

The Open-Response Chemistry Cognitive Assistance Tutor System: Development and Implementation

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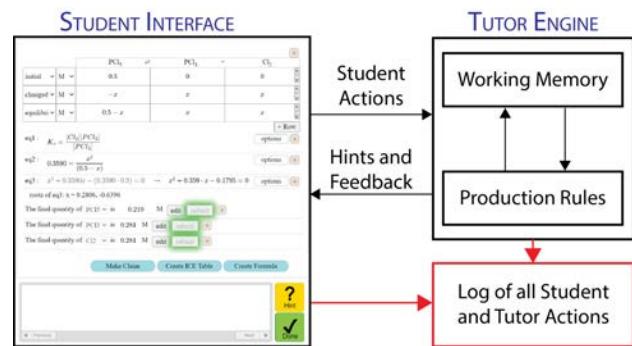
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ABSTRACT

This report showcases a new type of online homework system that provides students with a free-form interface and dynamic feedback. The ORCCA Tutor (Open Response Chemistry Cognitive Assistance Tutor) is a production rules-based online tutoring system utilizing the Cognitive Tutoring Authoring Tools (CTAT) developed by Carnegie Mellon University. In this report, we discuss the interface design and the production rules that allow for a multitude of chemistry calculations to be solved in a wide variety of ways by students. We discuss improvements of the software, already implemented or planned for the future, based on think aloud/interviews with students.

GRAPHICAL ABSTRACT (3.25 INCHES BY 1.75 INCHES)



KEYWORDS

First-Year Undergraduate/General, Interdisciplinary, Web-Based Learning, Thermochemistry, Equilibrium, Stoichiometry

The utility of computer-based homework systems for learning chemistry has been the subject of development and study for many years.¹⁻¹¹ The translation of student steps onto computer cards reported¹ in 1972, has given way to increasingly diverse and functional systems, including adaptive systems.¹⁰ The recent widespread pivot to remote learning has placed even more emphasis on computer-based homework systems.¹²⁻¹⁹ The parallel development of artificial intelligence technologies in the same time frame²⁰⁻²¹ suggests new ways that computer-based homework systems can be refined to assist students in novel, more flexible ways. This report describes one such system.

INTRODUCTION

A number of different artificial intelligence (AI) strategies may be used to develop online tutoring systems for general chemistry²²⁻²⁸. The production rule system developed here is a type of expert system that has some particular advantages. One advantage is the ability of a single set of rules to support a broad range of problems. This is in contrast to much current online homework where the author must, for each individual problem, develop supports such as hints, distractors for multiple-choice questions, and the logic needed to evaluate an entered response for correctness or common errors. Production rule systems can take a more general approach.

Here, we report on a production rule system for quantitative problems involving stoichiometry, concentration, gas laws, thermochemistry, chemical equilibrium, and acid/base chemistry. Although this corresponds to a broad range of problem types, these problems can be solved with a flexible understanding of a few key concepts, such as the use of molar mass or heat capacity. The rules in the tutor engine are closely associated with these individual concepts. This allows the tutor engine to support many problem types, multiple problem-solving pathways for each problem, and real-time monitoring of student work providing hints and feedback based on the unique pathway chosen by an individual student. Inclusion of “buggy” rules, corresponding to common student mistakes or misconceptions, allows the tutor engine to identify and provide specific feedback. Because the tutor engine links student actions with rules, the system gathers information on student learning of the key

underlying concepts. This tutor system combines two innovations: a set of production rules for chemical problem solving and a user-interface for free-form entry of student work. This combination is synergistic in that the production rules are what enable the tutoring system to interpret the free-form work input by the student. Here we describe the development and initial testing of this free-form production rule system.

DEVELOPMENT

Interface Design

This tutor system is designed to allow students to complete chemistry calculations as they typically would on paper while providing scaffolding only when needed. Current online problem-solving tools either provide feedback only on the final result (minimal scaffolding) or use a step-by-step question sequence that does not provide practice with how to develop broader problem-solving strategies (heavy scaffolding). By coupling a user interface for free-form entry of mathematical expressions with a production rule system that monitors student work, we aim to provide scaffolding only when needed (dynamic scaffolding). To achieve this, the student workspace in Figure 1 begins as a blank slate for input of student work. Immediately below this workspace is an area for the tutor engine to provide hints and feedback. The right side of the interface provides the problem statement (top) and controlled vocabulary (bottom). A detailed walkthrough of the problem in Figure 1 is provided in the Supporting Information. Along with the walkthrough, a website has been created to allow for the exploration of the tutor system (<http://orcca.ctat.cs.cmu.edu>).

