Integrating the Use of Commercial Simulators into Lecture Courses

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Abstract

Since commercial simulators are commonly used in the practice of engineering, we need to ensure they are included in engineering education. Computer laboratory sections were added to a "lecture" course to teach the use of a simulator and to give the students practice in solving realistic problems. By thinking about the computer lab as a problem-based learning environment, minimal lecture time was necessary to train the students on the simulator. Examples of instructions, problem statements and results from a student survey are presented.

I. Introduction

The modern practice of engineering often involves the use of specialized commercial simulation packages. Since student use is an excellent form of advertising, these packages are often available to schools at a considerable educational discount. Graduates need experience with simulators, but many educational questions about their use remain. Should students be trained explicitly to use a simulator or should they learn on their own? Which classes should use simulators? How many of the "bells and whistles" of the simulator should be taught? Must hand calculations be required? Must hand calculations use the same solution techniques as the simulator uses, or is it sufficient to use another solution technique? Is it necessary to use multiple simulation packages from competing firms or can one be used as an example of the type? How can students learn how-to-learn to operate simulators by themselves?

This paper discusses integrating a commercial simulator, ASPEN PLUS, into a junior level course in chemical engineering. The approach can be considered to be a form of Problem Based Learning (PBL) in a laboratory that is used to simultaneously teach the students how to use the simulator and to solve realistic, open-ended problems. The laboratory portion of the course also had the advantage of introducing modern computer techniques, group activities, and communication into a "lecture" course. Although applied to a specific simulator for chemical engineers, *the teaching technique will also be effective for teaching with simulation packages in other disciplines.*

II. The Course

CHE 306 is a three-credit lecture course for chemical engineering juniors and seniors covering separation methods such as distillation, absorption, extraction and membrane separations. Since these separations are very important industrially, many students regard this course as the first chemical engineering course that gives them a taste of real engineering. The relevance of the course is further reinforced by comments from students who work with separation techniques on co-op or internship assignments. Although a fair amount of work is involved, the students do not consider it to be a flunk-out course. As a result, the students are comparatively well motivated despite the large size of the lecture class (up to 150 students).

Chemical engineers have designed and performed separation techniques since the founding of the profession. The classical design methods involved graphical design procedures for binary separations and approximate, short cut methods for multicomponent separations (e.g., see Seader and Henley [1] or Wankat [2]). Current industrial practice is to use a commercial simulation package (e.g., ASPEN PLUS, ChemCAD, HYSIS, and PROSIM) or perhaps a simulator written in-house. Graphical methods are still employed for visualization and trouble-shooting. The current practice of engineering is similar in other engineering fields.

The classical course in separations taught equilibrium-staged separations (distillation, absorption and extraction) using graphical and short cut approaches. When computers became available, projects involving writing FORTRAN code were instituted. However, practicing engineers now use existing simulators and rarely write their own code to solve these problems. To prepare students for industrial practice, we need to teach students how to use one of the commercial simulators. Graduates and students on co-op or internship assignments will be at a competitive disadvantage if they do not have experience with one of the simulators used in industry. The first challenge is to incorporate the simulator into the course in such a way that students learn how to use it, but it is not just a black-box. The second challenge is to teach use of the simulator in a minimal amount of lecture time.

All of the separations covered in CHE 306 except for the membrane separations are included in the commercial simulation packages. We chose to use the ASPEN PLUS simulator because it is used in our senior design course and the site license had been purchased. Other commercial simulators are similar and could also have been used.
In the recent past students were assigned to learn a simulator on their own in order to do a homework assignment. They were told that they could see the teaching assistants (TAs) for assistance. Unfortunately, the results were, at best, mixed. Many students did not do the assignment or turned in incomplete or incorrect solutions. Those who did turn in correct solutions often collaborated, contrary to the rules, with a student who had used ASPEN PLUS on a co-op or internship assignment. Most students learned neither how to use the simulator nor the underlying engineering principles. This experience also did not prepare the students to use the simulator in their senior design course.

III. Course Redesign

In fall 1997 CHE 306 was restructured to have two lectures plus either a two-hour recitation or a one-hour computer lab every week. This restructuring required a streamlining of the lectures, but additional time for examples was available in recitation. The lectures were arranged on a Monday-Wednesday-Friday schedule. The Friday lecture period was used for a scheduled but optional help session taught by the course instructor. Each of the four recitation sections had roughly 36 students. The students were placed in groups of three or four students and solved problems with occasional help from the TA. Since the computer laboratory could hold at most 18 students, each recitation section was split into two parts for the laboratory. The students worked in the same groups in laboratory and recitation. Groups were selected to be as diverse as possible using the procedures discussed by Wankat [3]. In the six labs during the semester all students had computers and sat next to other members of their group. In both recitation and lab the students were supposed to ask their group members for help before asking the TA. Initially students wanted to ask all questions of the TA, but by half way through the semester they were relying more on their groups. Both the recitations and computer laboratory help the students learn.

