College Students Solving Chemistry Problems: A Theoretical Model of Expertise

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Abstract: A model of expertise in chemistry problem solving was tested on undergraduate science majors enrolled in a chemistry course. The model was based on Anderson's *Adaptive Control of Thought-Rational* (ACT-R) theory. The model shows how conceptualization, self-efficacy, and strategy interact and contribute to the successful solution of quantitative, well-defined chemistry problems in the areas of stoichiometry, thermochemistry, and properties of solutions. A statistical path analysis and students' explanations supported the model and indicated that the students' problem conceptualization and chemistry self-efficacy influenced their strategy use, which, in turn, strongly influenced their problem-solving success. The implication of these findings for future research and developing students' expertise in chemistry problem solving is that a strategy is advantageous when it is built on a foundation of conceptual knowledge and chemistry self-efficacy. © 2009 Wiley Periodicals, Inc. J Res Sci Teach 46: 1070–1089, 2009
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An essential component of students' education in chemistry, particularly students who wish to become chemists or scientists in fields related to chemistry, is expertise in solving chemistry problems. Linus Pauling is widely regarded as one of the greatest chemists of the 20th century. He is best known for his remarkable problem-solving skills, which led to his discoveries about the nature of the chemical bond. For these discoveries, Pauling was awarded a Nobel Prize in chemistry. According to Pauling, developing expertise in chemistry problem solving meant learning the knowledge of the discipline and, just as importantly, learning what he called *the scientific method of logical thinking* (Marinacci, 1995). For Pauling, the scientific method of logical thinking meant applying reliable methods of reasoning (strategies) to problems in the discipline. He believed this combination of knowledge and strategic reasoning led to his success in problem solving, and he stressed the importance of both in chemistry education.

Problem solving is "the process of moving from a situation in need of resolution to a solution, overcoming any obstacles along the way" (Sternberg & Williams, 2002, p. 319). Often, it is assumed by instructors that problem-solving practice will, by itself, result in students developing expertise in problem solving and a good understanding of the concepts in the problems (Tsaparlis, 2005). This assumption is not warranted in chemistry instruction, however, because research indicates that many students are leaving their chemistry courses with inadequate problem-solving skills and a poor understanding of the concepts in the problems (Bodner, 2003; Teichert & Stacy, 2002). In response to students' lack of expertise in problem solving, chemistry educators are calling for reform in the teaching and learning of chemistry problem solving because they would like all of their students to become, relatively speaking, "experts" in solving the problems posed in these courses (Cohen et al., 2000).

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Chemistry problems, like problems in many sciences, are characterized in a variety of ways (e.g., Bodner & Herron, 2003; Tsaparlis, 2005). One way of characterizing a chemistry problem is *quantitative* or *qualitative*. Quantitative problems are those that involve equations and ask for a precise numerical answer. Qualitative problems, on the other hand, often ask for an explanation rather than a numerical answer. Another way of characterizing a chemistry problem is *well-defined* or *ill-defined*. A well-defined problem has one correct solution and a prescribed method for finding it. An ill-defined problem, on the other hand, has a number of acceptable solutions and no universally accepted method for finding them. Chemistry instructors usually pose quantitative and qualitative problems that are well-defined, but sometimes pose problems that are ill-defined in order to challenge students, encourage reflection, and stimulate critical thinking. Ill-defined problems are also called *true* problems (Lyle & Robinson, 2001), *novel* problems (Bodner, 2003), and *creative* problems (Bromage & Mayer, 1981).

In the present study, we focus on quantitative, well-defined chemistry problems. These constitute many, if not the majority, of the problems presented in college chemistry courses as part of classroom instruction, homework, and examinations (Cohen et al., 2000; DeJong & Taber, 2007; Gabel & Bunce, 1994). These problems require students to set up chemical equations in order to solve for an unknown value. We recognize, however, that qualitative and ill-defined problems are also presented to students by instructors and textbook authors, often in an open-ended, *critical-thinking* format (Lemay, Beall, Robblee, & Brower, 2002). A focus on qualitative and ill-defined problems is beyond the scope of this article, but we refer readers to an article by Hollingworth (2001) that discusses qualitative and ill-defined problems.

Given the need to develop students' expertise in chemistry problem solving, our goal in the present study was to examine the research on expert and novice differences in problem solving in general, and in chemistry in particular, in order to formulate and test a model of expertise in chemistry problem solving. The model identifies the important cognitive components of problem solving, describes how these components influence each other, and quantifies the relative contributions of each component. This information is valuable to researchers and instructors who wish to improve the teaching and learning of chemistry problem solving. In addition, because some of the problem-solving components (e.g., conceptualization) in chemistry are similar to those in physics, biology, and other sciences (Chi, Feltovich, & Glaser, 1981; Williams & Noyes, 2007), the model will be informative to researchers and instructors in other sciences as well.

Theoretical Framework

Our model of expertise in chemistry problem solving is based on the *Adaptive Control of Thought-Rational* (ACT-R) theory, a cognitive-science theory about thinking and problem solving developed by Anderson and coworkers (e.g., Anderson, 2002; Anderson et al., 2004). ACT-R was developed to explain complex behavior in mathematics and scientific domains. The models derived from ACT-R quantify and visually depict relationships among cognitive variables involved in learning and problem solving.

Anderson and coworkers describe ACT-R as a *cognitive architecture*: A theory that provides a blueprint for understanding human cognitive processes and simulating them computationally. ACT-R provides a means to understand how humans acquire knowledge, organize it, and strategically use it to think and solve problems. Within ACT-R, problem solving involves identifying and applying knowledge and skills that result in the attainment of a goal. More specifically, problem solving is a process in which one "calls on knowledge to re-represent problems in a way that moves towards solutions" (Danker & Anderson, 2007, p. 1365).

We used ACT-R to develop and test our model of expert problem solving in chemistry. Because ACT-R was designed to examine and explain the interaction of quantitative components of problem-solving expertise, it has more explanatory power for our purposes than other cognitive architectures, such as the *Soar* symbolic cognitive architecture (Newell, 1990), or other depictions of problem solving, such as the *working-memory model of science problem solving* (Johnstone & El-Banna, 1986) or the *basic view of learning science problem solving* (Taconis, Ferguson-Hessler, & Broekkamp, 2001).