STUDENT WORKSPACE

| | PCl_5 | \rightleftharpoons | PCl_3 | + | Cl_2 |
|-------------|----------------|----------------------|----------------|-----|---------------|
| initial | M | | 1.5 | 0 | 0 |
| changed | M | | $-x$ | x | x |
| equilibrium | M | | $1.5 - x$ | x | x |

eq1 : $K_c = \frac{[\text{Cl}_2][\text{PCl}_3]}{[\text{PCl}_5]}$

eq2 : $1.450 = \frac{x^2}{(1.50 - x)}$

eq3 : $1.450 \cdot 1.5 \rightarrow 2.175$

eq4 : $x^2 + 1.450x - 2.175 = 0$

roots of eq4: $x = 0.9184, -2.368$

eq5 : $1.50 - 0.9184 \rightarrow 0.5816$

The final quantity of PCl_5 is 0.582 M

The final quantity of PCl_3 is 0.918 M

The final quantity of Cl_2 is 0.918 M

PROBLEM STATEMENT

Under certain conditions, the equilibrium constant K_c for the decomposition of $\text{PCl}_5(\text{g})$ into $\text{PCl}_3(\text{g})$ and $\text{Cl}_2(\text{g})$ is 1.450. What are the equilibrium concentrations of PCl_5 , PCl_3 , and Cl_2 if the initial concentration of PCl_5 is 1.500 M and the initial concentrations of PCl_3 and Cl_2 are 0.000 M, according to the following reaction?

$\text{PCl}_5(\text{g}) \rightleftharpoons \text{PCl}_3(\text{g}) + \text{Cl}_2(\text{g})$

Expression Symbols (click to insert)

| | | |
|-----------------------------|------------------------------|------------------------------|
| Variables and Operators | | |
| K_c (shift+K) | $[\text{PCl}_5]$ (ctrl+1) | $[\text{PCl}_3]$ (ctrl+2) |
| $[\text{Cl}_2]$ (ctrl+3) | x (x) | $\sqrt{}$ |
| Labels | | |
| M (ctrl+4) | mol (ctrl+5) | PCl_5 (ctrl+6) |
| PCl_3 (ctrl+7) | Cl_2 (ctrl+8) | |

CONTROLLED VOCABULARY

Make Claim
Create ICE Table
Create Formula

Previous
Next

Hints and Feedback
?
Hint
✓
Done

Figure 1: Screenshot of a completed problem using the graphical user interface for the ORCCA Tutor. Four main areas are depicted: student workspace, problem statement, hints and feedback, and the controlled vocabulary.

The number and type of buttons at the bottom of the student workspace varies with problem type. “Make Claim” and “Create Formula” are present for all problems while “Create ICE Table” is only for problems involving chemical equilibrium. “Create Formula” allows entry of a mathematical expression. The tutor engine acts as a calculator, simplifying the expression and providing the result; e.g. in eqs 3 and 5 of Figure 1 the expressions to the right of the arrows result from the tutor engine’s multiplication and subtraction respectively. The component used to support expressions is made possible by Guppy²⁹⁻³⁰, an open-source and well-tested JavaScript component that provides real-time formatting of mathematical expressions. To help ensure that the tutor engine will understand the expression, students construct the expression from numerical values entered from the keyboard and from terms selected from the controlled vocabulary. After a formula has been entered and evaluated,

an “Options” button appears for the user to optionally set units, substance, and context (e.g. mol PCl₅ initial) for the calculated value. The “Options” button can also be used to solve a quadratic equation e.g. eq4 in Figure 1, or to replace variables *e.g.* replace x with 0.9184, when applicable. Students are able to edit any entry in the student workspace at any time by double-clicking on the entry or navigating to the edit button in the “Options” tab. To remove an expression, the student can click the “Delete” button.

When a student clicks the “Create ICE Table” button, they first select a chemical equation from a list. The table initially has one row, with dropdowns to select context and unit. The boxes for entry of values use Guppy to allow students to perform calculations within the ICE table. Rows can be added, edited, and rearranged. To keep the format flexible, we allow each row to have different units but, for convenience, these default to the units of the first row.

