Introduction to Chemical Engineering Reactor Analysis:

A WEB-BASED REACTOR DESIGN GAME

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Since the beginning of the chemical engineering profession in late 19th century, ChE faculty have been frustrated when attempting to explain their field to college freshmen or high school students. When looking for information about a college major, high school students should be informed of the opportunities that ChE can offer in terms of applying chemistry, physics, and biological sciences to engineering problems. Freshman ChE students should be given an effective introduction to what they are going to encounter in their four years of education. Whereas civil, electrical, and mechanical engineers can illustrate their profession by having students construct model bridges, simple circuits, or a simple mechanical device, chemical engineers cannot ask students to build a "simple" model chemical plant.

We have developed an approach to address this issue. Our approach involves an interactive website and a business simulation game that demonstrate how to model a lab-scale experiment and use the results to design and operate a commercial chemical processing unit. When we applied this approach with high school students and freshmen ChE students at the University of Massachusetts, Lowell (UML), we received very positive student feedback. We believe that this effective approach will greatly aid in science, technology, engineering, and math education, which has been strongly emphasized in recent years.

Specifically, we implemented the Chemical Reactor Analysis Design (CRAD) Game, created by T.W. Fraser Russell of the University of Delaware and Becky Kinney of Moonlight Multimedia. This game utilizes a new teaching approach with a "technically feasible design" (TFD).[1] It was originally developed and operated with FORTRAN software.[2, 3] A combination of lectures and computer lab experience—employing personal computers (PCs) and an interactive website—was used to provide students with a hands-on approach to problem solving.

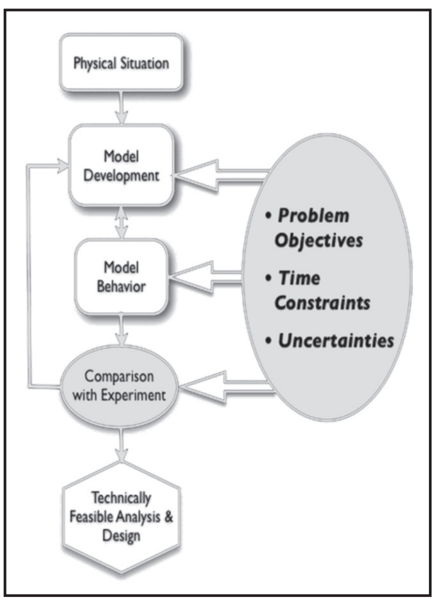

Figure 1. *Technically feasible design schematic.*[4]

The object of the game was to design a continuous-flow stirred tank reactor (CSTR) to produce a product and compete for market shares against three other companies producing the same product. Figure 1 outlines the ChE analysis required to

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solve the problem, as well as the model development, model behavior, and comparison with experimental data.[4] This last step is not trivial to perform, and is what makes engineering an art. All of the steps in the analysis must account for the objectives of the problem. In the game, constraints and uncertainties are illustrated by the competition, marketing, and financial aspects of the proposed process.

STUDENT PARTICIPATION

We tested our approach in two different settings for two different audiences: college freshmen at UML and high school juniors and seniors at Lowell High School in Lowell, MA. The approach varied due to the different math and science backgrounds of each group. The CRAD Game was used for three years at UML and one year at the Lowell High School.

Freshman students

The Introduction to Chemical Engineering Course at UML is a 3-credit, 3-hour-per-week required course for all incoming ChE students and is offered in the Spring semester. The class enrollment is about 80 students. The course is designed to give students an overview of the ChE curriculum and solidify their interest in the profession at an early stage in their education. The course lasts 13 weeks and consists of seven modules, ranging from 1 to 2 weeks per module. The CRAD Game was covered as one of the 2-week modules. Other modules describe options that are available in our program, such as biological engineering, nuclear engineering, and nanomaterials engineering.