In ACT-R, problem solving takes place within a theoretical *problem space*. A problem space is a mental representation of a problem that includes the initial state and the goal state of the problem, as well as the intermediate states (subgoals) attained when solving the problem. Our representation of a *chemistry problem space* is in Figure 1. For simplicity, we show a linear solution path, but there also may be multiple paths and nonlinear interactions among the intermediate states, depending upon the complexity of the problem. The

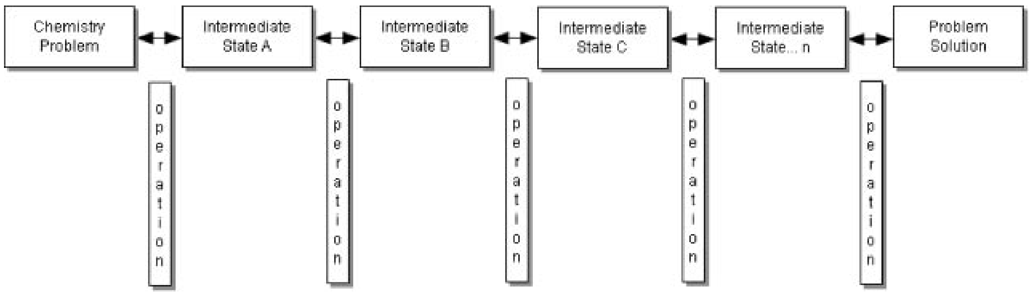

Figure 1. Chemistry problem space © 2008 Taasoobshirazi and Glynn.

bidirectional arrows indicate the possibility of recursion, or returning to previous states, when trying to solve the problem. This space can be applied to many quantitative, well-defined problems that students solve in an introductory college chemistry course, such as the following thermochemistry problem. We use this problem as an example throughout this article, and so we explain it in detail:

> When a 60.0-g sample of metal at 100.0°C is added to 45.0-g of water at 22.60°C, the final temperature of both the metal and the water is 32.81°C. The specific heat of water is 4.184 J/g °C. What is the specific heat of the metal? [Answer: 0.476 J/g °C] (Reger, Goode, & Mercer, 1997, p. 174).

This problem is asking for the *specific heat* of the metal, or the amount of heat required to raise the temperature of 1.0-g of the metal by 1°C, or $c_{\text{metal}} = Q_{\text{metal}}/m \times \Delta T$, where c_{metal} is the specific heat of the metal, Q_{metal} the amount of heat lost by the metal, m the mass of the metal, and ΔT the change in the temperature of the metal. The amount of heat lost by the metal, Q_{metal}, which is a negative value, is equivalent to the amount of heat gained by the water, Q_{water}, which is a positive value. The specific heat of a metal, or any substance, is an important physical property of it. Examples of other physical properties are density, color, and melting point.

Conceptualization of Chemistry Problems

In ACT-R, well-organized, easily accessed, conceptual knowledge structures called *schemas* are used by experts to recognize, mentally represent, and solve problems such as the example just given in thermochemistry. Taconis, Ferguson-Hessler, and Broekkamp (2001) define a schema as a "unit in human memory representing a functional package of knowledge" (p. 446). Experts in all scientific disciplines have more schemas, and better organized and more accessible ones, than novices do. The schemas are used to encode, store, retrieve, and apply knowledge when problem solving (Schunk, 2008). Schematic knowledge includes not only scientific facts, concepts, principles, laws, and theories, but problem solving strategies as well.

The differences between experts and novices in the amount, organization, and accessibility of their schematic knowledge are revealed in studies of problem conceptualization (Chi, 2006a,b; Chi et al., 1981). In these studies, conceptualization is operationally defined as the categorization (sorting) of problems by type (e.g., thermochemistry). When categorizing, experts tend to focus on the concepts, principles, laws, and theories underlying the problems, whereas novices tend to focus on superficial features of the problems such as terminology or objects in the problems. For example, Kozma and Russell (1997) asked 10 undergraduate chemistry students (novices) and 11 chemists and doctoral chemistry students (experts) to categorize a variety of chemistry representations that included equations. They found that the experts' categorizations were based on schematic knowledge of gas laws, kinetic theory, and precipitation reactions, whereas the novices' categorizations were incomplete, fragmented, and based on superficial features.

Stains and Talanquer (2008) asked 44 students who ranged in chemistry expertise—from beginning-level undergraduates, to senior-level undergraduates, to graduate students in chemistry—to perform categorization tasks involving symbolic and microscopic (particulate) representations of different chemical reactions. The students' level of expertise influenced the number and types of categories created, as well as how the categories were created. Many of the undergraduates (novices) based their categorizations on superficial features of the reactions and failed to create chemically meaningful categories. The more advanced undergraduates and the graduate students (experts) were more successful in using their schematic knowledge to build chemically meaningful categories for the reactions.

Chemistry Self-Efficacy and Problem Solving

Self-efficacy refers to a student's belief that he or she can organize and execute the course of action required to achieve in a specific area (Bandura, 2001). Self-efficacy differs from self-concept. According to Bong and Skaalvik (2003, p. 5), ''While self-concept represents one's general perceptions of the self in given domains of functioning, self-efficacy represents individuals' expectations and convictions of what they can accomplish in given situations . . . self-efficacy researchers thus emphasize the role played by specific contexts.'' For example, the expectation that one can achieve in a college chemistry course is an efficacy belief. It is not a belief about whether one is competent in science in general, but rather a belief about whether one can achieve in a particular scientific discipline, chemistry, in a particular chemistry context, a college course. Because self-efficacy refers to a belief, it is a cognitive problem-solving component, which we are examining within ACT-R. Although cognitive, self-efficacy is frequently described as *social*-cognitive because it is influenced more by social context than a component such as conceptualization.

Self-efficacy influences how students approach a task such as problem solving, the amount of effort they exert, and their levels of persistence—all of which influence students' performance (Crippen & Earl, 2007; Dalgety, Coll, & Jones, 2003). Students with high self-efficacy are more likely to work carefully, long, and hard on a task, whereas students with low self-efficacy are more likely to work half-heartedly and give up easily (Crippen & Earl, 2007).

In the present context, *chemistry self-efficacy* refers to a student's belief that he or she can achieve in a college chemistry course (Dalgety et al., 2003). Many studies have examined the role of students' self-efficacy when learning chemistry and other sciences (Anderman & Young, 1994; Koballa & Glynn, 2007; Lawson, Banks, & Logvin, 2007), but only a relatively small number of studies have examined the role of chemistry self-efficacy when solving chemistry problems. Although research on chemistry self-efficacy and problem solving is sparse, the studies that have been conducted suggest that it is an important variable. For example, Zusho, Pintrich, and Coppolla (2003) found that even after controlling for prior achievement, students' chemistry self-efficacy was the best predictor of their grades in an introductory college chemistry course, and those grades were based, in part, on problem solving.

Chemistry Problem-Solving Strategies

A problem-solving strategy is a plan or method to achieve a goal. Analogical reasoning, deductive reasoning, inductive reasoning, and abductive reasoning are examples of general strategies used in solving scientific problems (Sternberg & Williams, 2002). When solving well-defined, quantitative problems in a domain such as chemistry, specific strategies such as *working forward* and *working backward* are also commonly used.

Within ACT-R, working-forward and working-backward strategies are defined as goal-directed sequences of cognitive operations applied in a *problem space* similar to that in Figure 1 (Anderson, 1993; Danker & Anderson, 2007). To solve a problem, such as the one in thermochemistry presented previously, experts engage highly automatized schemas consisting of problem types, states, and operations. These schemas, derived from previous experience, enable the experts to work ''forwards'' when problem solving (see Anderson, 2005, for examples in physics). They start with unknown quantities that can be directly calculated and construct a set of equations that lead efficiently to the goal. Novices, on the other hand, often work ''backwards'' because they lack well-developed, automatized schemas (Heyworth, 1999; Williams & Noyes, 2007). They start with an equation that contains the goal and other unknowns that cannot be directly calculated. The novices then construct additional equations to calculate these unknowns. When the unknowns are calculated, the novices reverse, or ''chain backwards,'' inserting the values of the unknowns in the preceding equations, in order to solve the problem. Heyworth (1999) observed this when he asked 12 high-school students to ''think-aloud'' as they solved a stoichiometry problem. Of the six students who were considered ''experts'' (as indicated by a pretest), five used a working-forward strategy; the six ''novices,'' in comparison, all used a working-backward strategy, which Heyworth called a means-end strategy. Heyworth's findings should be considered tentative, however, because the number of students was small, and the students were asked to solve only one chemistry problem.