Students use the “Make Claim” button to report their answers and provide some argument for how they arrived at that conclusion. When a student clicks on the “Make Claim” button a menu opens, asking which type of claim they want to complete, *e.g.* final mass of a specific product. Once the students have completed the claim, the “Submit” button will turn green if the claim is correct and red if the claim is incorrect. If the claim is incorrect the student can edit the claim by clicking on the “Edit” button or double-clicking on their inputted value. Some problem types include claims regarding intermediate quantities, such as the identity of a limiting reagent. These have the advantage of providing feedback at early stages in the problem solving. The author of the problem can specify if entry of such intermediate claims is optional or required. Students must have all claims correct before they are done with the problem.

In the controlled vocabulary section of the interface, students can access variables and labels to help them in their calculations, by either clicking the button or using the assigned hotkey. Variables are used in an algebraic sense, *i.e.* to represent a quantity. Labels are used to annotate a quantity, *e.g.* by specifying the chemical substance and units. Students can use the labels to complete their mathematical expressions.

Below the workspace the interface contains hints and feedback from the tutor engine, which will appear directly below the workspace and expands as the student adds work. Both the hints and feedback are generated by the production rules. Hints are given in response to a request from the student, moving from more general, conceptual hints toward more specific hints, including “bottom out” hints that explicitly state the next step in the problem-solving. Students can use the “Previous” and “Next” buttons to navigate through the series of hints. Feedback is given in response to an incorrect student step. This includes specific feedback, when the tutor engine recognizes a value as resulting from a common error (i.e., you entered the answer in moles but it should be in grams), and more general feedback when the tutor engine does not recognize a value entered by the student (i.e., I do not recognize that value. If you are stuck, you can use the hint button to ask for a hint). This immediate feedback is meant to aid the student in realizing errors early in their calculations. Feedback is also provided on incorrect claims. This portion of the interface also includes the “Done” button, which students use to signal that they are finished with the problem.

CTAT

The tutor engine has been constructed using the Cognitive Tutor Authoring Tools (CTAT) system developed at Carnegie Mellon University³¹⁻³⁶. A CTAT rule-based tutor consists of a set of production rules, which operate on pieces of information called “facts” in order to predict solution paths (both correct and incorrect) and generate hints and feedback. Student input is checked against the steps generated by the rules, and hints/feedback are provided accordingly. In the case of the ORCCA tutor, the rules operate on the given values provided by the problem definition, using them to calculate the final values as well as any intermediate values. The rules also calculate values representing common mistakes, or “buggy steps” (discussed further below). These values (final, intermediate, and buggy) are all stored as facts in “working memory” and are available to the production rules. For example, consider the limiting reactant problem corresponding to mixing 300 g Cu₂O with 150 g Cu₂S which react according to 2 Cu₂O + Cu₂S → 6 Cu + SO₂. One of the first production rules to fire is *ConvertGramsToMols*, which adds the initial moles of the reactants to working memory, shown in Figure 2. These new facts cause additional rules to fire, such as

DetermineLimitingReagent. This populates working memory with a large number of quantities. When the student enters an expression, the computed value is compared to values in working memory to find a match.

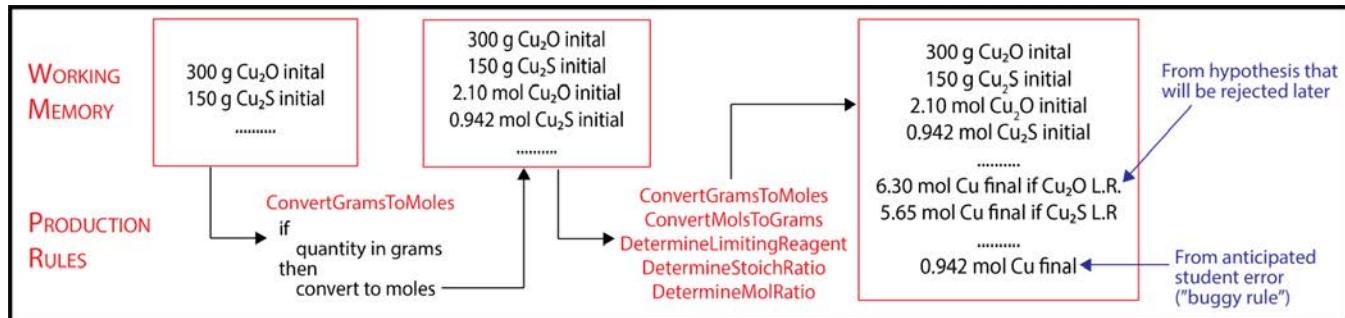


Figure 2: Example interaction between working memory and production rules.

