Students' Microscopic, Macroscopic, and Symbolic Representations of Chemical Reactions

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Abstract: This study examined the mental representations of chemical reactions used by six students (three male, three female) who achieved above-average grades in a college freshman chemistry class at a large midwestern university. The representations expressed by the students in structured interviews were categorized as microscopic, macroscopic, or symbolic representations of chemical reactions. The study revealed that the participants did make at least some use of each of the three representations; however, there were wide variations among participants in the sophistication of the various representations they used and in their understanding of the relationships between representations. Also, participants receiving very similar course grades sometimes demonstrated very different conceptual understandings of chemical reactions.

Rationale

Chemical reactions are a central focus in the study of chemistry, and it is almost universal for introductory chemistry courses to include the topic of balancing the equations representing these chemical reactions. Homework and exam problems in which the goal is to determine mathematically the missing coefficients for the chemical species in reaction equations are standard fare in nearly all courses, and courses with a laboratory component may incorporate experiments designed to allow students to balance chemical reactions empirically by quantifying the reactants and the collected products, relating these measurements to the molar amount of each species reacted or produced. Nonetheless, students doing exercises and experiments and viewing demonstrations do not necessarily recognize that these portions of the curriculum are interrelated and are based upon a common conceptual underpinning. Instead, it seems that many students view these experiences in chemistry class as unrelated events and as increasingly unpalatable repetitions of tiresome homework problems and tedious laboratory measurements. Even years after their high school or college chemistry course, what many people remember most negatively about chemistry courses is the amount of time spent balancing chemical equations [1]. Additionally, the demands that chemical stoichiometry problems place on students' problem solving skills can result in the intended conceptual development being thwarted as algorithms or trial and error approaches that replace concept-based problem solving [2].

From an instructional perspective, balancing chemical equations—both on paper and in laboratory serves a clear role in the logical development of a chemistry course. Crucial concepts embodied by chemical stoichiometry and equation balancing include conservation of mass; conservation of charge; writing correct ionic, atomic, and molecular formulae; and relating mass, gas volume, and solution volume and concentration to the number of atoms, ions, or molecules. A properly balanced chemical equation is a graceful quantitative statement of the behavior of matter on a submicroscopic scale (hereafter called simply microscopic), observed implicitly through macroscopic properties and recorded in a concise symbolic and algebraic language. Thus, in spite of the attitudinal and instructional barriers to students achieving a full understanding of chemical stoichiometry, the potential benefits justify the topic's inclusion in most curricula.

This study arose from the observation that in the chemistry classroom there is often a tacit expectation that students be able to routinely and quickly shift their thinking among several different representations within the three different levels into which chemistry may be conceptually arranged. A full understanding of chemistry generally requires that students use representations characteristic of the *macroscopic* level, the *microscopic* level, and the *symbolic* level [3, 4]. In addition, practical daily experience during non-school time principally involves the "real" macroscopic world, which sometimes seems to students to be inconsistent with the world of the classroom [5].

If it is recognized that each of these three levels typically has a different physical scale and different conventions—almost a different language—the potential for problems begins to be evident. The symbol NaCl is understood microscopically as an atom of sodium and an atom of chlorine, or more properly, as a three-dimensional array of alternating sodium and chloride ions; macroscopically it is a white or colorless crystalline solid weighing 58.5 grams per mole; in the real world it is kept beside the pepper on the dinner table. A further complication is that the same symbolic representation, NaCl, is applied to both the microscopic and the macroscopic levels; moreover, in much of chemistry the symbolic representation carries both algebraic and chemical significance, meaning that the symbolic level bridges the two other levels and has two languages of its own.

Macroscopic, microscopic, and symbolic representations are each appropriate for various aspects of chemical reactions. It is not necessarily realistic, however, to suppose that students have developed the same facility as teachers and chemists in

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choosing an appropriate representation for a given situation, particularly if teachers do not explicitly reveal that these representations exist. Moreover, even when a student can use and understand one or more representations, he or she may not understand how the individual representations are related to one another. Consequently, it is very important to examine what mental representations students use for chemical reactions and to explore what relationships students understand to exist among the various representations.

In this study we sought to understand the conceptual representations that high-achieving college freshmen developed concerning stoichiometrically balanced chemical reactions during routine instruction in a chemistry course. In order to focus the observations and analysis, we defined three contexts within which students' conceptual representations were grouped, namely (a) the macroscopic, empirical manifestations of stoichiometrically balanced chemical reactions; (b) the microscopic, atomic interactions occurring in these reactions; and (c) the symbolic language used to represent these chemical interactions. The students' concepts within these three realms and the relationships among them provided the basis for five guiding research questions:

1) What are students' conceptions of the macroscopic, empirical manifestations of the chemical interactions occurring in a stoichiometrically balanced chemical equation?
2) What are students' conceptions of the microscopic, atomic interactions occurring in a stoichiometrically balanced chemical equation?
3) What are students' conceptions of the information contained in the algebraic/symbolic equation used to represent a stoichiometrically balanced chemical equation?
4) What are the patterns and relationships connecting the macroscopic, symbolic, and microscopic representations held by each student?
5) What are the patterns in the macroscopic, symbolic, and microscopic representations held by a group of students?

Theory and Background

Constructivism is the epistemological theory which best describes our perspective in this study. Constructivism has received important contributions during the last decade, such as Osborne and Wittrock's [6, 7] Generative Learning Model and von Glasersfeld's [8] notion of human knowledge being a *fit* to the experienced world rather than a *match*. Because constructivism seeks to assess the nature of students' understanding, it is an ideal theoretical perspective for examining students' development of understanding about the microscopic, symbolic, and macroscopic representations of chemical reactions.