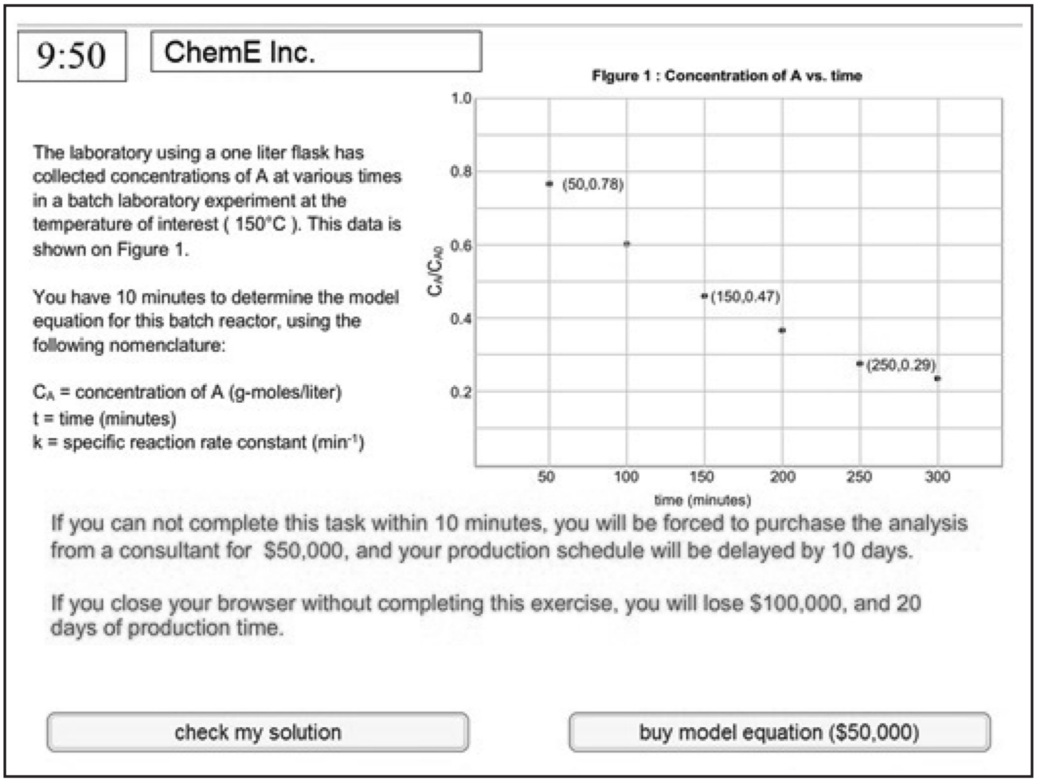

Figure 2. *Batch reactor problem.*

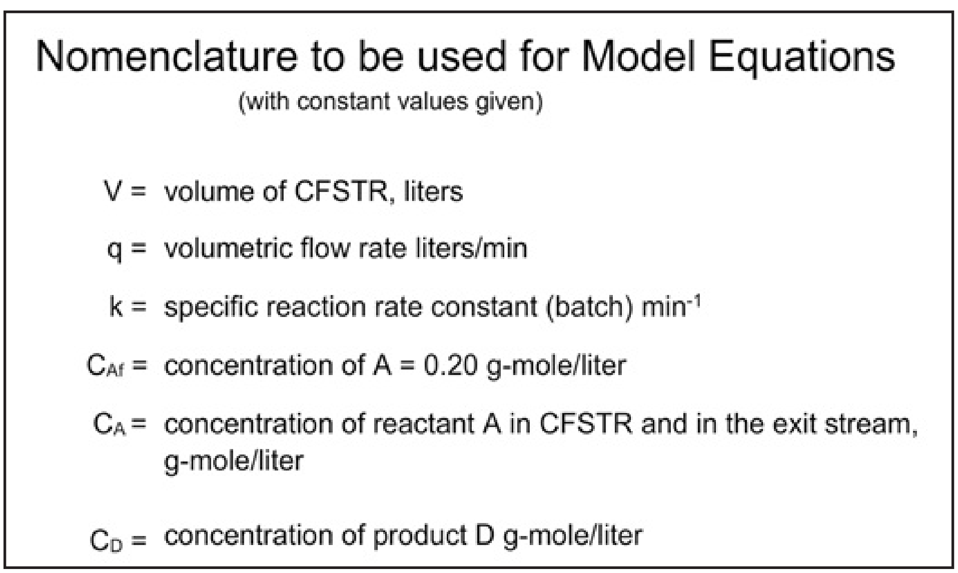

Figure 3. *Nomenclature.*

During the module that covered the CRAD Game, a general lecture was given each week to all 80 students. After the lecture, students were divided into four groups of approximately 20 students each. They participated in a 2-hour hands-on computer laboratory session, in which each student had access to a PC. Students were expected to derive all of the pertinent model equations. We used the reactor as an example, to emphasize the importance of obtaining lab-scale experimental data, modeling, and subsequent scale-up. However, the CRAD Game was not meant