A working-forward strategy and a working-backward strategy can lead to the same correct solution, but the former is more likely to lead to success than the latter because of its cognitive efficiency. A working-forward strategy exerts less cognitive load on working memory than a working-backward strategy and usually involves fewer equations (Chi, 2006b; Sweller, 2003). Working forwards is consistent with a constructivist approach to the problem-solving process because it is based on a strong conceptualization of the problem (Bodner, Klobuchar, & Geelan, 2001; Bunce, Gabel, & Samuel, 1991; Bunce & Heikkinen, 1986; Lorenzo, 2005). This conceptualization enables a student to build a mental model which results in efficient distance reduction: a path that moves directly toward the solution. Working backwards, in comparison, tends to place greater demands on working memory, relies more on trial and error, and often leads to detours or steps that are indirect as a student searches for a path toward the solution.

The Present Study

Having examined the research on expert and novice differences in problem solving in general, and in chemistry in particular, our goal is to formulate and test a model of expertise in chemistry problem solving. Based on ACT-R theory, we propose a model that depicts how conceptualization, self-efficacy, and strategy interact and contribute to the successful solution of quantitative, well-defined chemistry problems. There are other components that could be added to the model in an attempt to completely account for students' problem-solving performance, but our plan in this study is to begin with a relatively parsimonious model that could be expanded later.

Based on previous research, it is expected that each component of the model facilitates problem solving: In other words, the students with the highest problem-solving scores will be those who conceptualize problems well, have high chemistry self-efficacy, and use a working-forward strategy. But, more importantly, the innovative contribution of the model is that it shows how the components interact and the relative contributions they make to students' problem-solving success. The insight a model of this kind provides into the problem-solving process could lead to improvements in methods of teaching and learning chemistry problem solving.

The past research in chemistry problem solving has been characterized by studies that categorized participants in two groups: novices and experts. In these studies, novices are typically defined as those who have little knowledge and experience within a domain, whereas experts are defined as individuals with extensive knowledge and experience within a domain (Bodner & Herron, 2003). For example, novices are typically college students in an introductory-level chemistry course, whereas experts are students in an upper-level chemistry course, graduate students in chemistry, or chemists (Bodner & Herron, 2003; Kozma & Russell, 1997). The emphasis on extreme dichotomous groups that characterized past research in chemistry problem solving was informative in many respects, but it left important questions unanswered. In particular, what characterizes the relative problem-solving expertise of students *within* a large-enrollment chemistry class?

Expertise is, in reality, a continuous variable. To dichotomize expertise, by simply labeling some students as experts and others as novices, limits what can be learned about expertise. Dichotomizing a continuous variable in order to simplify analysis and interpretation was a methodological limitation of earlier studies of chemistry problem solving, when it was computationally difficult to carry out statistical procedures such as *structural equation modeling* (SEM).

In the present study, we improve upon past studies of chemistry problem solving by using SEM to examine expertise as a continuous variable among students in a large-enrollment, general-chemistry course. SEM is being used increasingly in science-education research, particularly when the research involves the testing of theoretical models (e.g., Nieswandt, 2007; Wang, Oliver, & Staver, 2008; Willson, Ackerman, & Malave, 2000). SEM allows us to examine the patterns of correlations among the components in our model and to explain as much of their variance as possible.

We are specifying our theoretical model by proposing that students' problem conceptualization and chemistry self-efficacy will influence their problem strategy, which, in turn, will influence their problem solution. Because all of these variables are *observed* rather than *latent*, because there is one measure of each variable, and because we have prior hypotheses about the causal relationships among our variables, we are using the SEM technique of *path analysis* to examine the hypothesized relationships among our variables (Kline, 2005). Using path analysis, our specific goals are to estimate the direct and indirect effects in our model, to control for the correlations among the hypothesized causal variables, and to "decompose" the correlations we observe into their component parts (causal and spurious). Although a correlation, in itself, does not imply causation, path analysis makes it possible to cautiously draw causal inferences from patterns of correlations.

Figure 2 depicts our theoretical model, with each of the hypothesized paths among the variables. In this model, problem strategy is an intervening (mediating) variable. An intervening variable serves a dual role because it "conducts" some of the causal effects of a prior variable onto a subsequent variable. For example, the problem-strategy variable is expected to conduct some of the causal effect of the conceptualization variable onto the problem-solution variable.

Method

At a public university with 21,962 undergraduate students in the southwestern United States, we studied 101 undergraduate students (41 men and 60 women) enrolled in an introductory-level, general-chemistry course for science majors. The average age of the students was 19.09 years old ($SD = 0.65$). There were a total of 169 students (70 men and 99 women) in the course, and 60% volunteered to participate to earn a small amount of extra credit and help the investigators "study how students solve chemistry problems." The course includes students majoring in the life sciences in addition to the physical sciences, and there are usually about 15% more women than men in the course. The instructor indicated that about 50–60% of the students usually volunteer when asked to participate in science-education research studies. Students' participation was voluntary rather than compulsory, as specified by the guidelines for research with human participants specified by the Institutional Review Board. The students participated during the 13th and 14th weeks of the 15-week fall semester: At this point in time, the students had already covered the types of chemistry problems that they were asked to solve in this study.

Procedure and Materials

Students were administered a packet that included chemistry self-efficacy questions, a problem-conceptualization task, and chemistry problems to solve. All students completed their work within 1 hour, and all reported that this time interval was sufficient to complete their work.

Chemistry Self-Efficacy. The students' chemistry self-efficacy was assessed using the following five items:

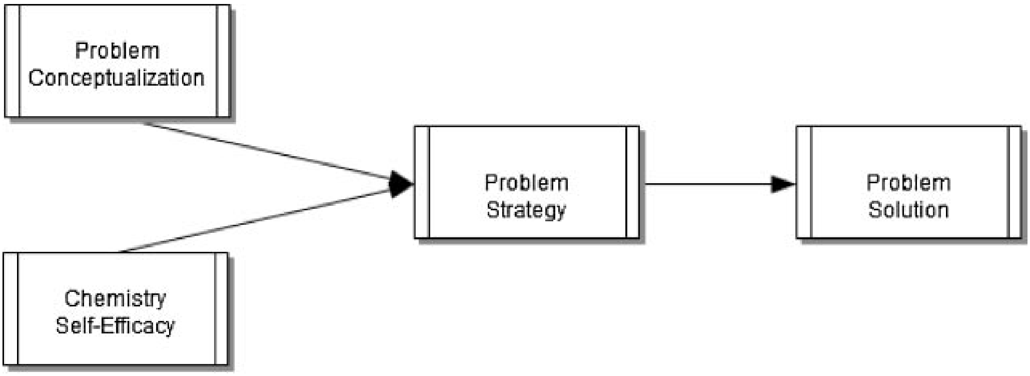

Figure 2. Theoretical model of chemistry problem solving.

- I believe I can master the knowledge and skills in chemistry courses.
- I expect to do as well as or better than other students in chemistry courses.
- I am confident I can do well on chemistry tests.
- I am confident I can do well on chemistry labs and projects.
- I believe I can earn a grade of "A" in a chemistry course.