In the course we studied, valid information about these representations was presented to the students, and relationships among the representations were shown, either explicitly or implicitly. The choice of a constructivist perspective had two major implications for our study. First, it drew our attention to the importance of carefully observing the constructions developed by individual students in response to their classroom experiences. Second, constructivism focused our attention on the process by which classroom instruction is transformed into individual personal knowledge rather than on the product alone, meaning that it was important to examine students' construction of ideas in addition to their final answers.

Previous Research

The literature investigating the teaching and learning of chemical equations and stoichiometry ranges from descriptions of rather mathematical, algorithmic approaches designed to help students produce correctly balanced chemical equations to highly conceptual investigations of students' conceptual understanding of chemical reactions on a molecular level. To impose some sort of order on this body of literature, we chose the following five categories which, while having obvious regions of overlap, were useful for summarizing the scope and results of previous research and framing the implications for the present study.

Methods for Balancing Chemical Equations. Blakley [9] demonstrated that almost every equation could be balanced with a FORTRAN program using matrix algebra. Jones and Schwab [10] and Rosen [11] also developed computer programs which returned the proper coefficients for chemical equations. Kennedy [12] presented a calculator-based procedure to find appropriate sets of coefficients. Other papers, such as Garcia's [13], typically have offered refinements on common algorithms, such as the oxidation number of half-reaction methods. While a mathematical approach can yield correct numerical answers, neglecting the subtle difference between a mathematical and chemical equation increases the likelihood of conceptual errors. Kolb [14] argues that a chemical equation is unlike a mathematical expression because the reactants and products are truly chemically different; therefore, they cannot be equivalent in a mathematical sense.

Concepts of the Particulate Nature of Matter. A distinctive line of research has attempted to determine whether students who succeed in finding correct numerical answers to problems do so because they understand the system at a molecular level or merely because they have used an appropriate algorithm but do not actually understand the physical system. Several researchers [15–20] found that even when students could correctly solve numerical problems, they often were not able to identify a pictorial solution representing the same physical system on a molecular level. This, along with a similar study of students' concepts of the particulate nature of matter [21], indicated that many students succeeded in solving problems by executing algorithms rather than by understanding basic concepts.

In a key study, Yarroch [22] presented very simple chemical reaction equations to above-average secondary students; the students were able to balance all of the equations correctly. He then asked these students to generate their own pictures of the reactions on an atomic scale and interviewed them about their understanding of the physical meaning of the correctly balanced equations and their drawings. Yarroch reported that nine of the fourteen students could balance the equations but could not explain what the equations meant.

Errors in Balancing Chemical Equations. Several studies have explored the causes of students' errors in balancing equations. Interestingly, mathematical errors and violations of mass conservation were seldom found to be reasons for incorrectly balanced equations. For example, Savoy [23] found that students lacked understanding of such concepts as oxidation numbers and atoms and that students did not understand the formalisms of writing formulas, that is, subscript numbers, brackets, and coefficients. Garforth, Johnstone, and Lazonby [24, 25] investigated ionic equations and found that concepts of spectator ions, oxidation numbers, and ionic charge posed the greatest obstacles for students.

Savoy [23] linked these types of errors to misconceptions about more fundamental concepts, such as atomic structure, electron configuration, and bonding. In addition, Herron and Greenbowe [26] reported that students' misunderstandings of chemical equations were also due to students' failure to "associate the symbols and numerical answers…with real objects and events". Thus, students' difficulties understanding chemical reaction equations have been attributed to misunderstanding the symbols themselves, to misunderstanding concepts related to the atomic and electronic structure of matter, and to not understanding the relationship between the equations and the macroscopic level.

Empirical Balancing of Chemical Equations. The laboratory provides an opportunity to apply quantitative and qualitative physical measurements and observations to the problem of chemical stoichiometry. Chemical reactions, such as the formation of copper (II) iodide [27], the thermal decomposition of potassium bromate [28], and the reaction of sodium borohydride with hydrochloric acid and water [29], have been used to empirically teach basic stoichiometry. These experiments illustrate an approach different than that typically used in the classroom, using physical rather than mathematical properties as the basis for balancing chemical equations.

Translating Between the Representation Levels of Chemistry. The purely mathematical approaches to balancing chemical equations essentially have focused on the algebraic aspect of the symbolic level without relating it to any of the other levels. Research dealing with the particulate nature of matter has principally dealt with students' ability to translate between the symbolic level's chemical meaning and the corresponding microscopic level. The investigations that examined students while they balanced chemical equations have addressed both the interplay between the mathematical and chemical aspects of symbolic representations and, especially in the case of Yarroch [22], the relationship between these symbolic representations and students' understanding of the microscopic level.

What is lacking is research relating students' ideas about the *symbolic* level to their ideas about the *macroscopic* level, such as is encountered in daily experience and in laboratory experiments. In addition, the work investigating the relationships between students' symbolic and *microscopic* ideas is relatively sketchy. Herron and Greenbowe [26] did careful interviews of students' problem-solving procedures, but they did not explicitly seek the students' own ideas about the microscopic level; rather, they inferred the nature of the students' ideas from their errors. Savoy [23] was far more vague in this respect, referring to "discussions" with students from which their misconceptions were apparently deduced. Thus, only Yarroch's [22] set of fourteen interviews provided an explicit investigation into both symbolic and microscopic representations. Yarroch's [22, p 456] observation that "students seemed to be more prone to conserve symbols…than mass or elementary particles" suggested the importance of studying students' ideas about the junction of the symbolic and microscopic levels more extensively.