Unfortunately, the two TAs were significantly overworked. Either I needed more TAs or the course had to be restructured. Since additional resources were not available, I restructured the course again. The lab portion appeared to be critically important to teach the students how to use the simulator. However, the one hour lab periods were clearly too short. The recitation sections helped improve student problem solving, but appeared to be expendable.

In fall 1999 the course was organized with Monday-Wednesday-Friday lectures and students were assigned to one of the seven two-hour computer lab sections. The Friday lecture became an optional help session during the seven weeks that lab met. A TA was present during the first hour of each lab section, and then left before the second hour. This reduced the work-load for the TAs and it reinforced the need for the students to learn on their own with some assistance from other engineers. This amount of help from the TA seemed to balance the need of students to have help available with their need to become independent learners.

IV. Teaching Method

Lectures talked about the fundamental concepts and problem solving. Graphical methods and short-cut methods useful for solving problems by hand were illustrated in class. The alternate solution methods (matrix based) used by the simulators were explained and the equations were set up. The theory in lecture was related to the simulation package when appropriate, but time in lecture was not used to discuss the details of the matrix solution or of running the simulator. Similar problems were solved by both hand calculation and the simulator albeit with different solution techniques.

A modified Problem-Based Learning (PBL) approach was used in the laboratory both years. In PBL students are given challenging, realistic problems that motivate them to learn the material [4,5]. Students were given realistic problems to solve and they were expected to learn how to operate the simulator essentially on their own with modest assistance from the TA. One of the big frustrations when first learning how to use a complicated simulator is the inability to get any results. Results for even very simple problems are motivating. Once a simple problem can be set up and run, students can add to it. The students were given written instructions in a recipe form (Table 1) that, if followed *exactly*, allowed them to start using the simulator. The TA was available to help students set up and get their first simulation running. They were expected to pick up other techniques by exploring problems and talking to other students. The TA was available when the entire group was stuck. Groups were encouraged to talk to other groups, but this was frequent only when one student was obviously quite skilled with ASPEN PLUS.

Three of the early labs were exploratory in nature, and no lab report was required. The students were given a basic problem statement and were asked to explore a series of "what if" questions (e.g., what happens if the pressure is changed?). I tried with mixed success to get the students to play with the simulator and discover for themselves what it could do and what all the bells and whistles were for. These exploratory labs were directly tied to the phenomena being studied in class, and they prepared the students for the design labs.

In this exploratory phase students were also asked to solve homework problems from the textbook that they had already solved by using hand calculations. Early in the semester when you want to increase student confidence in the simulator, select problems that will give good agreement between the hand calculations and the simulation. Later in the semester when the students need to be reminded that the simulator is not perfect, choose a problem where the simulator does not agree with the hand calculation.

Students were also asked to try calculations that they knew (or at least should have known) were incorrect so that they could see what the simulator did in these cases. For example, in addition to using the Non-Random Two-Liquid (NRTL) model students were told to use Raoult's law for the vapor-liquid equilibrium behavior of ethanol-water. They were told to produce a plot of the data and compare it to the data in their textbook. The simulator will do what it is told to do even though Raoult's law cannot predict azeotropes and is clearly inappropriate for this system. Hopefully, they learned from this exercise that the results are only as good as the information input into the simulator.

Attendance at each lab session was worth 5/7 of a percent of the course grade. This small fraction was sufficient to motivate the students to attend or arrange for a make-up if they would be out of town. Other than attendance, there were no student grades involved in the exploratory labs. Despite this, the students were motivated to learn how to use the simulator partly because using it is both challenging and fun (once one is past the frustration of getting it to work) and partly because they knew they would need to know how to use the simulator for the design lab, which was graded. Laboratories without grades ease the burden on TAs, and allow the professor to reuse the lab assignments every year.

