."

Often (36% of excerpts), participants relied on knowledge about the source of a fuel to infer the consequences of using it. For example, some students reasoned that substances are good if they are natural and abundant, or if they have good element combinations in them, and that fuels that were manufactured were worse. Many students noted that the more "chemicals" a substance has, the worse it is, and that even a small amount of "chemical badness" can spell dire outcomes. This approach is typified by the following excerpt:

U11: *Yeah. And it's also a natural gas.*

Interviewer: *What do you mean by it's also a natural gas?*

U11: *Well the name says natural gas, so I assume it's natural gas like, it's not made with like other artificial gas, so it doesn't have chemicals in it. So I think it's better 'cuz it's natural. It doesn't have chemicals in it.*

In some cases (31% of excerpts), participants made affective judgments based on the actual composition of the substances under consideration. For example, oxygen was associated with "goodness" because it is necessary for life, and therefore, a fuel containing oxygen would be better for the environment or human health. As described in more detail in the section on Structure−Property Relationships, the construction of simple associations between the known or perceived properties and structure of the chemical components of a fuel and the actual properties of the material was common among study participants.

More Advanced Judgments about BCR. In a significant fraction of the excerpts classified as above intuitive-relational (60% of these excerpts), students' reasoning was also focused on the consequences of using different fuels. However, in contrast with excerpts at the intuitive-relational level, which mostly focused on affective impressions about the perceived products of using a fuel, arguments and decisions at these other levels were mostly related to either the process of using a fuel or to the production of a fuel. As illustrated by the following excerpt, some participants considered that the production of some fuels created more toxic byproducts than others. For example,

U8: *I guess I would choose methane gas, because it's more renewable. I don't know if the ethanol is coming from corn and what the byproduct of it is, or how making the gasoline from wood pellets and what the byproduct of that would be, but I guess natural gas would be the best because it's more renewable... it comes from the ground, so um... it's probably gonna produce less damage to the environment than say drilling for oil or um, getting ethanol from corn which produces a sludge at the end that's really bad for the environment.*

Other students weighed various benefits and costs, such as energy efficiency and renewability against pollution. Some participants expressed concerns with process and production in several ways. They argued for minimizing impacts on agriculture, food supplies, and general economics. They framed hierarchies according to energy requirements for different feedstocks, e.g., recycled feedstocks like cellulose are more resource-intensive than grown feedstocks like corn. They also focused on the renewability timeline of fuel sources, e.g., corn grows faster than trees.

Many students reasoning at these higher levels integrated more nonchemistry prior understanding into their arguments, were more aware of the limits of their knowledge, and frequently recognized that they would need more information to make a decision. More sophisticated or complex reasoning about benefits, costs, and risks commonly focused on energy as a pertinent factor in decision making, whereas it was rarely mentioned or of inferential basis in intuitive-relational arguments. Energy was mostly inferential in arguments about the process of using or production of fuels, but it was sometimes invoked explicitly in reasoning patterns about components of the fuels and practical matters of usage and transport. Linear causal reasoning paired with intuitive conceptual sophistication often occurred in describing submicroscopic connections (e.g., fuels made from a gas, such as methane, have the greatest energy; fuels made from liquids, such petroleum and ethanol, have intermediate energy; and fuels made from solids, such as wood, have the least energy).

Structure−Property Relationships: How Do Properties of Matter Types Emerge? How Does Structure Influence Reactivity?

Close to 43% of all excerpts included ideas or concepts related to structure−property relationships (SPR). As was the case with BCR, the intuitive-relational co-occurrence was the dominant type of judgment among our study participants (see Figure 3).

Intuitive-Relational Judgments about SPR. Participants who expressed intuitive-relational reasoning about structure−property relationships to determine consequences of fuel usage commonly relied on an "additive framework" to think about chemical substances.[33] Within this framework, the properties of a chemical compound are thought of as the result of the weighted average of the properties of the compound's components (i.e., elements present in the compound, number and types of atoms that make up the substance, number and types of chemical bonds, etc.). For example, students often made associations between the properties of a given fuel and the presence of elemental components such as oxygen (e.g., more combustible because oxygen makes fire burn), carbon

