

A Cognitive Modeling Tutor Supporting Student Inquiry for Balancing Chemical Equations

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Abstract: Improved interactive tutoring capabilities in educational software for chemistry problem solving is an important need that has been clearly articulated by teachers and students. The purpose of this work is to examine the incorporation of new concepts from the field of artificial intelligence (AI) as a route to meaningful individualized tutoring. The basic shift is to replace specific foreknowledge of problems with a direct representation of chemical and pedagogical principles and then simulate reasoning using these principles to tutor students. To assess the potential of an AI-based approach, we have developed a prototype tutorial program for balancing chemical equations that contains two important advances. First, the system can create a worked-out solution with detailed explanations for any equation entered by the student or teacher. Unlike a conventional tutorial, this is done dynamically, without the equation being stored ahead of time. Second, the program can interactively answer a variety of detailed questions about its work at each step. Studying worked-out examples plays an important role in learning, and this approach to supporting interactive student inquiry is being investigated as a method of cognitive modeling and apprenticeship intended to foster the student's own self-explanation and question-asking abilities.

Introduction

Improved interactive tutoring capabilities in educational software for chemistry problem solving is an important need that has been clearly articulated by teachers and students. Most tutorial programs are termed “computer-assisted instruction” (CAI), an approach that has been used for a long time in chemistry [1, 2]. To deliver the next generation of enhanced capabilities that users currently demand, however, it will be necessary to go beyond this methodology.

The CAI approach contains inherent fundamental limitations that must be overcome. Existing programs typically limit the problems available for students to a fixed list, which rules out the possibility of providing tutoring for the teacher's own assignments, for example. More serious, however, is the shallow level of interactivity during the problem-solving process. Typically, the student only selects the final answer in multiple-choice form. Most programs also present a standard worked-out solution, but cannot provide instruction on an individualized basis. The student is not able, for example, to ask questions or get feedback and analysis on his or her own attempts at solving the problem.

These issues have led to criticism of CAI for a “linear” instructional approach that is too inflexible to support meaningful learning or add significant complementary value to other educational resources [3–6]. The crucial design weakness of CAI is the need for the problems and solutions to be programmed into the system ahead of time. Although this makes for straightforward computer implementation, the approach is not extensible. The student cannot work with problems that are not in the database, and the only way to give feedback on a specific mistake is for it also to be prestored. This severely narrows the ability to assist the student and to treat a significant number of problems with any depth.

A fresh approach is required to overcome these obstacles. The purpose of this work is to examine the incorporation of new concepts from the field of artificial intelligence (AI) as a route to meaningful individualized tutoring, which CAI cannot deliver because of its intrinsically rigid design. The basic shift is to replace specific foreknowledge of problems with a direct representation of chemical and pedagogical principles and then simulate reasoning using these principles for the purpose of tutoring students on problems given to the program.

To assess the potential of an AI-based approach, we have developed a prototype tutorial program for balancing chemical equations that contains two important advances. First, the system can create a worked-out solution with detailed explanations for any equation entered by the student or teacher. Unlike a conventional tutorial, this is done dynamically, without the equation being stored ahead of time. Second, the program can interactively answer a variety of detailed questions about its work at each step. Studying worked-out examples plays an important role in learning [7], and this approach to supporting interactive student inquiry on such examples is being investigated as a method of cognitive apprenticeship [8, 9] intended to foster the student's own self-explanation [10] and question-asking [11] abilities.

Balancing equations is a topic of considerable pedagogical interest as evidenced by the large existing literature, which has recently been thoroughly reviewed [12]. Several techniques have been proposed; however, most are concerned with “bulletproofing” a method for all possible equations. This is counterproductive for our purposes, because it necessarily pulls student focus from the concept of conservation, where it belongs, to the details of an overly complex procedure. It has been noted that such approaches are not beneficial for instilling and underscoring the fundamental concepts [13]. It was therefore decided that a simple inspection-based method

clearly motivated from conservation principles was the most desirable.