This minimalist approach to teaching students how to use a complicated commercial simulator can be adapted to any simulator and does not require a large amount of preparation time. The first draft of the detailed recipe for starting the simulator (see Table 1) took about two hours to write and about another hour to polish based on comments from the TAs. Each of the exploratory labs took about the same amount of time to prepare. These materials can be reused every year since there is no grade directly associated with them. An alternative approach is to use extensive teaching materials to help students learn to use the simulator if these materials are available. For example, a CD-ROM is now available to teach students how to use ASPEN PLUS and HYSYS [6]. The four design labs required the students to solve realistic, complicated separation problems requiring significant trial-and-error use of the simulator. An example design problem for lab is shown in Table 2. This particular problem illustrates the power of the simulator, since it is more difficult than the absorption problem I did for the course project in a graduate course thirty years ago. And now undergraduates can do it in less than two hours. This problem asks the students to explain what they observe and to develop a physical explanation. This part of the problem relates the computer simulation to the fundamentals covered in lecture and is at the comprehension level in Bloom's taxonomy [7]. Then they were asked to determine what happens when conditions are changed by doing a series of application and analysis level problems. Finally, they answered a design question. Some of the design questions were at the analysis level while others involved synthesis. Note that hints on operation of the simulator are interspersed throughout the problem statements.

The design labs were scheduled immediately after the exploratory labs, which were after the material was studied in the lecture portion of the course. Doing the labs after the material was studied reduced the tendency of the students to use the simulator as a black box. According to PBL theory [4,5], these problems will motivate the students to learn the material. The problems certainly motivated the students to learn how to use the simulator. Many of the students also were able to relate the laboratory exercises to the lecture material. Several students commented that lab was where they really learned how to solve the problems.

The problems for laboratory were designed so that they could be completed within the two-hour lab period. Most of the groups completed the design labs during the lab period and wrote their one to two page lab reports afterwards. The students were given an example report and told that since attaching ASPEN PLUS printouts will overwhelm the reader, they needed to summarize just the most important results. The lab reports were due a week after the labs. Groups received a group grade for the assignments. The computer labs constituted 10 percent of the course grade. Half of this was based on attendance while the remainder was based on the lab reports. The average grade on the four lab reports was 90.2, which is an A since 85 or better was required for an A.

V. Results

At the beginning of the last lab period in 1999 the TAs passed out a survey (Table 3). The students completed the surveys and returned them anonymously before the end of the first hour of lab. This procedure resulted in a high rate of return (82 surveys returned for the total of 106 students who received a grade in the course). The results of the survey are also recorded in Table 3. Six of the questions had a rating greater than 4.0 and very few negative scores, which is very favorable. The vote was very favorable on question J, retaining labs as part of CHE 306, and only four students were against this. This was my “bottom line” question in the survey, and I am gratified to see the large number of positive ratings.

There are parts where a significant fraction of the students would like to see change. Question B had the lowest rating and 24 students did want the TA available for both hours. Students were split on question C, whether lab helped them learn the lecture material; however, some students who did not think it helped commented that learning to use the software was useful. Students who disagreed on question G overwhelmingly thought that lab should be a higher percentage of the course grade.

A number of students wrote comments, which are listed in Table 4. Reading through the comments reinforces the impression that the students appreciated the opportunity to learn how to use the simulator. Unfortunately, they did not always see the connection between the theory and the simulator. Some students appear to want to use the simulator as a black-box. Some students reported that the lab helped them understand the material better, and that lab was where they really learned the material.

There is additional anecdotal evidence that the computer lab helped the students learn. Students have told me that those who had the 306 computer lab had a significantly easier time learning the number of new ASPEN PLUS sub-packages used in the senior capstone design course. These students often tutored the other students in their groups to teach them how to use the simulator. The use of a simulator in senior laboratory courses is optional. Students who took CHE 306 with the computer lab appeared to be much more likely to use ASPEN PLUS for these laboratory projects.

The instructor's reflections may also be of interest. I thought that the two-hour lab periods used in 1999 were much less hectic and more beneficial than the one-hour periods used in 1997. The absence of the TA from the second hour of lab caused some problems, but it seemed to force groups to work together. And certainly the TAs appreciated the break on lab days. Providing support for only the first hour of a multi-hour laboratory appears to be both an effective and cost-effective method of instruction in computer labs. It would not be appropriate in laboratories where safety is a major concern.

Unfortunately, relinquishing the recitation sections appeared to have a price. The students seemed to learn the material quicker in 1997 and did better on the homework that year. Two hours of group practice on problems with a TA present to answer questions clearly improved the performance of many students. However, student grades were higher in 1999, probably because a deliberate effort was made to cover less material and make the tests a bit easier.