Students responded to each of these chemistry self-efficacy items on a 5-point Likert scale ranging from 1 (never) to 5 (always), with the instructions: "In order to understand what you think and feel about chemistry, please respond to each of the following statements." A student's total score on these five items could range from a minimum of 5 to a maximum of 25. These five items were found to be reliable in terms of their internal consistency, as measured by coefficient alpha ($\alpha = 0.88$). These items were from the chemistry version of the 30-item Science Motivation Questionnaire (Glynn, Taasoobshirazi, & Brickman, 2007), which has been found in previous studies to be reliable ($\alpha = 0.93$), and valid in terms of positive correlations with college students' science grades, decision to major in science, interest in science careers, and number of science courses taken. The five items we used to assess chemistry self-efficacy were similar in nature to the five items used by Gungor, Eryilmaz, and Fakioglu (2007) to reliably and validly assess physics self-efficacy (e.g., I know I can do well in physics courses).

Problem Conceptualization. Three of the major categories of chemistry problems are *stoichiometry*, *thermochemistry*, and *properties of solutions* (Reger et al., 1997; Zumdahl, 1997; Zumdahl & Zumdahl, 2007). It is not particularly difficult for students to classify problems in these major categories, but to classify subcategories of problems requires greater expertise (Reger et al., 1997; Schunk, 2008). The subcategories of the major categories were: stoichiometry reaction with a reactant in excess, stoichiometry reaction with a limiting reactant, constant-pressure calorimetry, constant-volume calorimetry, colligative properties of non-electrolyte solutions, and colligative properties of electrolyte solutions. We presented each student with 12 problems (3 major categories $\times$ 2 subcategories $\times$ 2 problem examples) in a random order. The problems (see Table 1) were selected from three undergraduate-level chemistry textbooks (Reger et al., 1997; Zumdahl, 1997; Zumdahl & Zumdahl, 2007) that were not used by the students, to ensure that the problems were different ones than those the students had seen previously in the course. The problems are representative of those in their categories, both in terms of content and word length, as found in textbooks. Typically,

Table 1
Examples of chemistry problems categorized by students

Stoichiometry: Reaction with a reactant in excess
Determine the mass of Ga_2O_3 formed from the reaction of 14.5-g of gallium metal with excess O_2
Stoichiometry: Reaction with a limiting reactant
Calculate the mass, in grams, of H_2O that can be produced from the reaction of 10.0-g of H_2 with 99.8-g of O_2
Thermochemistry: Constant-pressure calorimetry
When 1.00 L of 1.00 M $Ba(NO_3)_2$ solution at 25.0°C is mixed with 1.00 L of 1.00 M Na_2SO_4 solution at 25°C in a calorimeter, the white solid $BaSO_4$ forms and the temperature of the mixture increases to 28.1°C. Assuming that the calorimeter absorbs only a negligible quantity of heat, that the specific heat capacity of the solution is 4.184 J/°C g, and that the density of the final solution is 1.0-g/mL, calculate the enthalpy change per mole of $BaSO_4$ formed
Thermochemistry: Constant-volume calorimetry
Camphor ($C_{10}H_{16}O_6$) has an energy combustion of −5903.6 kJ/mol. When a sample of camphor with mass 0.1204-g is burned in a bomb calorimeter, the temperature increases by 2.28°C. Calculate the heat capacity of the calorimeter
Properties of Solutions: Colligative properties of non-electrolyte solutions
A solution contains 2.00-g of the non-volatile solute urea (molar mass = 60.06 g/mol) dissolved in 25.0-g of water. Calculate the freezing and boiling points of the solution in degrees Celsius
Properties of solutions: Colligative properties of electrolyte solutions
A 3.4-g sample of $CaCl_2$ is dissolved in water to give 500 mL of solution at 298 K. What is the osmotic pressure of this solution?

Note. The stoichiometry and properties of solutions problems are from Reger et al. (1997, pp. 116; 122; 514–515); the thermochemistry problems are from Zumdahl and Zumdahl (2007, p. 239) and Zumdahl (1997, p. 281). The problems are typical of those in the categories, both in content and word length.

stoichiometry problems have fewer words than thermochemistry and properties of solutions problems, which are similar in word length.

The students were not required to solve the problems, but were asked to categorize the problems and explain in writing, in as much detail as possible, why they believed a pair they selected belonged to the same subcategory. The students' categorizations and explanations were scored as correct when they were based on underlying chemistry concepts, principles, or laws. The students' categorizations and explanations were scored as incorrect when they were based on superficial features of problems, such as vocabulary or objects. The students could achieve 1 point for each correct pairing and 1 point if the pairing was correctly explained, for a total of 12 possible points. For explanations, there was 97.03% agreement between raters (two science instructors), and the disagreements were settled through discussion.

Problems and Strategies. The students were asked to solve three quantitative, well-defined chemistry problems, showing their work, and producing the mathematical solution associated with each. As can be seen in Table 2, there was a *stoichiometry: reaction with a reactant in excess* problem, a *thermochemistry: constant-pressure calorimetry* problem, and a *property of solutions: colligative properties of non-electrolyte solutions* problem. These problems were representative of those in chemistry textbooks (Reger et al., 1997; Zumdahl & Zumdahl, 2007), both in terms of content and word length. The most frequent problem subcategories were used. The students had not seen these three problems previously.

We used strategy-scoring guidelines similar to those of Chi (2006a,b), Priest and Lindsay (1992), and Heyworth (1999) to score the students' problem-solving strategies. For each of the three problems, a working-forward strategy was identified as being used by a student when the first equation contained only a single unknown, and each subsequent equation provided the value of a single unknown (intermediate state) quantity, resulting in equations that led to the sought quantity. A working-backward strategy was identified as being used by a student when the first equation contained the goal and other unknowns that could not be directly calculated, and each subsequent equation attempted to solve for unknown quantities that were part of the previous equation(s); these newly found quantities were then inserted into the preceding equations in order to work backwards to solve the problem. Students received one point for using a working-forward strategy and zero points for using a working-backward strategy. Points were summed across the three problems, and a student's strategy score could range from 0 to 3. For strategy scores, there was 98.02% agreement between raters (two science instructors), and the disagreements were settled through discussion.

A student's problem-solution score could range from 0 to 3, with the student receiving 1 point for each of the three problems answered correctly. If a simple calculation error was present, full credit was still given for the problem—this occurred in only seven of the 303 possible instances (2.31%). A simple calculation error was computational as opposed to conceptual, and there was evidence in the work shown that indicated that the student understood the problem.

Table 2
The chemistry problems solved by students

Problem 1: Stoichiometry: reaction with a reactant in excess
Calculate the mass, in grams, of $Al(OH)_3$ (molar mass = 78.00 g/mol) formed by the reaction of exactly 500 mL of 0.100 M NaOH with excess $Al(NO_3)_3$
[Answer: 1.30-g $Al(OH)_3$]

Problem 2: Thermochemistry: constant-pressure calorimetry
When a 60.0-g sample of metal at 100.0°C is added to 45.0-g of water at 22.60°C, the final temperature of both the metal and the water is 32.81°C. The specific heat of water is 4.184 J/g °C. What is the specific heat of the metal?
[Answer: 0.476 J/g °C]

Problem 3: Properties of solutions: colligative properties of non-electrolyte solutions
Pure ethylene dibromide freezes at 9.80°C. A solution made by dissolving 0.213-g of ferrocene (molecular formula $Fe(C_3H_5)_2$, molar mass = 186.04 g/mol) in 10.0-g of ethylene dibromide has a freezing point of 8.45°C. What is the freezing point depression constant of the solvent ethylene dibromide?
[Answer: 11.8°C/*m*]

The three problems are from Reger et al. (1997, pp. 152; 174; 496).