Our concern is not balancing all possible equations; this problem has been solved for a long time. Rather, our goal is to successfully tutor students by computer, a much more complex task. All of the difficult objectives leading to the investigation of an artificial intelligence approach are pedagogical in origin. There is no shortage of programs that can balance chemical equations, but none of these can explain for the student a rationale by which he or she can learn to do the same, unless again, the specific equation has been scripted ahead of time. Typically, only the final result is provided with no indication of how it was obtained.

Prior applications of AI to chemistry tutoring are extremely sparse (only two in the past decade). One of these, for oxidation numbers [14], was in actuality equivalent to a database approach. The other, an online web-based tutor at the University of Massachusetts, was more sophisticated, dealing with Lewis structures [15] and stoichiometry [16]. Still, the available problems were restricted to a small list and the solution path was somewhat procedurally scripted; therefore, the approach chosen for investigation here was not similar to either.

Expert System Design

The many different approaches to intelligent tutoring system design are categorized as simulation-based or problem-based [5] with the latter sometimes also referred to as cognitive tutors [17–19]. Within cognitive tutor methods, the model-tracing approach [19] was chosen as the basis of this work. This approach has been successful in developing advanced tutors for algebra and geometry [20]. This first involves creating an expert system for the domain of interest, which is a model of how a skilled problem solver represents knowledge, to be applied by the computer to solve problems in a similar fashion. This method uses production rules (PRs), rather than a database or script, as the representation of knowledge. These rules examine a problem and take a step towards its solution dynamically. This is key, because foreknowledge of the problem is not required as with CAI. The technical details of expert system design and implementation are beyond the scope of the present paper, but interested readers may consult reference 21 as a good introductory reference on the subject.

Based on the career teaching experience of one of the authors (DAH), a set of PRs was developed for an expert system sufficiently powerful to balance all equations beginning students will encounter at the high school and university general chemistry levels, while remaining simple enough to show the underlying concepts clearly. Examples of the system's PRs include changing the coefficient of a single reactant or product to bring a particular element into balance, multiplying the equation by a constant to facilitate balancing an element, and removing common factors from the equation's coefficients.

During the course of solving a problem, the set of all possible next steps generated by the production rules is called the conflict set, and the process of deciding which of these steps should be taken is called resolution of the conflict set. The cycle of conflict-set generation and resolution is repeated until the problem has been solved. For conflict-set resolution, each step is classified as productive, counterproductive, or illegal. An illegal step is defined as one violating a

fundamental principle, such as using negative coefficients. These steps are never selected. A legal step is productive if it yields net progress towards solving the problem. Assessment of productivity entails analysis of elements balanced and unbalanced by the step (as well as other factors) and results in a score by which the legal steps are ranked.

Solutions can be found by always selecting the most productive step, but this is not entirely satisfactory for teaching purposes because it biases the system towards finding the shortest solution, not the most instructive one. The clarity of the solution for the student is another essential factor. For this, each step is also independently critiqued for teachability, a measure of simplicity and how clearly the underlying concept is illustrated. Productive steps that can be clearly explained are considered more desirable than complex steps that are more productive.

The system was validated for robustness on several hundred equations from current textbooks and Internet study pages. The bottom line is that the method implemented can readily handle essentially all equation-balancing problems given to general chemistry students, as well as several more complex equations considered beyond the introductory level.

Explanation of Solution

The next stage was to add the ability for the expert system to give a detailed explanation of its work in balancing an equation for students who could benefit from seeing a few more examples worked out in detail before attempting problems themselves. The key to achieving this goal is that the design shift to the PR-based representation has the link between problem work and its justification built in from the start. The system simulates reasoning by applying chemical principles to create a solution to a problem not known to the system ahead of time. This is in sharp contrast to CAI, which simply recalls the solution from a database or reads from a prestored script, with no real "understanding" of what goes into solving the problem.