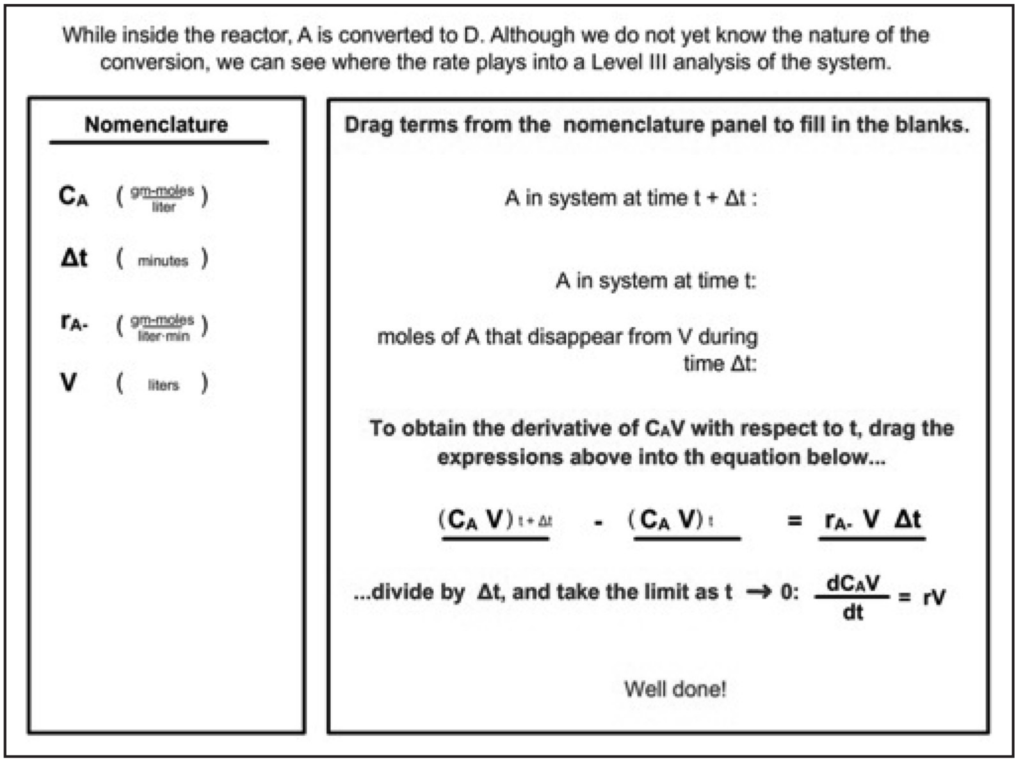

Figure 4. *Batch model equations.*

to replace the reactor engineering course that the students would take later in their education.

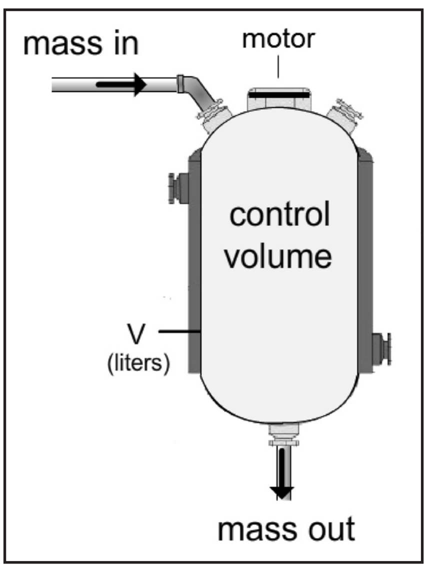

Figure 5. *CFSTR.*

High school students

High school students included in this study were enrolled in either an engineering or physics class at Lowell High School, and had an interest in chemical engineering or engineering in general. Eleven high school students voluntarily participated in this study, through a group that met once weekly after school for four weeks to test the CRAD Game. During the first week, a 45-minute lecture was presented in which the students were given the model equations (rather than having to derive the equations themselves). For the subsequent three weeks, the students met in a computer lab, with one PC for each student.

The web-based design game presented here has its roots in a pre-PC work.[2, 3] The same approach was used, but the students handed in papers and the results were entered into a FORTRAN program. The use of PCs and the web enables a much more effective interactive learning approach. Many excellent papers have described the development of web-based teaching tools in ChE, including a process dynamics and control exercise,[5] as well as a virtual laboratory for chemical experiments.[6] Newell[7] and Vestal[8] created web-based active-learning games that addressed different motivational styles and were loosely based on TV series. While similar to their approach, our game addresses economic and business aspects in addition to technical considerations. ChE educators have gone to high schools to lecture interested students in ChE curricula, as a part of outreach.[9-13]

INTRODUCTION AND REVIEW OF CHEMICAL REACTOR ANALYSIS[14]

In the college freshman course, the first lecture was a general introduction to reactor design. The emphasis was on the challenges of transitioning technology from lab-scale batch reactors to commercial-scale production in continuous flow reactors. The roles that experiments and modeling play in the scale-up and design were discussed, as these roles are key background information for using the website and playing the game.

The object of the game was presented as follows: "How can a chemical engineer design a reactor to manufacture a chemical, D, produced by the following chemical reaction:

$$A \rightarrow D \tag{1}$$

Students were tasked with designing and building a CFSTR. The reactor volume and the flow rate of the feed stream needed to be specified by applying the conservation of mass principle for each species and deriving the model equations. In addition to technical considerations, the amount of product that can be sold was influenced by the actions of other companies competing for the same market. This uncertainty was included in the game.

After the lecture, students were divided into four groups and began the hands-on computer session. Each student had access to a computer and opened the Introduction and Review of Chemical Reactor Analysis, Activities, section of the website.[14] Figures 2 to 12 are screenshots reproduced from the game website.[14]