Methodology

Choice of Research Paradigms. Based on this analysis of previous research, we designed a coordinated investigation of students' macroscopic, microscopic, and symbolic representations and the relationships among them for the same chemical equation in order to assess the representations developed by academically successful students during routine instruction. Our research questions were concerned with uncovering *how* students understood chemical reactions and *why* students had different understandings of these reactions. The studies cited above have shown that these differences exist; we wished to take the next step and gain some insight into the reasons behind students' difficulties. Therefore, a qualitative research methodology (interview-oriented, small sample, verbal data analysis, no control group) was more appropriate to our questions than the quantitative methodology (test-oriented, large sample, statistical data analysis, control group) with which most chemists are familiar.

We agree with Nurrenbern and Robinson [30] that quantitative data can be very useful in detecting differences in performance due to some intervening treatment; however, we argue that quantitative methods are not very useful in explaining *how* or *why* questions. Our work falls more in the qualitative research tradition that both Bowen [31] and Phelps [32] have stated is appropriate when investigating students' individual understandings of chemical concepts.

Bowen [31] discussed in depth the strengths of interviews as a research tool to investigate *how* and *why* questions. He noted that interviews are not haphazard; they are carefully constructed to provide maximum opportunity for students to reveal their understanding of a concept or phenomenon. The students interviewed can also be chosen to represent a particular segment of the population under investigation or can be chosen to represent a cross section of the population, depending on the research questions. Sample size is usually small; the idea is to probe deeply the understanding of a few students, to strive for depth rather than breadth. For example, we chose to interview a small sample of purposefully selected students in order to probe the conceptual understandings of students who were performing well in the course.

Bowen also described how taped interviews are transcribed and analyzed for patterns that arise from the verbal data. These patterns are then used to make general assertions that support or disconfirm the original research questions. We argue that the power of this interview technique lies in the way that interviews can confirm or disconfirm trends in the data or can even detect new trends emerging from the data that were not considered in the original research questions.

Phelps [32] argued that the internal validity of qualitative studies is very high because the researcher is able to interact with the students. For example, in our study the interview format allowed the interviewer to ask students probing questions in order to clarify their explanations. In the same vein, reliability and generalizability are important concepts in any research, but in qualitative studies these constructs come to have slightly different meanings. As Phelps noted, it is rarely possible to exactly duplicate the conditions of a qualitative study, but reliability is generally enhanced by

Table 1. Chemical Reactions Selected for the Interview

Reaction	Chemical Equation
Reaction 1. Synthesis	$H_2(g) + O_2(g) \rightarrow H_2O(l)$
Reaction 2. Decomposition	$NH_4NO_3(s, > 300\ ^{\circ}C) \rightarrow N_2(g) + O_2(g) + H_2O(g)$
Reaction 3. Metathesis	$Ca(NO_3)_2(aq) + NaF(aq) \rightarrow CaF_2(s) + NaNO_3(aq)$
Reaction 4. Laboratory Experiment	$NaBH_4(s) + HCl(aq) + H_2O(l) \rightarrow NaCl(aq) + H_3BO_3(aq) + H_2(g)$

careful description of the setting, the data, and the results. Therefore, qualitative research reports tend to be longer and more detailed that the concise, numeric reports of quantitative research.

The generalizability we sought was to see if students used any common models or patterns in their understandings of macroscopic, microscopic, and symbolic ways of representing chemical equations. We argue that intensive interviews of a small selected group of students allowed us to investigate these understandings. Our study was exploratory in nature, and we expect that the results from this study will inform other investigators using a larger number of students.

Participants. We conducted the study with six students during the first semester of their freshman year at a large midwestern land-grant university. The students came from a single chemistry course; total enrollment in the course was 853 students. The course was designed primarily for engineering majors who had already taken at least one chemistry class in high school. The course included lectures given by the professor twice weekly to groups of about 425 students, a weekly recitation taught by a teaching assistant (TA) in groups of 24, and a weekly three-hour laboratory with the same TA and same group of 24 students.

The six participants had the same TA, and they all attended the three components of the course with approximately the same frequency. An additional selection criterion was that the participants be receiving a grade of B or A at the time of selection in early November because we were concerned that students with lower grades at this late date in the semester might have such a limited understanding of chemistry that no useful data would be obtained. There was an even male-female mix among the participants, all were first-semester freshmen, all had taken one or two years of high school chemistry and a high school curriculum generally strong in mathematics and science, and all attended more than 90% of the laboratory and recitation sessions; all but Mandy also attended more than 90% of the lectures. All six participants were Caucasian Americans.

The Course. Two factors about the instructional environment were perhaps somewhat out of the ordinary. First, the teaching assistant (TA) was certified to teach secondary school and was pursuing a master's degree in chemistry education. Based on the first author's observation of the TA's teaching, her description of her approach to teaching, and the descriptions that participants, especially Jeni, gave of recitation, we concluded that this TA tended to emphasize conceptual understanding rather than simply getting correct answers. Moreover, the professor who lectured the first half of the semester explicitly made the distinction between macroscopic concepts and microscopic concepts. In fact, he consistently used two overhead projectors at opposite ends of the demonstration table to simultaneously display macroscopic and microscopic representations of the topic under discussion.