One week later, after the data were scored, students with high (top 10%) and low (bottom 10%) scores in self-efficacy and strategy use, respectively, were asked to explain how confident they were about their chemistry problem solving, and why they generated the equations they did.

Results

The Statistical Program for the Social Sciences, version 14.0 (SPSS Inc., 2005) was used to compute descriptive statistics, mean comparisons, and correlations among the variables in the theoretical model. SEM was used to test the model. Specifically, LISREL Version 8.80 (Jörkeskog & Sörbom, 2007), with a covariance matrix generated by PRELIS Version 2.80 (Jörkeskog & Sorbom, 2006) was used to test the hypothesized model. The students' explanations were used to interpret the results of the statistical analyses.

Descriptive Statistics, Mean Comparisons, and Correlations

The results of independent-samples *t*-tests indicated there were no statistically significant differences between men and women on any of the model variables; thus the means reported in Table 3 are on men and women combined. In addition, the means for the students' conceptualization and problem-solution scores were combined over the problem categories: We used the categories in order to generalize our findings, not to study differences among the categories. Dependent-samples *t*-tests indicated that there was no significant difference in the number of times students used working-forward and working-backward strategies when attempting to solve the three problems; however, students correctly solved more of them when using a working-forward strategy ($M = 1.03$, $SD = 0.98$) than a working-backward strategy ($M = 0.12$, $SD = 0.33$), $t(100) = 8.42$, $p < 0.001$.

As can be seen in Table 3, there was a statistically significant Pearson product–moment correlation between problem conceptualization and problem strategy, indicating that the students with high conceptualization scores tended to have high problem-strategy scores. Self-efficacy was also correlated significantly with problem strategy, indicating that the students with high self-efficacy scores tended to have high problem-strategy scores. Finally, strategy was correlated significantly with problem solution, indicating that the students who used a working-forward strategy tended to have higher problem-solution scores than students who used a working-backward strategy.

The preceding findings are all consistent with the hypotheses of this study. Two additional findings were that conceptualization was significantly correlated with problem solution, indicating that the students with high conceptualization scores tended to have high problem-solution scores, and self-efficacy was significantly correlated with problem solution, indicating that the students with high self-efficacy scores tended to have high problem-solution scores. While not hypothesized, these correlations are consistent with our model because we hypothesized that both conceptualization and self-efficacy would be correlated with problem strategy, which, in turn, would be correlated with problem solution.

Table 3
Correlation matrix, means, standard deviations, skewness, and kurtosis

Variable	1	2	3	4
1. Conceptualization	—			
2. Self-efficacy	0.15	—		
3. Strategy	0.35^{**}	0.30^{**}	—	
4. Solution	0.35^{**}	0.25^{**}	0.67^{**}	—
M	2.84	18.16	1.52	1.15
SD	2.12	3.89	0.82	0.99
Skewness	1.06	−0.17	−0.10	0.36
Kurtosis	1.53	−0.81	−0.47	−1.01

$^{**}p < 0.01$.

Model Testing

The data were analyzed by means of SEM, which refers to a family of related statistical techniques, not to a single one. SEM typically involves building or "specifying" a model, often depicted in a drawing, about how the variables in a set influence each other. SEM is most frequently used in correlational research in which neither the independent nor the dependent variables are manipulated, but SEM is also useful when variables are manipulated.

A core SEM technique, path analysis, was applied to the present data, consistent with guidelines provided by Kline (2005). Path analysis involves the estimation of hypothesized causal relations among observed variables. The path analytic technique involves building a model aimed at explaining why variables 1, 2, 3, etc. are correlated. This explanation should take into account effects that are causal (e.g., variable 1 causes variable 2) and non-causal or spurious (e.g., variable 2 and variable 3 are related, but only because they are both caused by variable 1). Thus, the main goal of a path analysis, such as the one conducted in this study, is to build a model that explains the causal and non-causal components of observed correlations in a set of variables.

To satisfy the conditions of path analysis for the inference of causality, our hypothesized relationships involved time precedence and a logical direction of causality, consistent with the research reviewed. Also, our relationships were hypothesized to remain intact when external variables were held constant. Finally, our model was *recursive*: the sources of unexplained variance (*disturbances*) were assumed to be uncorrelated and the causal effects to be unidirectional.

Before empirically testing the model, the data were examined for normality and homoscedasticity (constant variance). There were no missing data values. Based on the data plots (histograms of the variables), examination of skewness and kurtosis statistics (Table 3), and Mardia's coefficient = 0.98, the data were consistent with the assumptions of both univariate and multivariate normality, justifying the use of the maximum-likelihood estimation to test the model.

A number of statistical tests (indices) can be used to assess the "goodness of fit" of the model to the data, and thereby determine if the model should be accepted or rejected. Any single goodness-of-fit index evaluates only particular aspects of a model's fit. Therefore, to properly evaluate the fit of the model, it is recommended that several fit indices be used (Kline, 2005). The overall fit of the model was found to be very good, as indicated by the fit indices used, all which are described in detail in the following paragraphs.

First, the Chi-square statistic was used. The Chi-square is a fit index that addresses the degree to which the variances and covariances implied by the model match the observed variances and covariances. A *non-significant* Chi-square indicates that the model is a good representation of the underlying covariance matrix. The Chi-square, $\chi^2\ (2) = 3.09$, $p = 0.21$, indicated a good fit because the *p*-value was greater than 0.05. Further, the χ^2/df ratio was 1.55, indicating a good fit based on Kline's (2005) rule that values less than 3 indicate a good fit.

The standardized root-mean-square residual (SRMR) is an index based on the residuals between the observed and estimated covariance matrices (Hu & Bentler, 1999). The advantage of the SRMR is that it is sensitive to model misspecification, such as a mistake in the direction of causality between variables (Hu & Bentler, 1998). A value below 0.08 indicates a good fit (Hu & Bentler, 1999). The SRMR for this model was 0.04.

The Steiger–Lind root-mean-square error of approximation (RMSEA) assesses a lack of fit of the population data to the estimated model. It is an index that includes adjustments for model complexity so that evaluation of fit is not overly influenced by the number of parameters in the model (Steiger, 1995). Browne and Cudeck (1993) suggest that a RMSEA value of 0.08 or less indicates a good model fit. Our obtained value was 0.07.

The incremental fit index (IFI) is a fit index that is sensitive to model misspecification, but not to sample size (Hu & Bentler, 1999), making it a valuable indication of fit. The IFI compares the model to a baseline model in which all variables are assumed to be uncorrelated. This is the standard "null" model (independence model) that assumes zero population covariances among the observed variables. The IFI values range from 0 to 1, with larger values indicating a better fit. A value greater than 0.95 is considered to be a good fit (Hu & Bentler, 1999). The value for this model was 0.99.