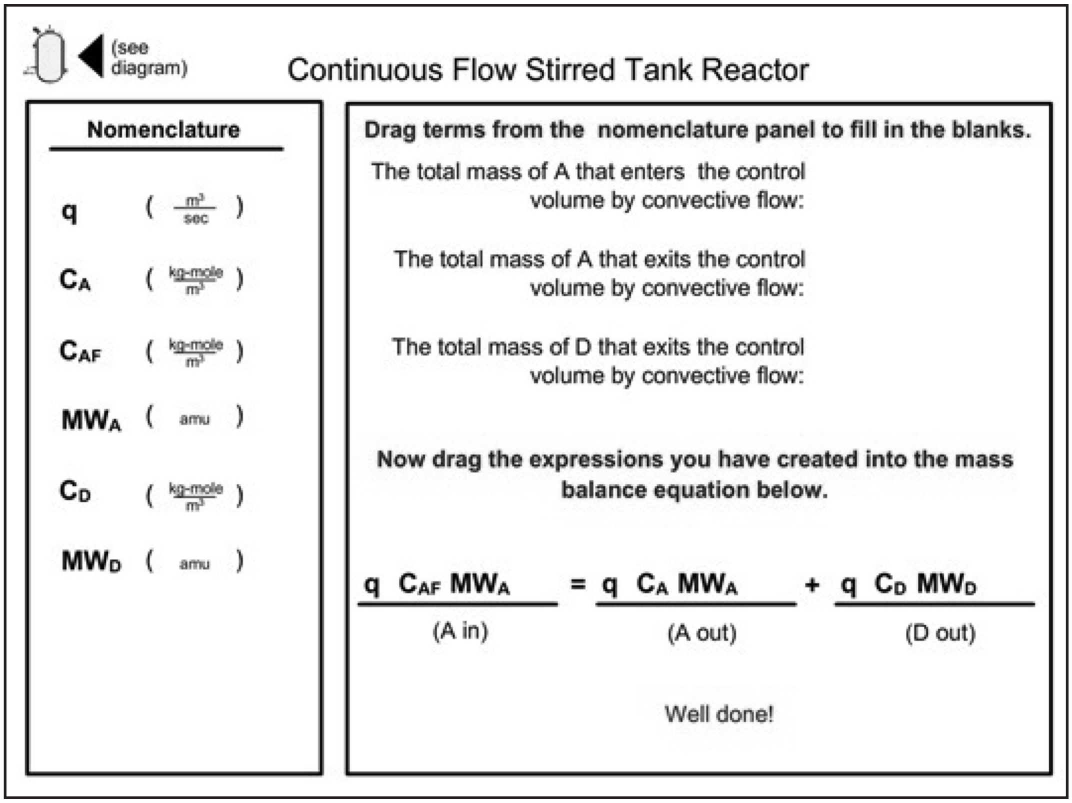

Figure 6. Manipulation of the model equations for the CFSTR.

Chemical engineers depend heavily on experiments, done by themselves or by others, that form the basis of any commercial-scale operation. These experiments need to be analyzed to determine the reaction parameters. The present case considered a single constant, k, obtained in a laboratory batch experiment in a flask at constant temperature. The amount of A (or D) was measured as a function of time, as shown in Figure 2.

As a first step, students had to determine the reaction parameters by deriving the batch reactor model equations from the conservation of mass and the nomenclature given in Figure 3. To develop the model equations for the batch reactor, the students used a drag-and-drop procedure on the website. They moved the symbol from the left-hand side of Figure 4 and placed it with the correct word statement on the right-hand side. If the student placed the symbol with the wrong word statement, then the program kicked the symbol back to the left-hand side, thus providing immediate feedback. The model equation was solved to obtain the specific reaction rate constant k for the reaction $A \rightarrow D$, assuming a first-order reaction.

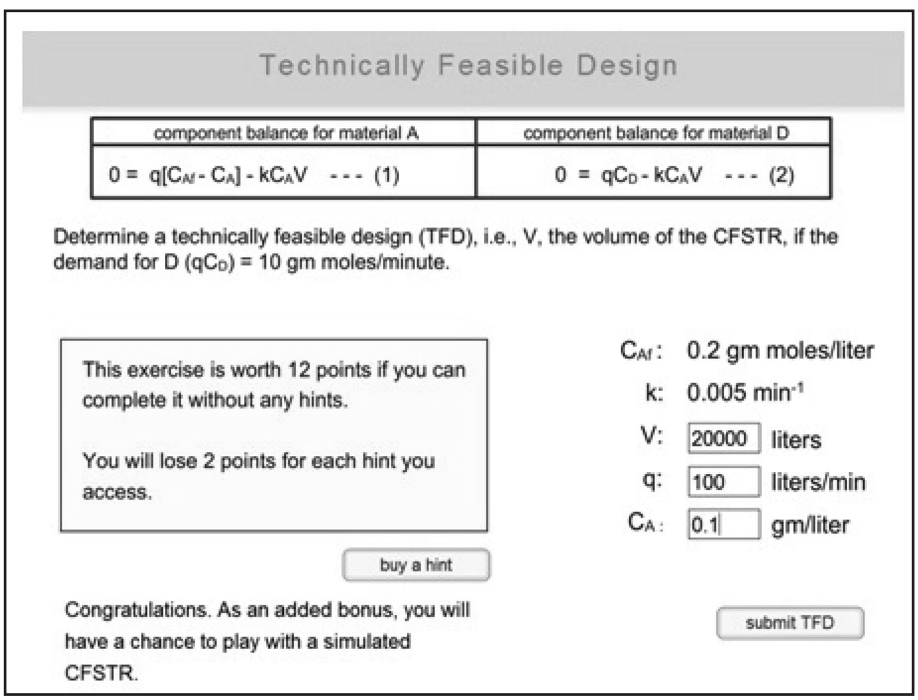

Figure 7. Technically feasible design.