Interviews. We used structured individual interviews, which were conducted by the first author, to investigate the participants' mental representations of chemical reactions following the standard lectures, homework, exams, and laboratories most directly addressing chemical reactions and stoichiometry. In the course of each individual interview, the first author presented the participant with four preselected chemical reactions. First, the written equation in unbalanced form was presented to the participant and also stated in words. Then the participant was asked to describe what he or she would expect to observe when the reaction occurred. Next, the participant was asked to balance the equation while verbalizing his or her thoughts in order to more fully reveal the thought processes behind his or her written answer. For one reaction, the first author deliberately balanced an equation incorrectly and allowed the participant to respond to his "errors" in order to further probe the participants' understanding of how to balance equations. Finally, the participant was asked to construct a diagram of his or her understanding of the microscopic meaning of the balanced equation.

The interview began with an introductory segment in which, prior to establishing the macroscopic/microscopic/symbolic context, the first author asked each interviewee to explain his or her understanding of the phrase "chemical reaction." The main body of the interview consisted of four iterations of the same basic sequence of questions for each of four preselected chemical reactions.

The four reactions were chosen to represent several broad classes of chemical reactions and several types of chemical compounds. Reaction 1 was a synthesis reaction with pure elements as reactants. Reaction 2 was a decomposition reaction involving a mixture of elements and compounds. Reaction 3 was a metathesis or double displacement reaction involving ionic substances. Reaction 4 was the basis of a laboratory experiment that all of the participants had recently completed (Table 1).

For each reaction, the first author presented the written equation in unbalanced form to the student, stated it in words, and asked the student to describe what he or she had observed or would expect to observe when that reaction occurred; this was primarily a macroscopic question. Then the student was asked how the discoverers of the reaction might have determined the equation for it, a question which explicitly addressed the symbolic representation of the reaction but also generally resulted in the student describing macroscopic properties and sometimes microscopic ones as well.

Next each student was asked to balance the equation, verbalizing his or her thoughts and actions while balancing it. For reaction number three, the first author deliberately demonstrated a wrong way to balance the equation, allowing participants to respond to the "errors" in order to further probe their understanding of how to balance equations.

Finally, participants were asked to make a diagram of what each reaction might look like if they were able to zoom in while the reaction occurred. The goal of this exercise was to elicite the participants' understandings of the microscopic meaning of the balanced equation. To conclude the interview, the first author asked the participants several questions concerning their personal use of microscopic and macroscopic ideas, their view of the role of the laboratory, and their academic background. Also, the participants made drawings during the interviews depicting what they would expect to see if the reaction could somehow be visualized.

Analysis Procedure

The analysis of the participants' macroscopic, microscopic, and symbolic conceptions was based upon the verbatim transcripts of the interviews conducted individually with each participant. Because the interview was designed not to provide explicit clues to direct the focus to macroscopic, microscopic, and symbolic representations, except for a direction question in the closing section, the participants did not necessarily identify their ideas about chemical reactions according to these representations. This was desirable because we wanted the participants to relate their ideas in a way most familiar to them. Nonetheless, in order to analyze their ideas within the framework of these representations, we regrouped their ideas into those three categories. Although a degree of inference was implicit in making such a reconstruction, it certainly was not done arbitrarily. Based on our operational definitions, statements were classified as *macroscopic* if they were based on empirical properties perceptible in a typical classroom laboratory, such as mass, density, and color. Statements were classified as *microscopic* if they were based upon the number of atoms or molecules present, the atomic structure of matter, or bonding theory. Statements were classified as *symbolic* if they addressed chemical processes primarily on the basis of coefficients and subscripts, atomic symbols, and algebraic manipulations on these numbers and symbols.

Identification of relationships between representations was based on the student's explicit statements of relationships and upon strong contextual and semantic indications that the student understood a relationship to exist. For example, if a single statement included two or more parallel explanations of a concept using different representations, we considered this to mean the student considered the two representations equivalent. Similarly, when one representation was used as a causal explanation of another representation (e.g., explaining macroscopic gas volume relationships on the basis of microscopic combining ratios of atoms), we considered this to show that the student understood that a relationship existed between the representations.

A detailed list describing the types of statements that were classified as macroscopic, microscopic, or symbolic was kept throughout the analysis and, using that classification scheme, another chemical educator (a graduate student in chemical education) independently classified the interview data for Adam and Jeni. After completing each section of the interview, the chemical educator and the first author (also a chemical education graduate student) compared classifications and resolved differences by discussion.

Results

Using the transcripts as the primary data source, the first author constructed descriptions of each of the six participants' macroscopic, microscopic, and symbolic representations of chemical reactions and of the relationships that each participant understood to exist between the representations. He then summarized the range of these conceptions across the group of participants and generated six assertions relating the data to the initial research questions. Table 2 summarizes the major trends in each category for each participant, and we also present a short profile of each participant with some relevant quotes to supplement the table.

Adam's Profile. Adam noted that he did not explicitly distinguish between the macroscopic or microscopic representations he used when analyzing chemical reactions. "…I don't really sit back and go 'hey, I'm thinking microscopic right now'" (Adam, lines 924–926). Yet Adam clearly articulated his understanding of the scope and function of both microscopic and macroscopic representations.

> …microscopic is just a way of…checking things that you observe…. It's like why…behind the macroscopic. I guess that…the labs were mostly the macroscopic part. And then when you…wrote the labs up, they got to the microscopic and why…. When you're talking about like electrons and stuff, then like the microscopic definitely comes in. (Adam, lines 900–906, 914–918)

Adam also used empirical properties to describe and explain reactions. Adam defined a chemical reaction as "two different substances [combining] to form something else…some kind of reaction you can see" (Adam, lines 33–36); he cited heat (absorbed or released) and crystal formation as evidence of a reaction. He later gave the precipitation of CaF_2 and the visible color change of an acid–base indicator as other macroscopic evidence for chemical reactions. When he was asked to speculate about how early chemists had determined equations for reactions, he relied upon macroscopic properties, particularly the volumes and densities of gaseous reactants and products (Adam, lines 184 ff, 359 ff).