The explanation capability is illustrated in Figure 1. After entering an unbalanced equation, the student gives the command for the tutor to take each step, so that the tutor's work can be studied one step at a time. At each step, a short explanation is given by default and the new resulting equation is displayed. This way, the student is not overloaded with information at first. Because more detailed explanation and querying facilities are provided, if the short explanation is not sufficient the student can follow up by asking the system for clarification. The longer explanations not only provide elaboration on how the step was carried out, but also explicitly bring in applicability conditions and the reason why the step was needed.

The information generated internally in the course of solving the problem is transformed into an explanation statement suitable for the student. A variety of wordings are available for these, selected at random to keep the dialogue fresh, and specifics from the problem at hand are directly instantiated in the explanations. In the following example, a more detailed explanation is requested for each step.

This simple example illustrates several pedagogical objectives. It continually reminds the student that conservation is the purpose behind the balancing process. It demonstrates that no single technique always works for balancing equations, so an attitude of trying different things is encouraged. At the

Tutor:	Here is our equation: $\text{NH}_3 + \text{O}_2 \rightarrow \text{NO} + \text{H}_2\text{O}$
	I will show you how to balance it.
Student:	Show me the next step.
Tutor:	I set NH_3 and H_2O in the ratio 2:3. This balances hydrogen. $2 \text{NH}_3 + \text{O}_2 \rightarrow \text{NO} + 3 \text{H}_2\text{O}$
Student:	Explain the last step you took in more detail.
Tutor:	With 3 hydrogen atoms in NH_3 and 2 in H_2O , balancing H requires changing two coefficients. Taking two NH_3 molecules and three H_2O molecules balances hydrogen with 6 atoms in both the reactants and products.
Student:	Show me the next step.
Tutor:	Then, I adjusted nitrogen monoxide to bring nitrogen into balance. $2 \text{NH}_3 + \text{O}_2 \rightarrow 2 \text{NO} + 3 \text{H}_2\text{O}$
Student:	Explain the last step you took in more detail.
Tutor:	I saw 2 N atoms on the reactants side but only 1 on the products side. The atoms are simply rearranged in a chemical reaction, so we need to have the same number of nitrogen atoms on each side. I placed a 2 in front of nitrogen monoxide, which brings nitrogen into balance.
Student:	Show me the next step.
Tutor:	I didn't balance or unbalance or anything with this step. I just multiplied through by 2. The reason I did this is that it sets up to balance oxygen easily in the next step. $4 \text{NH}_3 + 2 \text{O}_2 \rightarrow 4 \text{NO} + 6 \text{H}_2\text{O}$
Student:	Explain the last step you took in more detail.
Tutor:	Since there were 2 O atoms on one side and 5 on the other, oxygen was out of balance by 3 atoms. I would like to fix this by using O_2 , because this contains only oxygen and won't unbalance anything else. But, because each O_2 molecule contains 2 oxygen atoms, there is no way to make up 3 atoms, so I decided to multiply the whole equation by 2 first. Then I'll be able to make up the difference by adjusting O_2 on the next step.
Student:	Show me the next step.
Tutor:	To conserve oxygen, I then took five O_2 molecules on the reactants side. $4 \text{NH}_3 + 5 \text{O}_2 \rightarrow 4 \text{NO} + 6 \text{H}_2\text{O}$
	We now have the same number of atoms of each element in the reactants and products, so the equation is balanced.
Student:	Explain the last step you took in more detail.
Tutor:	We didn't have the same number of oxygen atoms in the reactants and products. Since we must end up with the same number of atoms we start with, I put five O_2 molecules on the reactants side. That balanced the oxygen by giving 10 O atoms in both the reactants and products.

Figure 1. Expert system solution with step explanations.

same time, excellent thought patterns and self-explanation skills are modeled for the student. Opportunities are also taken to reinforce terminology and meaning of notation. For example, it is clear from the discussion that the products side is the right side of the equation and, though nomenclature is not the focus of this tutor, occasionally names are used instead of formulas for reinforcement (as in the second step).