The next step was transitioning this knowledge to large-scale operation. Batch experiments are done at the laboratory scale in flasks and beakers, which are too small to produce large, commercial-scale quantities. It is the role of a chemical engineer to analyze and scale-up batch data to produce commercial-scale quantities of a chemical. For this step, students had to derive the model equations for a CFSTR from the conservation of mass equations for components A and D, using the nomenclature in Figures 3 and 5, as well as the drag-and-drop procedure in Figure 6. The resulting model equations were as follows:

$$\text{Component A} \qquad 0 = qC_{AF} - qC_A - kC_A V \tag{2}$$

$$\text{Component B} \qquad 0 = kC_A V - qC_D \tag{3}$$

After the students had derived the model equations, the website illustrated how the equations could be applied via a TFD problem. A TFD is a design that defines the size of a piece of equipment (in this case, the reactor volume) to meet a stated production rate (in this case, for D). In so doing, it initiates an analysis of factors affecting optimal design. This critical teaching tool is described in detail in a previous publication.[1] The TFD question on the website (Figure 7) was as follows: "Using the model equations above, determine the reactor volume (V) if the demand for D (qC_D) is 10 gmol/min, given that the feed concentration of A (C_{AF}) is 0.2 gmol/L and the reaction rate constant (k) is 0.005 min^{-1}." Eq. (2) can be rearranged as follows:

$$V = \frac{qC_D}{kC_A} \tag{4}$$

Students were asked to determine the reactor volume individually, while being closely monitored by the lecturer and teaching assistants who walked around the computer lab. There were two equations [Eqs. (2) and (3)] with three unknowns (reactor volume, V; outlet concentration of A, C_A; and flow rate, q). After considerable individual discussion and trial-and-error manipulation of the equations, the students, with the help of the instructor, realized that they could not solve for V without knowing C_A or q. The class then discussed which variable was best suited to make a realistic initial guess for its value. Picking a flow rate would be a more difficult choice because the upper and lower limits of q are not obvious at first sight without manipulating the two equations. On the other hand, C_A needs to be between the feed concentration (C_{AF}) and zero. At high conversions, the value of C_A approaches zero, requiring infinitely large reactor volumes. Any other value of C_A requires a separation unit after the reactor to purify the product and/or recycle unused reactant. C_A cannot be higher than the concentration of A in the feed stream (in this case, 0.2 gmol/L).

For each value of C_A, different values of V and q will be obtained; in other words, there is no one "right" answer. The value should be selected depending on the design and other criteria for the process. This concept can be a difficult one for students to understand because until now, their entire educational experience has included problems with only one "right" answer. Students can go through this problem (in Figure 7) as many times as they want until they are comfortable with the concept. Each time they repeat the problem, the computer changes the parameter values. When a TFD is completed, the simulation on the web allows students to have an interactive experience, in which they can change V and q and visually observe how the production of D is affected by the different values. A separation unit is included for better visualization of the process. Figure 8 is a screenshot from the simulation that shows this interactive exercise.

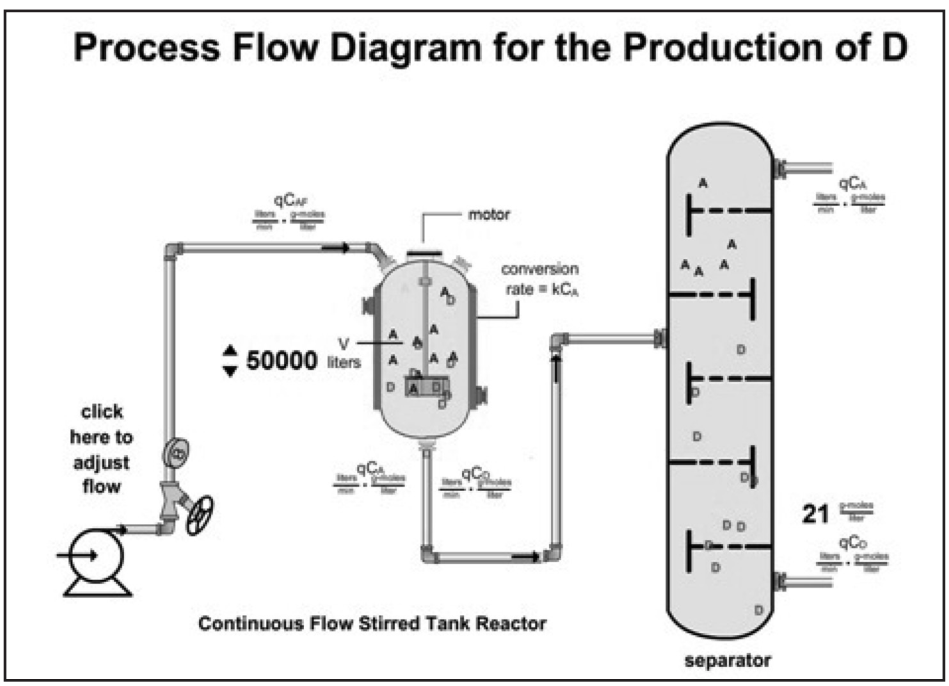

Figure 8. *Interactive process flow simulation.*

At the end of the lab session in the first week, the students were assigned homework on the TFD under the Non-Graded Activities option on the website. The homework was intended to solidify the concepts covered, as well as to help the students feel comfortable with the use of the website and the simulation.