In the microscopic level, Adam focused on the sharing and transfer of electrons among atoms. Each time he made a drawing, he specifically identified the nuclei and the electrons, drawing the electrons as a sort of cloud surrounding the nucleus, noting that "the electrons are just like all kind of combining in with each other…" (Adam, lines 303–304).

Adam exhibited some understanding of the relationships among the three representations. For example, he explained that if two volumes of a gas reacted to give one volume of a product "then you'd know that…two different, ah, atoms or molecules combined to form one, one single type" (Adam, lines 191–192). He then demonstrated the relationship in the opposite direction, noting that "you could somehow…find the densities of the two different gases…at the same temperatures or…they could just like find the properties of the gases themselves and…distinguish between them that way. And then they could name them after that…" (Adam, lines 199–210).

Jeni's Profile. Jeni also stated that she did not consciously distinguish between microscopic or macroscopic representations. The primary attribute she used to select between the two representations was physical size.

> …when you talk about electrons, it's not like you're going "oh, there just went an electron." Most of it, to me, is microscopic anyways…what's macroscopic is obvious…. If you *see* some gas being given off, I understand without thinking about it: "I can see it, I'm not using a microscope…". It's not something that you have to think about. (Jeni, lines 1261–1275)

Jeni defined a chemical reaction in terms of macroscopic properties. "If you start with two compounds…and then they

Table 2. Summary of the Use of Macroscopic, Microscopic, and Symbolic Representations in Interview Data for All Participants

Participant	Macroscopic	Microscopic	Symbolic	Cross Relations
Adam Used all three representations with appropriate understanding and demonstrated an ability to make meaningful transitions among the three representations. Grade was 72% (low B)[a]	1. Used empirical properties to explain reactions.	1. Focused on sharing and transfer of electrons among atoms. 2. Consistently used *atoms* and *molecules* in explanations.	1. Correctly balanced the three equations by manipulating coefficients.	1. Stated that macroscopic properties corresponded to the number of molecules or atoms reacting and vice versa. 2. Distinguished between a number in an equation used as a coefficient and a subscript.
Jeni Made at least some use of all three representations, but her discussion focused on macroscopic or symbolic examples. Her macroscopic ideas often seemed constrained or distorted by her ideas about the other levels. Grade was 70% (high C)[a]	1. Related to physical size. 2. Physical change means that only the form of an element changes.	1. Mentioned electrons, Lewis structures, and oxidation numbers, but these seemed to be algorithms rather than concepts. 2. No mention of atoms or molecules.	1. Correctly balanced the three equations by manipulating coefficients. 2. Used symbolic reasoning to decide between NaF or NaF_2 rather than bonding.	1. Seemed to use macroscopic knowledge to determine appropriate symbolic representation. 2. Had difficulty in extracting microscopic representations from symbolic information. 3. Used the arrangement of symbols in a formula to infer molecular structure.
Ed Used all three representations with appropriate understanding and demonstrated an ability to make meaningful transitions among the three representations. Grade was 75% (midrange B)[a]	1. Used empirical properties to explain reactions. 2. Recognized that one could use macro measurements to quantify reactions.	1. Mentioned the electronic nature of reactions but did not use the concept to explain reactions. 2. Consistently used moles in the sense of moles of atoms and mole ratios to balance equations. 3. Did not carefully discriminate between *atom*, *ion*, and *molecule* unless he was making a definition. 4. Explicitly represented the location and distribution of molecules in solids, liquids, and gases.	1. Correctly balanced the three equations by manipulating coefficients. 2. Stated that he first compared the left side with the right side to get a general idea of what was needed.	1. Demonstrated relationships across the three levels by tying weights of reactants to moles to their molecular weights to the balanced equation. 2. Used qualitative macroscopic properties to select an appropriate symbolic representation. 3. Used the balanced equation to generate correct molecule ratios for drawings, which were larger than the simplest set used to balance an equation. 4. Provided a microscopic explanation of macroscopic density.
Mandy 1. Used representations from the three levels, but the symbolic level seemed dominant. 2. Stated that she was better in math and that was why she liked redox, halff reactions, and stoichiometry. Grade was 69% (high C)[a]	1. Stated that macroscopic physical properties might change as a result of a chemical reaction. 2. Used chemical properties to predict reaction products rather than physical measurements. 3. Demonstrated understanding of macroscopic stoichiometry. 4. Had trouble distinguishing between macroscopic chemical and physical changes.	1. Used the terms *atom* and *molecule*, but she also used *chemical* and *element* which sometimes seemed to mean atoms/molecules and at others seemed to be simply substance. 2. Demonstrated an understanding that O_2 molecules split and recombine with H atoms when forming water. However, she did not recognize the ionic nature of NH_4NO_3 and other ionic substances.	1. Correctly balanced the three equations by manipulating coefficients. She stated that hydrogen and oxygen were always saved for last. 2. Oxidation numbers seemed to be fundamentally a symbolic concept used for balancing equations. She never described a causal link between electrons and oxidation numbers. 3. Appropriate molecular formulae were deduced from oxidation numbers that in turn were deduced from the Periodic Table.	1. Demonstrated most relationships in terms of the macroscopic and symbolic levels.