DOI: 10.1021/acs.jchemed.5b00119
J. Chem. Educ. XXXX, XXX, XXX−XXX

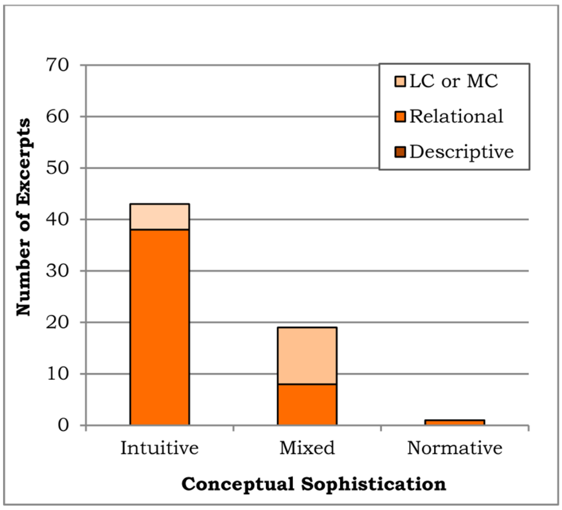

Figure 3. Number of excerpts coded within the Structure−Property Relationships (SPR) category distributed by level of conceptual sophistication (intuitive, mixed, normative) and mode of reasoning (descriptive, relational, linear causal or multicomponent).

(e.g., more harm-causing because CO_2, which damages the planet, contains carbon), and hydrogen (e.g., imparting water-like properties to the fuel). Consider the following excerpt:

HS8: *(long pause) Do you by any chance know what wood pellets are made out of? Do they have oxygen in them?*

Interviewer: *So... wood pellets, what I know is they're just little pieces of wood. That's all I know.*

HS8: *No, but like chemical formation. Do they have oxygen in them or not? Because if they do, then ethanol can definitely be burned, but at a relatively low temperature.*

Interviewer: *So you're asking if the wood itself has oxygen in it?*

HS8: *Yeah. In the formation of the molecules.*

Interviewer: *So you think if they did have...*

HS8: *Yeah. It would just have a similarity with ethanol, because methane and octane do not have any oxygen. And I'm thinking it's possible to burn something with oxygen.*

In this case, the student built a direct association between the presence of oxygen in the substance and its ability to burn. In other cases, the presence of particular components was used to infer the types of products that the fuel could generate. For example, student U4 eliminated ethanol as a choice because she thought that CO_2 could be produced from it because it contains oxygen. She considered that CO_2 could not be produced from use of the other fuels. Several study participants did not express awareness of products of a reaction as resulting from the interaction of different reactants, but rather seemed to conceptualize products as fragments or rearrangements of existing components in a fuel.

Several students also built associations between the size or shape of a molecular structure, or the number or types of bonds in it, and the effectiveness, efficiency, or amount of energy that could be obtained from the fuel. Consider this example in which a student analyzed the drawings of the molecular structures of different fuels:

Interviewer: *So which one do you think is best?*

HS2: *Ok, oh, ethanol.*

Interviewer: *Ok, because?*

HS2: *I guess, carbon, if you have three types of bonds then it makes it stronger for it to, no it makes it longer and makes it last longer.*

Interviewer: *Ok and that makes it a better fuel?*

HS2: *Yeah.*

Interviewer: *Ok and how does that help? Making it last longer, how does that help?*

HS2: *I think if you have like a variety of, well I think that the carbon, and hydrogen, and oxygen, they're all working together, but like create a strong, how do I say, strong gas.*

In this case, the student associated the presence of bonds between different types of atoms with "strength" or "ability to last longer," transferring a perceived molecular property into an expected macroscopic property. This type of reasoning involves the direct association of explicitly noticeable features of molecular representations of a substance to macroscopic properties of the actual fuel. Relying on these types of associations, other students thought that longer molecules would result in more lasting fuels or that shorter molecules would lead to fuels that burn more easily. Within this schema, the numbers of chemical bonds in molecules were used by some students as cues to predict the amount of energy that fuels could produce (the more bonds can be broken, the more energy can be released).

More Advanced Judgments about SPR. Over half of the excerpts in the more advanced categories involved reasoning about ways that properties and behaviors of fuels derived from features, mostly submicroscopic, of the substances that comprised the materials under consideration. As in BCR reasoning, consideration of energy also became more prevalent in this area. More conceptually sophisticated reasoning was marked by noticing features of molecules that were implicit rather than explicit. For example, several students reasoned about how differing bond strengths would occur in different bonds, leading to differences in energy inputs for breaking bonds or energy released when breaking bonds. For example, U7 considered C−O bonds to be different from C−H bonds: "*Like, in... like breaking it down I feel like that's important to know if the bonds are easier to break or not. Like so what will require less energy to break down. I feel like that would be important. And you could tell that by looking at the shapes and the bonds and whatnot... Um... I want to say ... (pause)... that this carbon−oxygen bond is...isn't it pretty strong?*" She then used this to account for why ethanol would produce less energy than methane or octane.