Finally, the adjusted goodness of fit index (AGFI) is a measure of the proportion of the observed covariance that is accounted for by the model. The AGFI is adjusted for degrees of freedom so that evaluation of fit is not overly influenced by the number of parameters in the model. The AGFI values range from 0 to 1, with larger values indicating a better fit. A value greater than 0.90 is considered to be a good fit (Schumacker & Lomax, 1996). The value for this model was 0.93.

Decomposition of Effects

Path analysis was used to estimate the direct and indirect effects in the model, control for the correlations among the hypothesized causal variables, and ‘‘decompose’’ the observed correlations into their component parts. The standardized path values and their associated t-values for the model are reported in Table 4; the model with standardized path values can be seen in Figure 3. A cutoff value of $t = 1.96$ for a two-tailed test was used to determine if direct and indirect path values were statistically significant. In terms of size and influence of the standardized path values, we used Keith’s (1993) recommended criteria: Standardized path values ranging from 0.05 to 0.10 are small, but meaningful influences; path values ranging from 0.11 to 0.25 are moderate in size and influence, and path values above 0.25 are large in size and influence.

The three direct path values were significant and large in influence. The decomposition of effects is shown in Table 4. Problem conceptualization had a significant and large influence (0.31) on problem strategy. Thus, students who conceptualized problems well tended to use a working-forward strategy. Self-efficacy also had a significant and large influence (0.26) on problem strategy, indicating that students with high self-efficacy tended to use a working-forward strategy. Problem strategy had a significant and large influence (0.66) on problem solution, indicating that students who used a working-forward strategy were more likely to arrive at the correct problem solution. In terms of proportions of variance (R^2) explained by the direct paths, self-efficacy and conceptualization together explained 0.19 in problem strategy, which, in turn, explained 0.44 in problem solution.

The indirect path values and their associated t-values are also shown in Table 4. Problem conceptualization, through its influence on strategy use, had a significant and moderately sized influence (0.21) on problem solution. This suggested that a deeper understanding of the concepts underlying the problems was associated with a working-forward strategy, which increased correct solutions. Self-efficacy, by means of its influence on problem strategy, had a significant and moderately sized influence (0.17) on problem solution. Thus, students with high self-efficacy tended to use a working-forward strategy, which increased correct solutions.

Students’ Explanations of Problem Solving

The correlations and path analysis indicated that the students who conceptualized problems well, had high chemistry self-efficacy, and used a working-forward strategy had the highest problem-solution scores. Students’ explanations provided insight into these results.

Table 4
Decomposition of effects in the model

		Effect			
		Direct		Indirect	
Predictor	Criterion	PC	t	PC	t
Conceptualization	Strategy	0.31	3.40		
	Solution			0.21	3.17
Self-efficacy	Strategy	0.26	2.77		
	Solution			0.17	2.65
Strategy	Solution	0.66	8.80		

Note. PC refers to standardized path coefficient. All t-values were significant, $p < 0.05$; tests were two-tailed. In terms of the relative size and meaningful influence of the path coefficients: those between 0.05 and 0.10 are small, those between 0.11 and 0.25 are moderate, and those above 0.25 are large (Keith, 1993).

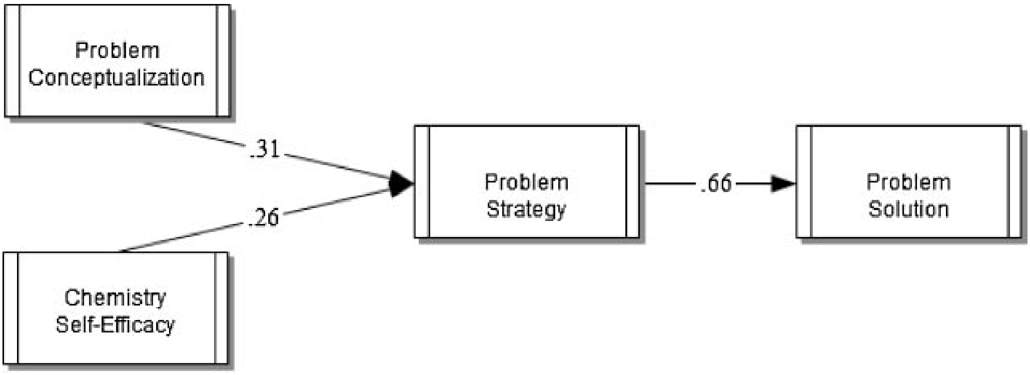

Figure 3. Tested model of chemistry problem solving, with standardized path coefficients.

During the conceptualization task, where students categorized pairs of problems as to subtype, the students explained in writing why they believed the pairs belonged together. The students who provided correct explanations referred to the chemistry concepts, principles, or laws underlying the problems. For example, a student who correctly paired thermochemistry (constant-pressure calorimetry) problems wrote: ‘‘These two problems are similar because they both deal with situations where the pressure is constant.’’ The students who provided incorrect explanations based the explanations on superficial features of problems, such as vocabulary or objects. For example, a student who incorrectly paired thermochemistry (constant-pressure calorimetry) problems wrote: ‘‘Both of these problems involve an M which stands for molarity of something, and the temperature of something looks like it's changing.’’

After problem solving, the students who scored high or low in self-efficacy and strategy use, respectively, were asked to orally explain how confident they were in their problem solving and why they generated the equations they did. Examples of what the students said about their self-efficacy and strategy use appear in the Discussion Section when interpreting the findings. In general, the students appeared to candidly reflect on their self-efficacy and strategy use. They mentioned a number of factors that contributed to their self-efficacy and strategic skill in chemistry problem solving. These factors included family members who are scientists, a high-school chemistry course, their current college chemistry course, hard work, perseverance, interest, enjoyment, grades, and science-career goals. The students who scored low in self-efficacy or strategy use, however, appeared to accept their low confidence or poor strategic reasoning as an unfortunate, predetermined, unchangeable condition, which they often attributed to an inadequate high-school chemistry course or lack of ability. These students did not mention steps they could take to improve either their self-efficacy or their strategy use, not did they mention a desire to do so.

One of the students, Susan, conceptualized problems well, had high self-efficacy, and used a working-forward strategy on all problems: She correctly solved all three problems. Relatively speaking, she's an ‘‘expert’’ problem solver, having acquired proficiency in solving the kinds of problems routinely posed in her college general-chemistry course. Jason, on the other hand, conceptualized problems poorly, had low self-efficacy, and used a working-backward strategy on all problems: He only solved one of the three problems correctly, the thermochemistry problem. Relatively speaking, he remains a ‘‘novice’’ problem solver because he did not acquire proficiency in solving the kinds of problems routinely posed in the course. To illustrate Susan's use of a working-forward strategy and Jason's use of a working-backward strategy, their explanations and equations for the thermochemistry problem, which they both solved correctly, are reported in Table 5. As can be seen in the table, Susan required only two equations to correctly solve the problem, using the cognitively efficient working-forward strategy. Jason, on the other hand, required five equations to correctly solve the problem, using the less efficient working-backward strategy. Although both students in this example correctly solved the problem, the additional cognitive load associated with the working-backward strategy often led to errors in students' problem-solving equations and solutions.