Participant	Macroscopic	Microscopic	Symbolic	Cross Relations
Robert 1. Stated that he focused on microscopic representations rather than macroscopic masses of reactants. Grade was 83% (A)[a]	1. Used macroscopic properties appropriately. 2. Temperature and pressure were important factors in vaporization and condensation phase changes.	1. Used microscopic concepts to explain bond rearrangement, dynamic equilibrium, and precipitation. 2. Sometimes exchanged the terms *atom* and *molecule*. 3. Mentioned *ionic bonding* but did not represent NH_4NO_3 as an ionic compound.	1. Balanced more complicated equations by making a table showing the number of each element in the reactants and products so that he could see relationships.	1. Gave microscopic explanations of microscopic phenomena. 2. Could describe relationships between the symbolic level and the other levels. 3. Could use equations to extract macroscopic information about volume. 4. Explained the arrow symbol in both microscopic and macroscopic terms as representing both a change (volume) and equality (numbers of atoms).
Nancy 1. Demonstrated an understanding of each level and made many relationships between levels. Grade was 78% (high B)[a]	1. Used macroscopic properties (DT, bubbles, precipitates) to indicate a chemical reaction. 2. Could identify products and reactants with tests for gases and could measure mass and gas volumes. 3. Drew an analogy between a gas mixture and a liquid mixture by stating you could separate gases by densities.	1. Described chemical reactions in terms of breaking and making bonds. 2. Distinguished between double and triple bonds and stated that some bonds are stronger than others. 3. Used a series of steps to explain the rearrangement of bonds. 4. Recognized that microscopic associations other than bonding can occur.)	1. Correctly balanced the three equations by manipulating coefficients. 2. Compared the iterative process to computer looping.	1. Extracted macroscopic information from symbols, such as (g) and (s). 2. Used macroscopic information to choose a correct symbolic representation. 3. Correctly related subscripts to the microscopic ratio of atoms. 4. Related macroscopic measurements of mass and gas volume to microscopic numbers of molecules and to symbolic balanced equations. 5. Used microscopic ideas to explain macroscopic phenomena, such as vaporization and the formation of water.

[a] The average score in the class was 64% (C).

react…you come out with something different…. You'll either have heat, like exothermic or endothermic…but you'll always come out with different products from what you started with" (Jeni, lines 33–38). She latter added color changes, formation of precipitates, and seeing gases given off as other manifestations of chemical reactions. She also differentiated reactions according to the macroscopic properties of reactivity and stability, saying that some substances were especially reactive, or reacted more violently, and that some substances occurred naturally.

Jeni named several concepts in her explanations, such as electrons, Lewis structures and the octet rule, oxidation numbers, and moles, but she did not provide further explanations to indicate whether she regarded these concepts as macroscopic, microscopic, or symbolic. Instead, these terms seemed to be components of rules or algorithms; it was unclear if these terms were simply part of the language of the rules or if they had deeper conceptual meaning for her. Interestingly, Jeni did not use the terms "atom" or "molecule" a single time in the entire thirty-page interview.

In her drawing of the synthesis of water, Jeni used the concept of bonding microscopically. Indicating the juxtaposition in her drawing of a hydrogen's lone electron dot and an unpaired electron dot on an oxygen, she said "this makes, bonding here, this one" (Jeni, lined 295–296) and drew a circle around the newly paired electrons. She further explained her drawing with the a microscopic-level discussion of valence electrons:

> The last shell…for hydrogen it wants to be two, but for…all the other ones, they want to get eight in their last shell…so it will like complete the shell. (Jeni, lines 307–312)

Ed's Profile. Ed offered this distinction between macroscopic and microscopic.

> …chemical reactions have properties that we can actually see, but that actually underlying cause of the reaction is something that's…too small to be able to actually view [with] the naked eye…. You can see the effects from the chemical reactions, but the actual reasoning behind that reaction…is unseen. (Ed, lines 72–86).

Ed, however, stated that he often had difficulty remembering which term corresponded with which representation and that he had probably checked his lecture notes twenty times during the semester trying to remember which was which. Nonetheless, he found the distinction helpful "in organizing how you think about things…." (Ed, lines 669–670), and it appeared that he could use the terms appropriately when necessary.

Ed named many macroscopic manifestations of chemical reactions, including color changes, phase changes, bubbling, and formation of a solid precipitate, and he recognized that one could use various macroscopic measurements, such as volume, to quantify chemical reactions. He seemed to understand the mole concept in both the macroscopic and microscopic representations because he explained that balancing chemical equations meant "getting it so that the number of…atoms…of reactants side equals the number of atoms on product side and…that gives you the mole ratios of the molecules" (Ed, lines 184–188).

Ed also discussed the location and distribution of molecules in his drawings. For example, in drawing the decomposition of ammonium nitrate, he said "I just put…solids, I should probably have put a little smaller as if they were more condensed and then showed the right side as a gas being less dense and more spread out, and I just put that on [water at top center] up there because I didn't want you to think that I was putting nitrogen and oxygen and water vapor as if they weren't mixed together. They're all mixed in together, not separated" (Ed, lines 350–360).

Mandy's Profile. Mandy stated that "microscopically, I think of the actual structure of the molecule, like h-2-oh…contains one oxygen and, and two hydrogens…. Macroscopically, you look at h-2-oh, you see water. That's just, a homogeneous mixture." (Mandy, lines 987–994) This potentially useful distinction, however, might not have been as important for her as the mathematical aspect of chemistry because she later mentioned "I'm better at math; so, in chemistry things like balancing equations and then…and reactions, half reactions, things like that, I always liked doing those kind of things, too" (Mandy, lines 1096–1105).