PLAY THE GAME[14]

During the lecture hour in the second week, the concept of and factors affecting process design were discussed, as shown on the website. Students were given a brief introduction to the economic and marketing aspects of design. Again, the lecture hour was followed by a 2-hour hands-on computer lab session consisting of 20 students per group.

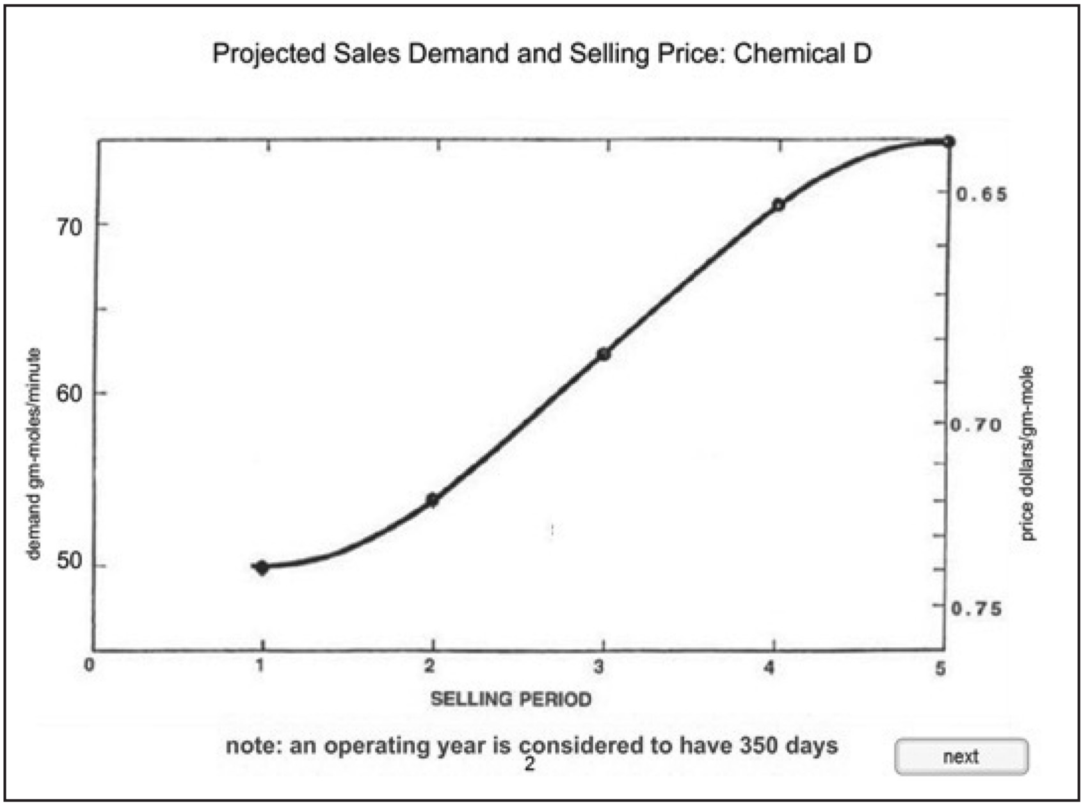

Figure 9. *Demand curve for product D.*

Yearly Manufacturing Costs

- Capital Cost Depreciation, Maintenance, Operation, and Waste Disposal = \$45.00/ reactor volume (liters)
- Raw Material Cost = \$0.20/gram-mole
  - note: unconverted raw material can not be recycled.
- Cost of storing unsold inventory = \$0.10/gram-mole

Sources of Income

- Sales (price of D*market share)

Figure 10. *Financial summary of game.*

Students were shown the market demand curve of component D for a period of five years (Figure 9) on the website. This demand curve is slightly different than the one normally seen in an economics course; specifically, it shows how the demand for D will vary with time, in an effort to quantify production and selling price. The website gave a simplified version of manufacturing cost (Figure 10). Capital equipment costs (*e.g.*, reactor, separation unit, pumps, valves, piping) and yearly manufacturing costs (*e.g.*, maintenance, operation, waste disposal) were considered to sum up to an approximate value of \$45 per reactor volume (in L). The website specified the raw material cost, cost to store unsold inventory, and sale price of product D. Although presented in a simplified manner, the manufacturing cost was realistic and derived from actual experience. Students were given some time to practice with the Activities website and calculate the profit they could make based on their design.

PLAY THE GAME: THE COMPETITION[15]

The Graded Activities and Activities sections are the same program, with the exception that tasks in the Graded Activities section are completed sequentially, and the user cannot go back to change/revise a design parameter. The first two questions reviewed what the students learned in the first week. Students were asked to calculate the volume and flow rate of a reactor for a given C_A. Then, they were asked to calculate the profit they would make for this particular design, assuming that they could sell all that they produce. Students were permitted to repeat the activity as many times as they wanted before starting the competitive game, to become comfortable with using the website. Whenever a student attempted a Graded Activity, a new set of input parameters was given; thus, no two trials were the same. A screenshot of the Graded Activities section is shown in Figure 11.