The explanation of the third step is the most involved. This focuses on the rationale for scaling the equation to allow oxygen to be balanced using an integral number of O_2 molecules. A noteworthy feature is that the AI directly incorporated the reasoning behind manipulating a free element into the discussion. This has the advantage of illustrating this "free element rule" in a context when it is needed in a concrete example provided by the student, clarifying the motivation for this strategy. The fourth step shows how the idea begun in step three was followed through to balance oxygen in a two-step process, completing the problem.

Student Inquiry of Tutor

In conventional intelligent tutoring system design, the usual approach is to proceed directly to analysis of student work with the expert system once it has been built. In applying AI principles to chemistry education software, our end goal is clearly that students work the problems for themselves with the tutor's guidance. One important innovation in this research, however, is investigation of a novel variation on the typical design path, creating a new category of tutor that itself addresses an important need. Again, one of the key motivations is to support students who are not yet able to attempt the problems on their own. The problem-solving process may seem reasonable when reading the examples in the textbook or following the teacher, but upon trying the same problems for

themselves many students find that they are unable to make a start.

How can intelligent software be designed to help bridge this gap? The ability to provide a quality explanation of a solution for any problem "on the fly" is itself a significant step forward, but this is not entirely sufficient. We should not rely on the student understanding the system's explanations "as is," for example. More generally, it is possible that a given problem situation could raise multiple different questions in the student's mind, and similarly, the same situation could raise different questions for different students. These cannot all be addressed by the step explanations, but in typical software, if the explanation given is not enough there is no way for the student to get more help.

Because the expert system operates by simulating application of chemical principles, a considerable level of detail is generated internally in the course of solving each problem. A new way to leverage the products of this reasoning process was developed by exporting them in the form of various questions the system can answer for the student. This provides a further dimension of interactivity allowing students to conduct exploratory inquiry even before they can attempt the problems. The questions generated are intended to model good scientific thinking and illustrate that asking questions is an essential part of learning; this is very important in fostering the development of the student's own question-asking ability [11].

Generation of the questions was implemented in the expert system framework in a similar fashion as the production rules. Again, a direct benefit of an AI-based approach is that the circumstances under which particular questions are useful can be determined dynamically without foreknowledge of the problem. The criteria for question activation can include pedagogical considerations as well. As a result, the questions

and answers can be generated dynamically and made highly targeted and context-specific, changing at each step.

A very important factor is that the tutor offers the additional question-and-answer capabilities by permitting the student to direct the inquiry [22] by deciding which questions to ask. At each step, the questions that the tutor can answer are placed in a menu (Figure 2) that the student can choose from as needed to query the tutor in different ways. In this way, at every step the student can explore, selecting as many or as few questions as desired and use the questions and answers in conjunction with the step explanations.

The dialogue in Figure 3 revisits the problem in Figure 1 using the questions menu. While the first dialogue focused on the mechanics of balancing the equation, this dialogue brings in some more advanced and conceptually oriented questions. Though the path followed in this dialogue was deliberately taken in order to illustrate specific tutor features discussed below, it is representative of actual interactive student sessions we have observed.

After a couple of relatively straightforward steps (for which further explanations could have been obtained if desired), a rich opportunity for discussion of some seemingly reasonable alternative steps for balancing oxygen arises. Relevant points in the dialogue are labeled for discussion.

(1) After balancing nitrogen, upon counting the oxygen atoms from left to right, it might be thought that the two oxygen atoms from the two NO molecules "already" balance the two O atoms on the reactants side. Thus, it might seem that oxygen can be successfully balanced by setting the coefficient of H₂O to zero to eliminate the three "unnecessary" O atoms. The answer relates the interpretation of the notation to the representation of a definite chemical reaction and directly connects to the meaning underlying the notation.