The production rules include “buggy” rules that represent common mistakes, e.g., forgetting to include the stoichiometric coefficients when determining the amount of product formed. When a value calculated by a student matches a value in working memory that was generated by a buggy rule, the tutor engine generates feedback associated with that buggy rule. For the calculation of Figure 2, if a student calculation led to 0.942 mol Cu final, the tutor engine would provide feedback that reminds the student the stoichiometry of the reaction is not one to one. In addition to the buggy rule stated here, more examples can be seen in the supporting information (Table S1). The production rules also determine intermediate values based on hypotheses that may later be rejected, such as assuming a reactant is limiting and then later rejecting that assumption (see upper right of Figure 2).

The tutor system is intended to allow free-form input resembling that of paper-and-pencil paper problem solving. Figure 3 illustrates a variety of ways different students successfully completed a thermochemistry problem. All of these students arrive at the final answer but the paths they take vary. One means through which we support such a wide range of student input is by considering only the quantity resulting from algebraic input. This includes units, substance and context (e.g. mol NaOH initial) attached by the student to the computed quantity. However, the expression name, shown to the left of the algebraic input, and the form of the algebra itself are not considered. By comparing the student’s quantity with those in working memory, the tutor engine can identify the correct, or

incorrect, pathway being followed by the student and provide specific hints and feedback. To support free-form input, we do not require students to fully label all quantities, i.e. they may enter “0.125” or “0.125 mol” instead of “0.125 mol NaOH initial” in Figure 3. This makes it more challenging for the tutor engine to follow the student work because it must consider all possible matches for “0.125”. However, mandating that students fully annotate all intermediate quantities would be unnecessarily tedious and not reflect our goal of mimicking paper-and-pencil work.

Supporting free-form input leads to a few complexities in matching quantities input by the student to those generated by the tutor. Students differ considerably in the extent to which they attach units and substance labels to intermediate quantities, e.g. compare Figure 3B and 3C. When comparing student input to quantities in working memory, the tutor engine only considers aspects of the quantity (i.e., substance and unit) that the student has explicitly set. If the student enters only a numerical value, that step will be considered by the tutor to match every quantity in working memory with that value. This list of matches is then pared down as the student attaches more information. Students may also delete/edit previous work, requiring the system to note that previously entered quantities have been overwritten by the student. Analysis of log files (see below) is being used to determine the extent to which this quantity-matching approach is able to successfully support student work in actual classrooms.

A

```

eq1: 70.0°C - 27.0°C → 43°C
eq2: 80g · 4.184 J/g°C · 43°C → 14390 J H₂O
eq3: 80mL · 1g/mol → 80 g H₂O
The value of qH₂O is 14.4 kJ   
eq4: 14.39 · -1 → -14.39
eq5: 5g · 1/40 g/mol → 0.125
eq6: -14.39 → -115.1
The change in enthalpy for the dissolution process is -115 kJ/mol   

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C

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mol h2o: 80mLH₂O · 1g · 1mol / 1mL · 18H₂O → 4.444 mol H₂O
qh2o: -4.444 mol H₂O · 75.38 J/g°C · (70.0°C - 27.0°C) → -14410 J
mol NaOH: 5.0gNaOH · 1molNaOH / 40gNaOH → 0.125 mol NaOH
qNaOH: -0.125 mol NaOH · 75.38 J/g°C · (70.0°C - 27.0°C) → -405.2 J NaOH
enthalpy change for NaOH: -14410 J - (-405.2 J) → -14000 J
The value of qH₂O is 14.4 kJ   
Temperature change: 70.0 - 27.0 → 43°C
qH₂O (try 2): 80gH₂O · 4.184 J/g°C (43°C) → 14390
qNaOH (try 2): 4.0g · 4.184 J/g°C · (43°C) → 719.6
enthalpy change for NaOH (try 2): 0.7196 kJ - 14.39 kJ → -13.67
The change in enthalpy for the dissolution process is -115 kJ/mol   
Change in enthalpy H₂O: 14.39kJ / 4.444mol → 3.238 kJ/mol H₂O
Change in enthalpy NaOH: 0.7196kJ/NaOH / 0.125molNaOH → 5.757 kJ/mol NaOH
delta H: 14.39 · -1 → -14.39
Name: 5.757kJ/mol - 3.238kJ/mol → 2.519
delta H: -14.39kJ / 0.125molNaOH → -115.1

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B