The competitive game was designed so that there were four companies competing for the same market share of chemical D over a 5-year period. Initially, each student played against three other computer-generated players. The company (student) with the highest profit at the end of the fifth year won the game. Students were encouraged to pick a name for their company.

To design the reactor, each company (student) had to determine the market share they were going to pursue and the year they were going to base their design on, using the demand curve for product D. These decisions are critical uncertainties in any process design. The strength of the game is that these uncertainties are incorporated in the simulation.

The game followed a similar course as the Graded Activities. Each company must first start with lab experiments to determine the rate constant k. Once a reactor size was selected, it could not be changed over the 5-year production period. However, the flow rate can be changed from year to year to influence the profits. Students who cannot do these steps by themselves have the option of "hiring" help (*i.e.*, consulting chemical engineers) to make these calculations for them. However, they will have to pay these employees a salary, which will appear as a "debt" in the first year. A screenshot from the game illustrating this aspect is presented in Figure 2.

Students were able to view the year-end report for their companies after each year, and determine whether the flow rate of the feed stream should be changed. This decision was based on several factors, such as the market share, profit, and amount of unsold inventory. At the end of the 5-year period, students printed out and handed in their final report for all five years. A sample of the year-end report is shown in Figure 12. In each lab section, students with the four highest profits at the end of the five years were selected and played against each other on the same computer. The winner of the second round of the competition received a small prize. Other students had the option of playing against three other students if they wished. The outline of the two weeks of the CRAD Game course is summarized in Table 1.