(2) Another step that seems to balance oxygen is setting the coefficient of NO to -1. This answer underscores that atoms and molecules are physical entities and points out the implication of this on the solution. It also emphasizes that balancing chemical equations is more than just solving an algebra problem or puzzle. As in (1), it shows that the reason for positive coefficients is chemical, not mathematical. Such "why didn't you" questions provide a particularly powerful way to model good cognitive strategies.

The next step completes the problem. Before moving on, however, there is an opportunity for the student to ask additional questions dealing with the "big picture." Typically, the question list is longest after the problem is finished.

(3) This question gives a reminder of what the equation notation represents and focuses attention on the chemical meaning, rather than on superficially manipulating symbols and numbers.

(4) This directly illustrates the mass conservation concept on the student's own problem. The fact that seemingly unrelated numbers add up to the same value is compelling evidence that something must be at work. If the student does not yet understand why this happens, he or she is primed by this demonstration for the explanation that follows. An important point is that this is a good example of a question the student is not likely to think of on his or her own, yet is beneficial for study.

(5) This question gives a timely reinforcement of why we would need to do this type of problem.

These examples show several useful attributes of the question-and-answer approach. Comparing Figures 1 and 3

illustrates that many different paths of inquiry are made possible for the same problem, with the student leading the inquiry. Support can be readily provided on several different levels of student proficiency, from initial "hand-holding" to advanced strategic questions. We do not take for granted, for example, that the student can answer elementary questions like "Is H balanced?" or even necessarily realize their relevance or importance if they are not made available for examination. The inability to obtain this level of detail and justification has long been recognized as a hindering factor in studying worked-out examples [7]. For the struggling student, this type of help is critical to building a solid foundation. This is simply not practical in a non-interactive medium (textbook) or a non-intelligent software format like CAI.

What if the student's question (or one equivalent to it) does not appear in the list? In this case the system assists in a cognitive apprenticeship fashion [8, 9] by modeling good questions to ask, prompting the student towards productive directions of thought. Often the most beneficial question to consider is one the student does not yet know how to ask. Many times, when confronted with a new problem a student will be unable to formulate any meaningful questions and getting examples of good questions is of tremendous benefit. Showing how to ask good questions is an important technique used by successful human tutors, and it is an important metacognitively-oriented capability of the question technique. At the same time, this approach contains a built-in mechanism for building self-efficacy as students progress, as they become able to answer the questions for themselves and confirm their answers using the tutor.

The use of context-dependent questions and answers for cognitive modeling and apprenticeship on user-supplied problems is a new feature in intelligent tutoring system design in general [23], not just in application to chemistry. This research dovetails well with other ongoing work on third-generation intelligent tutors supporting and promoting student self-explanation as an important key to learning with understanding [24–26]. By first modeling for students good approaches to self-explanation and question asking, they will be better prepared to do quality work.

Conclusion

This study has established the feasibility of a proposed AI-based approach to creating advanced new tutoring software for chemistry problem solving. Based on these results, we are excited about the continued investigation and development of these techniques, including extension to direct analysis of student work and development of tutors for additional chemistry topics. This technology has been implemented as a tutoring "engine" that can easily be interfaced to add interactive tutoring capabilities to any existing educational program or curriculum, such as those oriented around practical real-world applications of chemistry.

The capability for students to ask questions of the tutor is particularly promising. This new cognitive modeling functionality based on an expert teacher's knowledge provides interactive inquiry at a level not previously attained in chemistry software tutorials. This directly supports the goal of better teaching and learning of chemistry. The techniques developed here can be broadly applied as a powerful method for challenging head-on and in context the opportunities for misconceptions to take hold and develop.

Quantum - Cu(NO₃)₂ -> CuO + NO₂ + O₂ - Microsoft Internet Explorer

Address: http://localhost/cgi-bin/hrw/eqbal/process_response.pl

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$$2 \text{Cu}(\text{NO}_3)_2 \rightarrow 2 \text{CuO} + 4 \text{NO}_2 + \text{O}_2$$

Next, I'll balance oxygen with one molecule of O₂ on the products side.