```

eq1: 70.00 - 27.00 → 43
eq2: 80 · 4.184 · 43 → 14390
eq3: 14390 / 1000 → 14.39
The value of qH₂O is 14.4 kJ   
eq4: 14.39 · -1 → -14.39
eq5: 5 / 40 → 0.125
eq6: -14.39 / 0.125 → -115.1
The change in enthalpy for the dissolution process is -115 kJ/mol   

```

B

```

eq1: 70.00 - 27.00 → 43
eq2: 80 · 4.184 · 43 → 14390
eq3: 14390 / 1000 → 14.39
The value of qH₂O is 14.4 kJ   
eq4: 14.39 · -1 → -14.39
eq5: 5 / 40 → 0.125
eq6: -14.39 / 0.125 → -115.1
The change in enthalpy for the dissolution process is -115 kJ/mol   

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Figure 3: Renderings of three different student workspaces after completing a thermochemistry problem during a think-aloud session.

Types of Problems

The tutors within the system currently cover concepts associated with: limiting reactant, equilibrium, thermochemistry, concentration, and ideal gas law calculations. These concepts represent many of the difficult calculation problems that students will face during a general chemistry course. An advantage of production rules is that they can handle the wide range of problems arising from various combinations of these concepts. A description of each of the tutor types is below with a summary in Table 1.

Table 1: List and status of ORCCA Tutors

| Concept | Variations (Quantity) | Development Status | In Class Deployment |
|--------------------------|-----------------------------|----------------------|---------------------|
| Limiting Reactant | Forward (5) | Completed | Ongoing |
| | With Molarity (2) | Completed | Ongoing |
| | Inverse (3) | Ready for Deployment | Planned |
| Equilibrium | Using Quadratic Formula (1) | Completed | Ongoing |
| | Weak Acid | | |
| | Finding pH (1) | Completed | Ongoing |
| | Finding Concentration (1) | Completed | Ongoing |
| | Buffer (1) | Completed | Ongoing |
| Thermochemistry | | Completed | Ongoing |
| Concentration | | Hint Development | Planned |
| Ideal Gas Laws | | Rule Development | Planned |

The first tutors to be developed were for the limiting reactant concept, which currently has ten different problem variations. In addition to problem variations, randomization of starting values and reactions allows for a greater volume of distinct problems, all supported by the same production rules. There are varying levels of complexity ranging from traditional limiting reactant problems to problems involving molarity and inverted problems where the mass of products are the given quantities (the inverse limiting reactant calculations have not been tested by students yet, but are ready for deployment). These problems may require students to make a claim regarding the identity of the limiting reagent, and support this claim with intermediate values. After making the limiting reactant claim students will move to the second part of the problem which consists of determining the final quantities for each of the species in the equation.

Within the equilibrium concept, there are four variations of tutors. In the first tutor, students use the quadratic equation to determine the final quantities for each of the species in the reaction at equilibrium. Two other tutors involve a weak acid where students must calculate the H_3O^+ concentration at equilibrium or the pH of the solution. In these tutors, students may be required to make, and later justify a “small x” claim. In the final equilibrium tutor, students must determine the

final pH of a buffer solution.

Recent expansions to the ORCCA tutor involve thermochemistry, concentration, gas laws, and inverse limiting reactant concept tutors. This expansion of the production rules allows for the coverage of a broader range of chemistry. A thermochemistry problem, in which students determine the enthalpy for dissolution of NaOH in water (Figure 3), has been tested by students with another version under development. The remaining tutors are in development and will be tested in classes over the next year.

IMPLEMENTATION

OLI and TutorShop

Currently, students have been accessing these online tutors through the Open Learning Initiative (OLI)³⁷⁻³⁸ and through TutorShop³⁹⁻⁴¹ both of which were developed at Carnegie Mellon University. Most student interaction with the tutor system has come from within OLI and in a classroom setting, however, think alouds have been conducted using TutorShop. While both of these applications provide students with access to the tutors, OLI embeds the tutor in instruction that includes explanations and other practice opportunities.