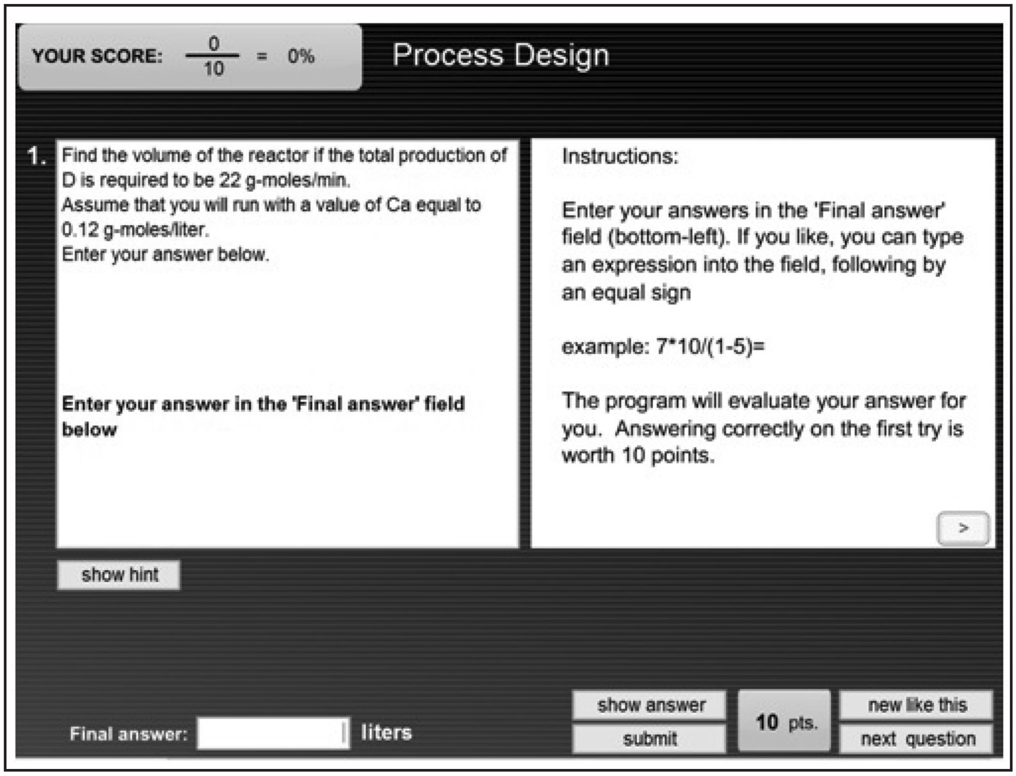

Figure 11. *Example of practice question.*

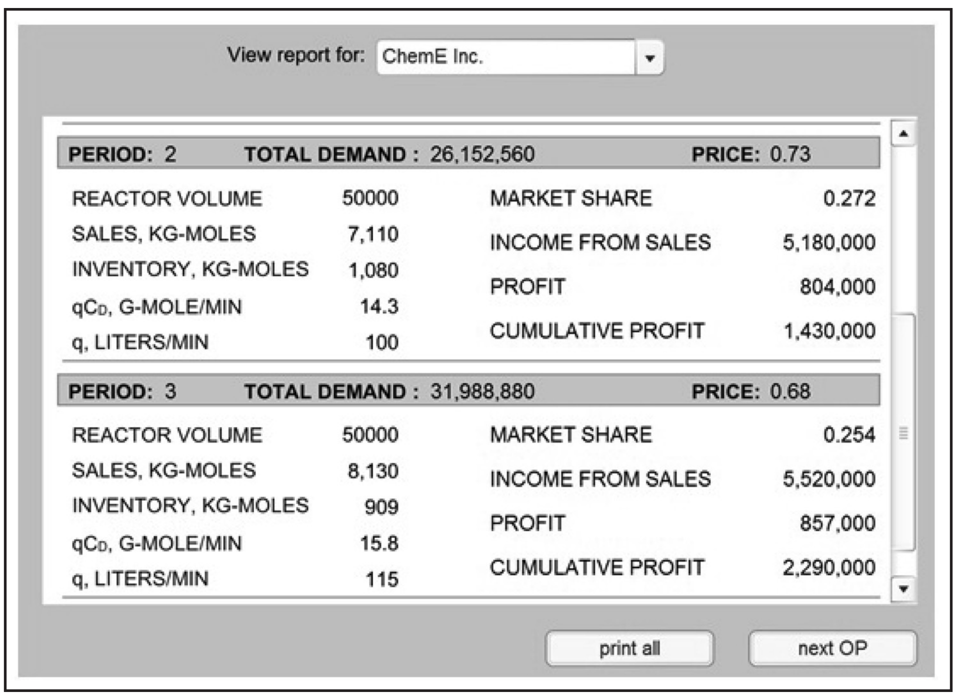

Figure 12. *Example of a year-end report.*

HIGH SCHOOL JUNIORS AND SENIORS

Whereas college freshmen spent part of the hands-on computer laboratory sessions deriving the model equations, the high school students were not asked to derive the batch reactor and CFSTR mass balance equations. The derivation was explained in detail by the instructor and the final equations were given to students. The remainder of the procedure for using the website and playing the game was the same with the high school students as with the university freshmen.

STUDENT FEEDBACK

All three authors of this article were present during the computer sessions of the class. Because the class size was small (20 students), it was possible to obtain immediate feedback while the students were learning to use the website, derive the equations, and make the required calculations. The students showed great interest in the game, and they were all actively engaged in the class. The web exercises "made the problems easier to understand with the visual aid" of the game. Each student had his or her own computer, allowing students to understand concepts at their own pace. Interactions between students and with the instructors were encouraged.

TABLE 1
Outline Followed During Computer Lab Sessions For Introducing and Playing the Game

	Topics covered in Computer Lab	Corresponding screenshot
Week 1	Description of problem	Figure 2
	Lab scale experiments	Figure 3
	Nomenclature	Figure 4
	Batch reactor model equations	Figure 4
	Calculation of rate constant	Figures 5 and 6
	Model equations in CSTR	Figure 6
	TFD	Figure 7
	Interactive simulation	Figure 8
Week 2	Demand Curve	Figure 9
	Economic aspects - costs and sales	Figure 10
	Graded Activities	Figure 11
	Game	Figures 12 and 13

At the end of the second week and at the conclusion of the game (March 2012 and 2013), the ChE freshman students were asked to respond to the following questions:

A. *Did the lectures provide an effective introduction to the exercises that followed?*
B. *Did the non-graded and graded activities prepare you for the game?*
C. *Was the game effective in demonstrating what chemical engineers do and the challenges they face?*

Students were asked to rate their answers on a scale from 1 (poor) to 5 (excellent). The results of the survey are presented in Figure 13, in which the percentage of students giving a particular rating for each question is shown as a bar graph.

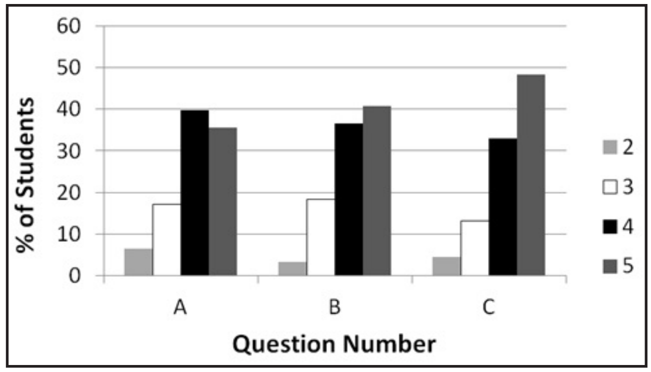

Figure 13. *Bar graph of students' ratings on survey questions. 1 = poor, 5 = excellent*

Most students rated their experience as positive, with more than 80% of students giving high ratings (4 or 5) to all questions. For Question A, 81% of students rated the lectures as an effective introduction for the exercises that followed, and 83% of students found the graded and non-graded activities to be useful. About 89% of the students gave the highest rating to the game being an effective learning tool. Overall, students "enjoyed practicing [problems] using real-life-based situations."

Involvement in the study and playing the game might have had some influence on the choices made by high school students, as five of the 11 participants went on to study engineering in college. However, in addition to the game, these students had other exposures to engineering concepts, which were included in the physics course and a separate engineering course taught by Mr. Anthony Iarrapino and Dr. William Jumper in their high school. Although the high school students responded favorably to the after-school class and game, we felt that more time was required to make it as effective as it was for the freshman engineering students.

ACKNOWLEDGMENTS

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