We now have the same number of atoms of each element in the reactants and products, so the equation is balanced.

Ask a Question

What does this balanced equation tell me?
Interpret this equation for me in terms of mass.
Why didn't you consider the question above until after the equation was balanced?
Why did you write just "O₂" instead of "1 O₂" in the equation?
Could you also have taken 0 CuO to balance O?
Give me a more detailed explanation of the last step you took.
What are the conservation conditions for this equation?
Is the equation balanced yet?
Is N balanced?
Is O balanced?
Is Cu balanced?

Figure 2. Example questions menu.

Tutor:	Here is our equation: $\text{NH}_3 + \text{O}_2 \rightarrow \text{NO} + \text{H}_2\text{O}$
	I will show you how to balance it.
Student:	Show me the next step.
Tutor:	I put NH ₃ and H ₂ O in the proportion required to balance hydrogen. $2 \text{NH}_3 + \text{O}_2 \rightarrow \text{NO} + 3 \text{H}_2\text{O}$
Student:	Show me the next step.
Tutor:	Next I'll take 2 molecules of nitrogen monoxide to balance nitrogen. $2 \text{NH}_3 + \text{O}_2 \rightarrow 2 \text{NO} + 3 \text{H}_2\text{O}$
Student:	Show me the next step.
Tutor:	I multiplied everything by 2. Multiplying by 2 doesn't balance or unbalance anything. It just sets up the equation to balance oxygen more easily. $4 \text{NH}_3 + 2 \text{O}_2 \rightarrow 4 \text{NO} + 6 \text{H}_2\text{O}$
(1) Student:	Why didn't you set the coefficient of H ₂ O to zero to balance oxygen?
Tutor:	This might look like a good move since it gives 2 oxygen atoms on each side. However, writing 0 H ₂ O amounts to eliminating H ₂ O from the equation. The original equation told us that water is involved in the reaction. That's why all the coefficients must be positive.
(2) Student:	How about taking -1 NO to balance O instead?
Tutor:	Taking -1 NO might seem to balance oxygen mathematically, since it appears to give 2 O on each side, but the problem with writing this is that it doesn't have any physical meaning. You can't have negative numbers of molecules. Writing -1 nitrogen monoxide molecules would be like saying you have -1 pieces of candy. That's why chemical equations use only positive numbers.
Student:	Show me the next step.
Tutor:	I balanced oxygen by putting five O ₂ on the reactants side. $4 \text{NH}_3 + 5 \text{O}_2 \rightarrow 4 \text{NO} + 6 \text{H}_2\text{O}$ The equation is now correctly balanced.
(3) Student:	What does this balanced equation tell me?
Tutor:	It tells you that 4 moles of NH ₃ plus 5 moles of O ₂ will react to form 4 moles of NO plus 6 moles of H ₂ O.
(4) Student:	Interpret this equation for me in terms of mass.
Tutor:	The mass of the reactants is: 68.1216 g NH ₃ + 159.9940 g O ₂ = 228.1156 g of reactants. The mass of the products is: 120.0244 g NO + 108.0912 g H ₂ O = 228.1156 g of products. It should be no surprise that the products have exactly the same mass as the reactants. The atoms that formed the reactants were rearranged to form the products, but all of them are still there.
(5) Student:	Why didn't you consider the question above until after the equation was balanced?
Tutor:	Balancing the equation determines the quantitative relationship between the amounts of reactants and products. An unbalanced equation tells you what is in the reaction, but it cannot tell you how much. Only after the equation is correctly balanced can we make any connection between the amounts of reactants and products.

Figure 3. Example student inquiry dialogue.

Access to a Web-based demonstration of the equation-balancing tutor (depicted in Figure 2) can be obtained by writing to us [27]. We are very interested in constructive feedback from readers of *The Chemical Educator*.

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