Widespread Use

All of the tutors discussed, except the inverse limiting reactant, concentration, and gas laws problems, have been used in general chemistry classes multiple times by students from different experience levels with chemistry and from different universities. Students typically major in a STEM related field and the session dates are from both on-semester and off-semester courses. Some students have AP chemistry knowledge and/or credit. The tutors were implemented in eight universities with a variety of students. One university was an R1 state institution in the Midwest, one was a private R1 university in the Northeast, one is a four-year public university in the west, and the remaining five were 2-year colleges in the West. Of these, four are considered Hispanic Serving Institutions. In total, approximately 650 students from across the United States have engaged with the tutors.

MOVING FORWARD

Logbook Analysis

The detailed log gathered by the CTAT system provides a detailed look at the steps students performed to complete a given problem (e.g., what they typed in the formula space, what buttons they pressed) as well as the tutor engine's interaction with the student work (e.g., matching values and production rules used). This allows us to evaluate the extent to which our approach, based on production rules that match only computed quantities, can successfully monitor and support student problem solving. An example of a full logbook file can be seen in the supplemental information, including both the raw file and more readable version. We are also working on ways to gain insight into student problem solving from large volumes of field data. In particular, we are working on automated ways to determine the paths most followed by students, critical stages in the problem solving beyond which most students move quickly to successful completion, and how the students use the tutor to aid them in their understanding of the topic. This detailed information on student problem solving may also be of use for selecting the next set of problems for a student to work on, as in the adaptive learning approach of ALEKS²⁵.

Qualitative Data

Focus groups, think alouds, and interviews were conducted to complement information gathered from analysis of logbook files. These studies, conducted with appropriate institutional review board approvals, give insight into the degree to which the tutor engine supports free-form problem solving and ways to improve this support. A detailed discussion of these studies will be published in a different article. Here, we briefly note some key changes to the tutors that were prompted by the results.

Think alouds, gathered while students were using the tutor system, prompted us to make some substantial changes to the user interface. The panel for hints and feedback was originally at the bottom of the user interface, but some students failed to notice the provided feedback or the availability of a hint button. These studies also revealed instances where students wanted, but were not able, to rearrange an expression or easily add units and substances to quantities. The user

interface was modified to make such operations more facile.

Our most recent round of focus groups and think aloud/interviews surfaced new features that would ease use of the tutors. One feature is the addition of a pop-up reference/equation sheet. We are implementing this, but allowing instructors to turn this feature off and on based on their preferences. Another feature is a note taking space where students can freely document their thoughts. Our plan is to allow students to turn this feature on and off. A note taking feature has the additional advantage of providing information on student reasoning that can be saved in the log file and later analyzed.

These studies also provide information on the extent to which students found the ORCCA tutor to be of use to their learning. One student had this to say about the tutor system, "...this one is quite different. I like this one a lot because it gives you a place to like work out your thought process but then it also had unlimited tries which I think just kind of takes the weight of each try off and it encourages just like hey if you think this is if this is your process we'll tell you what's wrong but you can rethink why your process is wrong and not think about losing points along the way." Another student stated this about their experience with the tutor system: "But I think it [the adaptive hint stacks] definitely helps you learn by explaining and then showing it [the calculation steps] and then you actually do it yourself. It's kind of like a four-step process where you're actually reading and then applying it and I think that definitely helped me learn.".

CONCLUSION

With the use of the CTAT rule engine, the ORCCA Tutor provides students with a more adaptive and supportive online experience for completing homework problems. By providing a freeform workspace, students are able to work through the problem as they typically would on paper. Production rules then allow for hints and feedback to be given to the student whenever asked for or needed during the problem-solving process. Currently, the tutor engine supports a variety of calculation steps which allows for a large number of chemistry problems to be added to the system. Adding a new problem of a supported class requires only a problem statement, including initial and

final quantities; the rules in the tutor engine are used to generate the problem solving pathways from these initial to final quantities.

Based on the feedback that has been gathered from students using the tutor system, a variety of changes have been made. In addition to working on improving the systems to fit the widest variety of student needs, work is also being done to analyze log data and evaluate how the system is aiding the students' learning and improving their understanding of chemistry concepts. The process students take to complete the problems and the places the students run into issues are also being evaluated to aid instructors in the discussion of these problems. Overall, this tutoring system provides a new approach to online homework by allowing for a more dynamic scaffolded approach.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI:

10.1021/acs.jchemed.XXXXXXX. [ACS will fill this in.] Example brief descriptions with file formats indicated are shown below; customize for your material.

Supporting Information includes: a PDF file with a full walkthrough of an equilibrium problem in the ORCCA Tutor, a table of example buggy production rules, and a readable version of a logbook file; and a CSV file with the raw version of the logbook file.

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