Mixed reasoning often included intuitive assumptions mixed with academic knowledge, as demonstrated by the following excerpt in which a student mixed academic knowledge about molar mass with intuitive ideas about the effect of the density of the fuel on energy consumption, i.e., the denser fuel would weigh down the car more thus require more fuel usage:

HSAP1: *I think that I would choose methane because it would give the most energy per, like, weight measure because I think that like gasoline from petroleum would be the most energy per gallon because it's really heavy so that methane would be lighter and the GoKarts would be faster.*

Interviewer: *So when you talk about it being heavier or lighter what are you, can you tell me more about that?*

HSAP1: *About the molar mass of the methane, is less than the molar mass of octane.*

Whereas intuitive reasoning about chemical reactivity primarily focused on what products would be formed, more conceptually sophisticated reasoning focused more on the reaction processes. The most prevalent intuitive-relational argument was that if oxygen was present in the reactant, then it would be present in the products. Conceptual sophistication

DOI: 10.1021/acs.jchemed.5b00119
J. Chem. Educ. XXXX, XXX, XXX−XXX

Table 4. Assumptions That Constrain Students' Thinking When Evaluating Fuel Choices, as Well as Stepping Stones That Are Conjectured Based on the Findings and May Facilitate Reconceptualizations toward More Advanced Thinking

	Intuitive Thinking	*Stepping Stone*	More Advanced Thinking
• *Benefits-costs-risks thinking*	Judgments based on affective impressions about system components	*Recognizing and thinking about energy changes*	Judgments based on analysis of material and energetic consequences of production and use of materials
• *Structure–property relationships*	Direct association between explicit features of chemical representations and macroscopic properties of substances	*Noticing implicit features of chemical entities*	Recognition of implicit features of submicroscopic particles that determine macroscopic properties
	Additive view of properties of substances based on properties of components	*Seeing mechanisms as multiple causal links*	Recognition of causal links based on interactions between different components of a system

that was at a mixed level (a mixture of intuitive and academic knowledge) tended to focus more on the complexity of a reactant in determining both reaction products and what processes could occur.

There was also greater multicomponent reasoning as conceptual sophistication increased from intuitive to mixed. Evolution in reasoning about SPR seemed to be marked by increasing numbers of causal linkages. This can be seen in conjunction with the ways that students reasoned about reaction processes. Typical intuitive-level explanations were:

- HSAP5: *Bigger molecules have more bonds, which releases more energy when the bonds are broken*; and
- HS5: *Ethanol should react more similarly to octane because it also has a carbon with three hydrogens around it.*

In contrast, mixed conceptual sophistication explanations included many more causal links, as students based reasoning on conjectures about reaction rates and mechanisms that could result from structural features of the reactants. For example, consider the following arguments:

- HSAP4: *Ethanol would react more slowly initially, because more energy is required to break C–O and O–H bonds than to break C–H bonds, but then after a while the reaction would go to completion because enough energy is getting generated*; and
- U2: *Ethanol has CO in it so would produce CO, which could then react with ozone, O_3, in the atmosphere, removing an O from it to make CO_2, thereby depleting the ozone layer.*

DISCUSSION

This study was designed to explore the assumptions and modes of reasoning that characterize less and more sophisticated understandings of students as they make decisions about what fuel to use in a particular situation. Our study sheds light on students' ways of thinking about chemical substances that are likely to affect their decision making in other contexts. Our results also provide insights into the nature of "stepping stones" in students' learning that instructors should scaffold to support changes in students' conceptualizations of chemical substances and processes.[34] In what follows, the reader is referred to Table 4, in which the results are summarized along with conjectured stepping stones.