Mandy recognized that, as a result of a chemical reaction, macroscopic "physical properties might change" (Mandy, line 59), and she specifically mentioned formation of a residue (precipitate), evolution of a gas, and the release of heat; however, Mandy noted that "I don't see things—I can't…*deduce* things from a chemical reaction" (Mandy, lines 112–113).

Mandy's microscopic language included such terms as "atom" and "molecule," but it also included "chemical" and "element," which sometimes seemed to mean atom or molecule, but other times seemed to have a more generic connotation of a "substance." Mandy also seemed to have a basic understanding of the nature of bonding because in explaining the formation of water she stated "this is just one oxygen molecule, but the oxygen will split apart because they are attracted more to the hydrogen molecule cause it can satisfy their valence electrons all together. So I see one, the oxygen molecule splitting apart and moving toward the hydrogens" (Mandy, lines 304–308).

Symbolic representations seemed to dominate Mandy's understanding of chemistry. For example, her concept of oxidation numbers seemed to be fundamentally symbolic. Although she explained that knowing a compound's formula revealed "how many valence electrons they had and what their oxidation states were" (Mandy, lines 404–406), she never described a causal link between electrons and oxidation numbers. Instead, she tended to use oxidation numbers symbolically, being certain "that the oxidation numbers balance out" (Mandy, line 206). She even stated that the ammonium nitrate reaction "must have been discovered after the periodic table" (Mandy, lines 200–201). In part, her rationale appeared to be that the periodic table could be used to figure out oxidation numbers, which in turn could be used to determine appropriate molecular formulae. Finally, the majority of the relationships she demonstrated were between macroscopic and symbolic representations.

Robert's Profile. Robert focused on microscopic representations, such as number of molecules, rather than on macroscopic masses of reactants; however, he could also use macroscopic representations appropriately. He mentioned acid–base properties, color changes, precipitates, heat changes, and the evolution of gases as macroscopic evidence for a chemical reaction.

Robert used microscopic language to explain bond rearrangement in reactions, dynamic equilibria in aqueous solutions, and precipitation reactions. Sometimes he interchanged the terms "atoms" and "molecules;" however, the context of Robert's explanations suggested that, in spite of his imprecise vocabulary, his microscopic conceptions were accurate. Interestingly, although he mentioned "ionic bonding" (Robert line 111), and the charges on ions, he never gave an electronic explanation of ions.

Probably the best example of Robert's dynamic microscopic mental picture of chemical reactions was his description of the formation of products in the metathesis reaction (Reaction 3 on Table 1).

> The calcium ions and the fluoride…ions. Ah, when *they* come in contact with each other and form a molecule for that brief period of time, it becomes insoluble, since calcium fluoride is insoluble in water. It separates out from the solution and forms [a] precipitate; however, the sodium nitrate, every time a sodium and—sodium ions and nitrate ions—meet, they are soluble and so they will break apart into their ions again and no precipitate forms (Robert, lines 497–505).

Nancy's Profile. Throughout the interview, Nancy used macroscopic, microscopic, and symbolic representations and showed many relationships among them. In the macroscopic level, she mentioned bubbles, changes in temperature, and precipitates as being indicators of a chemical reaction. In the microscopic level, she had many accurate ideas, particularly with respect to bonding. She consistently described chemical reactions in terms of breaking old bonds and forming new ones. Summarizing the decomposition of ammonium nitrate, Nancy said "You're *breakin'* a *lot* of bonds, that's the bottom line" (Nancy, lines 631–632).

Nancy represented the breaking and forming of bonds in her drawing for the water reaction by drawing x's through the bonds of the oxygen and hydrogen molecules and then drawing new lines to represent the new bonds between two hydrogen atoms and an oxygen atom. She also tried to represent this dynamic rearrangement of bonds for the decomposition of ammonium nitrate.

In addition to bonding, Nancy recognized that microscopic associations other than bonding sometimes occur. As she finished her drawing of the water reaction, she added a line between the two water molecules, explaining that it represents "networking it all, like to get your actual like liquid or your ice or whatever" (Nancy, lines 380–381). She also used the terms "dipole" and "polarity" in conjunction with the idea of networking.

Findings Across Cases

We have developed six assertions that indicate trends observed across participants. These assertions also address the research questions with which we began the study.

Assertion 1. All Of the Participants Successfully Identified Several Physical, Macroscopic Manifestations of Chemical Reactions. This assertion relates to the first research question, which addressed students' macroscopic representations of chemical reactions. All of the students were able to identify three or more macroscopic phenomena that provided evidence of a reaction; however, not all of the participants could describe ways to determine the stoichiometry of a reaction on the basis of macroscopic measurements.

Assertion 2. All of The Participants Were Successful at Mathematically Balancing the Chemical Equations. This assertion relates to the third research question, which addressed students' symbolic representations of chemical reactions. The six participants correctly balanced three equations, generally using a similar algorithm of manipulating coefficients. The thought processes verbalized during the process of balancing were generally confined to commentary on the symbolic and algebraic aspects of the equation. In responding to the first author's deliberate errors in balancing the equation, some participants based their disagreement on symbolic reasons while others gave microscopic reasons.