Table 5

Examples of working-forward and working-backward strategies used by students when solving the thermochemistry problem

Problem:

When a 60.0-g sample of metal at 100.0°C is added to 45.0-g of water at 22.60°C, the final temperature of both the metal and the water is 32.81°C. The specific heat of water is 4.184 J/g °C. What is the specific heat of the metal? [Answer: 0.476 J/g °C]

Susan, who used a working-forward strategy to correctly solve the problem, constructed the following 2 equations and explained:

$Q_{\text{water}} = (4.184\,\text{J/g}\,°\text{C}) \times (45.0\,\text{g}) \times (32.81\text{-}22.60°\text{C}) = 1.92 \times 10^3\,\text{J}$

"First, I'm solving for the heat gained by the water, 1.92×10^3 J, because that tells me the heat lost by the metal, -1.92×10^3 J."

$c_{\text{metal}} = -1.92 \times 10^3\,\text{J}/(60.0\,\text{g}) \times (32.81\text{-}100.0°\text{C}) = 0.476\,\text{J/g}\,°\text{C}$

"Next, I'm using the heat lost by the metal to calculate its specific heat, 0.476 J/g °C, and solve the problem."

Jason, who used a working-backward strategy to correctly solve the problem, constructed the following 5 equations and explained:

$c_{\text{metal}} = Q_{\text{metal}}/(60.0\,\text{g}) \times (32.81\text{-}100.0°\text{C})$

"I've got to solve for the metal's specific heat, but I've got to solve for the heat lost by the metal too."

$Q_{\text{metal}} = c_{\text{metal}} \times (60.0\,\text{g}) \times (32.81\text{-}100.0°\text{C})$

"I've rearranged terms in the equation."

$Q_{\text{water}} = c_{\text{water}} \times (45.0\,\text{g}) \times (32.81\text{-}22.60°\text{C})$

"I can find out the amount of heat lost by the metal if I can find out how much heat the water gained."

$Q_{\text{water}} = (4.184\,\text{J/g}\,°\text{C}) \times (45.0\,\text{g}) \times (32.81\text{-}22.60°\text{C}) = 1.92 \times 10^3\,\text{J}$

"The problem said the specific heat of water is 4.184 J/g °C, so I can plug that in. So, now I've figured out the heat gained by the water, which is the same as what the metal lost."

$c_{\text{metal}} = -1.92 \times 10^3\,\text{J}/(60.0\,\text{g}) \times (32.81\text{-}100.0°\text{C}) = 0.476\,\text{J/g}\,°\text{C}$

"And now I can go back to my first equation and plug in the heat the metal lost and get the answer, 0.476 J/g °C, for the metal's specific heat."

Susan required only two equations to correctly solve the problem, using the cognitively efficient working-forward strategy. Jason required five equations, using the less efficient working-backward strategy. Even though both students correctly solved this problem, the heavy cognitive load associated with the working-backward strategy often led to errors in the equations of students who used it.

Discussion

By means of SEM, we tested and validated a model of expertise in chemistry problem solving based on ACT-R theory (Anderson, 2002; Anderson et al., 2004). A model is an important theoretical tool in understanding a process as complex as chemistry problem solving. By providing insight into this process, the model can be used to improve programs for teaching and learning chemistry problem solving. Our model quantitatively and visually depicted the interaction and relative contributions of conceptualization, self-efficacy, and strategy to the successful solution of quantitative, well-defined problems. The components interacted as hypothesized: The students with the highest problem-solving scores were those who conceptualized problems well, had high chemistry self-efficacy, and used a working-forward strategy. The relative contributions of the model's components to chemistry problem solving are discussed in the following sections.

Strategy Use: Central to the Model

Strategy use played a central role in the model, influencing problem-solving success more than any other model component. We found that the students who used a working-forward strategy tended to answer the problems correctly, whereas those who used a working-backward strategy tended to answer the problems incorrectly. The work of the students using a working-forward strategy appeared to be conceptually driven, goal directed, and consistent with a constructivist view of chemistry problem solving (Bodner et al., 2001). Students using a working-forward strategy constructed equations based on the information provided in the problem statement, systematically working forwards toward the goal state. One of the students, who successfully used a working-forward strategy to solve the thermochemistry problem, explained her work in this way:

> I knew that ultimately I'd need to solve for specific heat of the metal. But in order to get the specific heat of the metal, I'd need the heat gained by the water. So I started to solve for the heat gained by the water first, and then getting that allowed me to solve for the specific heat of the metal.

Compared to the students using a working-forward strategy, the students using a working-backward strategy appeared to lack planning and focus. The latter began by forming an equation that contained the problem goal and one or more other unknowns. These students then created additional equations to solve for the unknowns. When values for the unknowns were obtained, the students worked backwards, inserting the values in the preceding equations, in order to solve the problem. Even when the solution was correct, it was inefficiently arrived at. For example, one of the students, who used a working-backward strategy to solve the thermochemistry problem, explained his work in this way:

> Well, let's see. I started out trying to solve for specific heat of the metal. Then I realized I had everything to solve the equation except for the heat lost by the metal, which is the same as the heat gained by the water. I needed this before I could solve for the specific heat of the metal. So I formed an equation, actually a few, to set things up so I could solve for the heat gained by the water. After I got that value, I then went back and stuck it into my first equation in order to get the specific heat of the metal.

We are not stating that working backwards is a bad strategy. We are stating that it is an inefficient strategy for solving the quantitative, well-defined problems typically posed in introductory-level chemistry courses. Such problems in areas such as stoichiometry, thermochemistry, and properties of solutions lend themselves to a working-forward strategy because students (and professional chemists) who are knowledgeable and well prepared can apply familiar schemas to the problems and mentally represent them in terms of a problem space. Schema application and mental representation become highly automatized through guided practice in problem solving, and the cognitively efficient working-forward strategy becomes the default strategy that knowledgeable students use with quantitative, well-defined problems. In effect, working forwards becomes second nature for knowledgeable students solving such problems.

Although working backwards is inefficient for solving quantitative, well-defined problems, it is a good strategy for students to use when they encounter problems for which they have not yet developed schemas, such as ill-defined problems. In fact, chemists frequently use a working-backward strategy to solve problems. A famous example is Elias J. Corey, who received the Nobel Prize in chemistry in 1990 for his contributions to synthetic organic chemistry. Corey's work led to new methods of synthesizing compounds, and these methods have facilitated the production of pharmaceuticals. When awarding him the Nobel Prize, The Royal Swedish Academy of Sciences (1990) noted the important role that a working-backward strategy played in Corey's problem solving. Using a working-backward strategy can, therefore, prepare students for possibly making their own discoveries in the field of chemistry someday. For this reason, we recommend introducing students to a working-backward strategy, in addition to a working-forward strategy, and occasionally presenting them with problems for which they do not yet have schemas (Bodner, 2003; Lyle & Robinson, 2001).

Model Components Influencing Strategy Use

Problem conceptualization influenced students' strategy use. We found that the students who conceptualized the chemistry problems well tended to use a working-forward strategy and solve the problems successfully: Written explanations by these students indicated that they used schemas to recognize and mentally classify the problems in terms of the categories of stoichiometry, thermochemistry, and properties of solutions. These categories were based on the concepts, principles, and laws underlying the problems—not on superficial features of the problems, such as terminology and objects. We used subcategories, in addition to categories, to create a more challenging and valid conceptualization task than had been used in previous studies, but the task proved a bit too challenging because the average student's score was about 24% instead of a psychometrically desirable 50%. This restriction in score range means that the observed influence of problem conceptualization on strategy use, while significant, probably underestimated the actual influence.