Stepping Stones

Intuitive benefits-costs-risks thinking in our study was strongly influenced by an affect heuristic triggered by familiarity with the substances under analysis or by surface characteristics of their molecular representations. Progress in BCR thinking was characterized by increased attention to the source of fuels and to the byproducts and imperfect yields of processes involved in fuel production. Recognizing and thinking about energy changes involved in such processes seemed to be a critical stepping stone in the progression toward more sophisticated decision making.[35]

Intuitive thinking about chemical substances was characterized by the direct association of explicitly noticeable features of molecular representations of a substance to macroscopic properties of the actual fuel. Participants at this level seemed to assume that bulk properties derive from the explicit properties of submicroscopic components and vice versa, which is consistent with previous studies.[27,33] In contrast, students who exhibited more advanced reasoning about the properties of substances tended to cue on implicit features in building explanations and making decisions. While the features they paid attention to were often inappropriate, the act of noticing these implicit characteristics of chemical entities (e.g., relative bond strength) seems to be a stepping stone in transitioning toward more sophisticated chemical thinking about how a substance's properties emerge from structural features. Prior research has shown that this transition does occur with increasing content acquisition.[36]

Students' intuitive thinking about SPR was characterized by reliance on an additive framework in which the properties of chemical compounds were seen as a linear combination of the properties of their individual components.[27,33] This way of thinking led students to focus on the characteristics of individual components and reaction products rather than on the interactions that occur during reactions. A transition toward thinking about reactivity in more sophisticated manners appeared to occur when students began to focus on interactions and on the ways in which chemical structure can influence such interactions. Such reasoning was commensurate with students building more causal links in their explanations. Thus, it may be that the ability to see mechanisms through multiple causal links is a stepping stone toward increased conceptual sophistication in reasoning about reactivity.

Implications for Teaching Chemistry

Evaluation of consequences and decision making is core to the discipline of chemistry. However, students will not learn to apply their chemical knowledge to benefits-costs-risks reasoning if they do not practice it. To prepare students for thinking and learning outside the confines of school, educators must provide opportunities for students to see the relevance of chemistry in their daily lives and to use chemistry knowledge in their daily decisions. Context-based learning[5−9] affords opportunities for change on the scale of the whole curriculum. However, teachers who use other instructional materials can also provide theoretically grounded relevant chemistry learning experiences to enrich students' engagement with chemical thinking.[37] For example, a chemical thinking lens can be focused on the use and production of consumer goods by asking questions such as: Which toilet paper production

DOI: 10.1021/acs.jchemed.5b00119
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methods are better than others in terms of byproducts? What is the quality of the water from drinking fountains in the school? As in the formative assessment tool used in this study, there is not a single answer to such questions. Teachers can learn much about their students' benefits-costs-risks thinking by critically looking at students' approaches to answering such questions.[38]

Our results suggests that students' judgments and evaluations are strongly influenced by intuitive assumptions about the benefits, costs, and risks of using synthetic versus natural chemicals, and about the effect of chemical composition on the physical and chemical properties of materials. These assumptions should be elicited and openly analyzed and discussed in chemistry classrooms at all educational levels. Students should be offered opportunities to develop and test models of matter based on these assumptions, and to evaluate their limitations compared to other models that are based on assumptions that are more aligned with modern chemical thinking. Engaging in the development, testing, and evaluation of models has proven to be an effective approach to increase students' conceptual sophistication and ability to apply mechanistic reasoning.[38,39]

Limitations of the Findings

The research reported here benefits from the data having been collaboratively analyzed by teachers and educational researchers. However, the findings also have limitations in generalizability due to the sample size and the situated nature of the participant pool. The middle school students came from two schools, and the high school students came from four schools, two of which are high-achieving magnet schools, and one of which is on the cusp of being closed due to low performance. The university students were all from one university. All were public institutions in the same city, serving ethnically diverse and relatively economically disadvantaged populations. Students' thinking was likely influenced by their life experiences, and may be representative of some extremes rather than average experiences in the U.S. For example, experiences with agriculture and deforestation may be more hypothetical for students who have always lived in the city, but highly relevant to participants who were immigrants from countries where agriculture and deforestation impact daily life. To know whether our findings about chemical thinking are representative of a broader population would require more participants, and from different types of places (e.g., rural, suburban locations, private or elite schools).

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

Supporting Information includes a table of all axial codes, with examples of intuitive-relational and above-intuitive-relational themes that fell into each axial code. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

The authors acknowledge important contributions by Scott Balicki to data collection and initial discussions of data analysis. The authors acknowledge the leadership and vision of Pamela Pelletier, Senior Program Director for Science in the school district. The authors also wish to acknowledge the funding sources, US NSF awards DRL-1221494 and DRL-1222624, that support our work. We thank all of the students who participated in the interviews, as well as Anahid Johnson, who drew the abstract graphic. The author order is alphabetical because all contributed significantly to the paper.

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