Assertion 3. None Of the Participants—Including Those with Otherwise Strong Microscopic Understandings of Molecular Structure and Chemical Reactions—Demonstrated a Clear Understanding of the Microscopic Nature of Polyatomic Ions. This assertion relates to the second research question, which addressed students' microscopic representations of chemical reactions. It might also be related to participants' interpretation of symbolic formulae, addressed by the third research question. Most of the participants expressed doubt that their drawings were accurate microscopic representations of ammonium nitrate, and none of them drew a structure which accurately represented its ionic nature. It is important to emphasize that the participants were not explicitly told that ammonium nitrate is an ionic substance; they were provided only a macroscopic description of its decomposition reaction and the symbolic representation "$NH_4NO_3(s)$" Even for simpler ionic substances, however, such as sodium fluoride and calcium fluoride, only Robert described the substances as ionic and "not together most of the time" (Robert, lines 489–490), and he did not represent the ions as separated in his diagram.

Assertion 4. Participants Who Generally Demonstrated Inexact Use of Microscopic Vocabulary (e.g., "Molecule," "Atom," and "Ion") Could Sometimes Provide Accurate Definitions of The Terms and Did Not Necessarily Demonstrate Poor Understanding of Microscopic Concepts. This assertion also relates to the second research question concerning students' microscopic representations of reactions. Robert and Ed are good examples of participants who tended to use the terms for various microscopic entities interchangeably, yet they could use the terms accurately and define them correctly when specifically asked to do so. Moreover, the ideas they related throughout the interviews indicated that they both had good understandings of many microscopic aspects of chemical reactions.

Assertion 5. The participant who did not use the terms 'atom' or 'molecule' also had some substantial misunderstandings of microscopic aspects of chemical reactions. This assertion also relates to the second research question. Although Jeni did use the microscopic concept of bonding and a Lewis structure representation to explain the water reaction, her explanations of the other reactions did not involve microscopic concepts. She also provided only a macroscopic explanation of the mole concept. Moreover, Jeni's drawings representing microscopic aspects of the ammonium nitrate and metathesis reactions utilized the symbols for the elements or the letters A, B, C, and D for different ions, which we interpret as further evidence of a rather poor understanding of the microscopic interactions involved in those reactions.

Assertion 6. Participants Receiving Very Similar Course Grades Sometimes Had Very Different Conceptual Understandings of The Macroscopic, Microscopic, and Symbolic Representations of Chemical Reactions. This assertion relates to the fourth and fifth research questions, which addressed the relationships individual participants understood to exist between different representations and the patterns in the representations used by different students. Jeni and Adam provided the strongest evidence for this assertion. Their course grades differed by only two percent, yet their case studies indicate that Adam had one of the strongest conceptual understandings of chemical reactions, while Jeni had one of the weakest.

Conclusion

Our goal in this study was to describe the conceptual understandings of stoichiometry that a small group of students exhibited during routine instruction. These results, like those of any study revealing the understandings of students, raise important issues for educators. Chemistry educators generally believe and try to convey to students that understanding basic physical concepts is important. This study showed that among six students receiving above average grades in a reasonably typical class, some students developed solid conceptual understandings of many fundamental principles of chemistry while other students' understandings were less developed. The academic rewards that students generally seek were not necessarily closely linked with the cognitive development that educators value.

Admittedly, there are many other factors, such as motivation and discipline, that are implicit components of typical academic evaluation. Nonetheless, an educator who valued conceptual development would probably agree that Robert's relatively high grade was appropriate and would also experience some concern that Adam and Jeni received similar grades, although their conceptual understandings were very different. Ed expressed similar frustration from a student perspective at what he considered to be a mismatch between what he believed he understood and his grade: "I'd say a good majority of points I've lost in the course are more just not knowing how to display my information…I mean, I *know* the stuff, it's just more of how to present it" (Ed, lines 690–692 and 696–697).

Implications for Chemistry Education. Having studied the macroscopic, microscopic, and symbolic representations used by the participants in this study, two principles for teaching emerge. First, helping students develop facility in using multiple representations requires that educators help students become explicitly aware of these representations and provide opportunities in the classroom for students to use these representations. These opportunities could come in the form of group work on conceptual problems in either recitation or lecture. Nakhleh, Lowrey, and Mitchell [33] present several ideas for group problems that are open-ended and/or conceptual.

Second, educators must develop assessments designed to reveal students' macroscopic, microscopic, and symbolic ideas. Nakhleh et al. [33] also present several types of examination questions that could be used to test students' knowledge of the microscopic and macroscopic levels of representation. The American Chemical Society Examination Institute also has a conceptual exam for general chemistry that could be useful for large lecture courses.

The fact that these students were enrolled in a course in which the professor identified many concepts explicitly using the three representations underscores the notion that careful, thoughtful instruction does not guarantee that students will incorporate that information completely or accurately into their own mental structures. Rather, the constructivist perspective suggests that students must actively operate on that information in their own minds. It is important that educators present ideas accurately; however, it is also important for educators to provide opportunities for students to use these ideas and to extend upon them so that students can develop their own abilities to use the different representations.

A major barrier to achieving this goal is that most methods of evaluation are not well adapted to assessing ideas that are not represented in written form. Most classroom communication occurs through written and spoken language. This poses no particular obstacle to using symbolic representations in evaluation, but microscopic and macroscopic representations are less easily communicated using language. Pictorial language is one option for communicating these representations; another option is using written or spoken language to describe mental pictures of these representations. Effective use of assessments will ideally inform both educators and students about the status of the students' understanding.

Students who recognize that (1) multiple representations of chemical phenomena exist (because these representations have been explicitly presented) and (2) they can monitor their own use of those representations (because of classroom practice and effective assessment) are far more likely to gain an appropriate understanding of chemical concepts.

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