In other words, problem conceptualization probably has an even bigger influence on problem solution than the influence we found.

Our problem conceptualization findings are consistent with the general literature in problem solving which suggests that schematic knowledge enhances performance (Kozma, 2003; Mason, Shell, & Crawley, 1997; Taconis et al., 2001). Our findings are also consistent with the relatively small number of studies conducted so far on the conceptualization of chemistry problems. Those studies found that experts tended to categorize chemistry problems based on laws, principles, and concepts, whereas novices tended to categorize problems based on superficial features of the problems (Stains & Talanquer, 2008).

Chemistry self-efficacy also influenced students' strategy use. We found that the students with relatively high chemistry self-efficacy tended to use a working-forward strategy and solve problems successfully. This finding suggests that students who believed they were capable in chemistry were more likely to exert strategic effort and persist with this effort until they solved the problems. One student, who scored high in self-efficacy, said this about the thermochemistry problem:

> At first I wasn't sure what I needed to do, but then I just kept thinking about it and realized, okay, I need to find the heat gained by the water first. It took me a minute to get it, but I really wanted to solve it and knew I could. After that I knew what to do to get the specific heat of the metal.

We found that students with relatively low chemistry self-efficacy tended to use a working-backward strategy and solved the problems incorrectly. One student, who scored low in self-efficacy, said this about the thermochemistry problem:

> I knew when I looked at the problem that I would probably get the wrong answer. I'm not too good at chemistry, and I'm not doing too well in the class. I just came up with an equation to solve for the problem, but I think I plugged in the wrong values or something, and I'm sure my answer is wrong.

Our finding that chemistry self-efficacy influenced strategy use and problem solving is consistent with the general literature concerning self-efficacy (Crippen & Earl, 2007; Schraw, Brooks, & Crippen, 2005; Zimmerman & Campillo, 2003). Self-efficacy contributes to the acquisition of expertise in problem solving by predisposing students to work on challenging problems, and to persist longer when goal attainment is difficult. In explaining the powerful influence of self-efficacy on behavior, Bandura and Locke (2003) state:

> Among the mechanisms of human agency, none is more central or pervasive than beliefs of personal efficacy. Whatever other factors serve as guides and motivators, they are rooted in the core belief that one has the power to produce desired effects; otherwise one has little incentive to act or to persevere in the face of difficulties. (p. 87)

Our finding that chemistry self-efficacy influenced strategy use and problem solving is also consistent with other studies conducted on students' chemistry self-efficacy, such as that of Zusho et al. (2003), and with historical accounts of the role that self-efficacy played in chemistry achievement. For example, Dorothy Crowfoot Hodgkin received the Nobel Prize in Chemistry in 1964 for using X-ray crystallography to determine the structure of penicillin and vitamin B12. While studying chemistry at Oxford, her self-efficacy enabled her to persevere in the face of difficulties such as "the chemistry club uniting Oxford's chemists did not permit women to belong or attend meetings" (McGrayne, 2001, p. 235).

More research needs to be done on how to improve students' chemistry self-efficacy. The general literature concerning self-efficacy suggests at least three techniques that could be helpful (Zeldin, Britner, & Pajares, in press). First, the concept of self-efficacy should be explained to students, and they need to understand the circumstances that help or hinder their chemistry self-efficacy. Second, students should have the opportunity to interact with peer models that started at a similar level and, over time, improved their chemistry self-efficacy. And third, students should be encouraged to self-regulate their chemistry learning; this means students should take responsibility for their metacognitive awareness, strategy use, and motivational control.

Implications for Future Research and Practice

In future research, the model we developed should be expanded to provide a more comprehensive understanding of expertise in chemistry problem solving. We developed a parsimonious model as a prototype, one that we and other researchers could use to explore how other cognitive and social-cognitive components interact and contribute to chemistry problem solving. For example, a student's *interest in chemistry*, a social-cognitive component, could be added to the model. How is interest related to the other components, such as self-efficacy? Does interest contribute more to successful problem solving than a component such as self-efficacy? These are examples of questions that merit attention in future research with the model.

Comprehensive, open-ended, individual interviews should be conducted in future research to gain an in-depth understanding of students' understanding of the components of the model. This understanding is an aspect of students' *metacognition*, or their "thinking about thinking" (Nielsen, Nashon, & Anderson, in press). In the present study, we asked a sample of students to explain "how confident they were in their problem solving" and "why they generated the equations they did." The students' responses were informative, but more could be learned about students' understanding of the components of the model if extensive open-ended interviews were conducted (Patton, 2002).

Our model has implications for practice because it provides insight into the process of chemistry problem solving. In particular, our findings indicate that that the use of the working-forward strategy is tied to effective conceptualization. Students should not be taught a working-forward strategy without first attending to students' conceptual knowledge. A working-forward strategy is a tool that enables students to efficiently apply their knowledge of problem schemas and to mentally represent problems well. Without conceptual knowledge driving it, a working-forward strategy is no more advantageous than a working-backward strategy.

One way to help students develop conceptual understanding is to ask them to compare and contrast concepts, identify valid similarities and differences, and then arrange the concepts hierarchically through instructional activities such as categorization tasks or concept mapping (Ruiz-Primo, Schultz, Li, & Shavelson, 2001). The concepts that students categorize or map should not be limited to those they are currently learning, but should also include those they learned in the past. Helping students to reflect on the relevance of concepts they learned in the past to those they are presently learning will increase the cohesion of the students' knowledge, develop their conceptual understanding, and foster the construction of schemas that support effective strategy use.

When teaching a working-forward strategy, instructors should ensure that students activate their relevant conceptual knowledge when learning and implementing the strategy. We encourage instructors to show students the difference between the working-forward and working-backward strategies, the connection between the strategies and conceptual understanding, and the advantage of working forwards when solving quantitative, well-defined problems. Doing this will support students' metacognitive understanding of their problem solving (Wilson & Clarke, 2004).

Our findings suggest that instructors teaching chemistry problem solving should take into account students' chemistry self-efficacy and the factors that likely support it, such as students' belief in the relevance of chemistry to their lives, both inside and outside of the classroom. Without this social *contextualization* of chemistry, students often perceive it as a particularly abstract and difficult subject (Bloom & Halpin, 2003). If chemistry is contextualized, it may be easier for instructors to develop students' self-efficacy and problem-solving expertise (Dalgety et al., 2003; Teichert & Stacy, 2002).

In conclusion, we return to Linus Pauling's view that developing expertise in chemistry problem solving means learning the conceptual knowledge of the discipline and how to apply strategic reasoning to problems in the discipline. Historians of science have documented that these qualities of Pauling, in combination with his chemistry self-efficacy, contributed to his phenomenal success in chemistry (Marinacci, 1995). We found these same qualities to be influential in the model of expertise in chemistry problem solving that we tested. We want students in introductory chemistry to develop expertise in problem solving. To help them do so, it is important to identify the cognitive and social-cognitive components involved in this expertise, determine how these components interact, and quantify the contributions that these components make to successful problem solving. This knowledge is essential in order to improve the teaching and learning of chemistry problem solving.

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