VI. Summary and Conclusions

Use of a modified form of Problem Based Learning (PBL) to teach engineering students to use a simulation package in a computer laboratory attached to a "lecture" course is effective. The students learned how to use the simulator better and they learned the course material better than in the lecture course without the computer laboratory. The most important point is that *simulation packages can be integrated into engineering lecture courses without requiring a large amount of lecture time.*

Acknowledgments

The outstanding performance of my teaching assistants, Praveen Gunaseelan and Will Walters in 1997 and Shawn Adair and Paul Fanson in 1999, is gratefully acknowledged. The assistance of Mrs. Marcella Maynard in analyzing the surveys is gratefully acknowledged.

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Bio Sketch

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Table 1. Portion of Recipe to Start Doing Simulations

In the “Start” button menu choose the following in order: ecn software, AspenTech, AspenPlus, and the Aspen User Interface.
On the “Connect to Engine” screen use the menu to scroll to “local PC.”
Click OK.
Click OK when the screen message is “Connection Established.”
You should see an Aspen Plus blank screen.
On the bottom menu click “Separators.”
Left click Flash 2 (a flash drum with two phases).
Move your cursor to the center of the blank screen and left click. This gives you the basic module of a flash drum.
Try left-clicking the mouse on the module (this selects it for attention) and then right click the mouse to see the menu of possibilities.
To add a feed line and two outlets: Move to the bottom menu and left click the mouse on the icon labeled “material streams.” Move cursor to the inlet arrow on the flash module and hold it over the arrow until the arrow lights up. Left click on the arrow and drag the cursor away from the flash drum. Left click again to obtain a labeled material stream for the feed.
Repeat these steps for the two outlet streams
Once you are happy with your flow sheet, click the Next button (blue N with an arrow). This will tell you if the flow sheet connectivity is complete. If it is, click OK.
…..[instructions continue].

Table 2. Problem for Lab 6 (Absorption)

1. You wish to absorb ethylene oxide (EO) from a nitrogen stream into water. The column and feed streams are at 275 psia. The solvent used is pure water. The inlet gas stream is 1.8 mole % EO and 0.5 mole % water. Flow of inlet gas is 100 kmol/h. Basic problem: Water flow rate is 50 kmoles/h. Inlet water temperature is 20 ^{o}C. The inlet gas temperature is 20 ^{o}C. N = 35. Answer the following:
   a. Why is the amount of nitrogen in the liquid so high? [Isn't nitrogen essentially insoluble?]
   b. Where does the temperature maximum occur and what is the maximum temperature?
   c. Where is the water mole fraction in the gas the highest? Why?
   d. What are outlet flow rates and mole fractions?
   e. How much liquid is in the inlet gas feed? Does this liquid negatively impact the operation?

2. Try inlet gas and liquid at 50 ^{o}C. Everything else is the same as the base case (problem 1). Start with the 20 ^{o}C run, and do 30 ^{o}C and 40 ^{o}C to approach 50 ^{o}C while always converging. How does increasing the inlet temperatures change the performance?

3. The pressure is high because the reactor pressure to make EO is high. Return to the base case (problem 1) and try a pressure of 137.5 psia. What happens to the EO absorption if the pressure is reduced?

4. Thirty-five stages is high. Return to the base case (problem 1) and try N = 25, 15, 10, 5 and 3. Look at both the leaving vapor mole fraction of EO and the component split fractions, focusing on EO.

5. Suppose we return to the base case (problem 1), but with N=10 and an inlet EO mole fraction of 0.036 and water 0.005 in the vapor. Find the outlet mole fractions and the split fractions of the components. Look at the temperature profile in the column. Compare to the base case (but with N = 10).

6. Suppose we choose N=10, T inlet (liquid and vapor) = 20 ^{o}C, p = 275 psia, and want 95.0 % of the EO fed to the system recovered in the outlet liquid. If the inlet vapor flow rate is 100 kmole/h, what inlet water flow rate is required? [Inlet vapor is 1.8 mole % EO, 0.5 mole % water, and the remainder is nitrogen. Inlet water is pure.] Report outlet mole fractions and flow rates, and recovery of EO in the liquid.

Table 3. CHE 306 Lab Survey. November 1999

Incorporation of a computer lab is an experiment. Please answer these questions based on your experience with the previous 306 labs. Do not put your name on the survey. Return it this period to your lab TA. Thank you.
Please respond using a scale of 1 = strongly disagree, 2 = disagree, 3 = neutral, 4 = agree and 5 = strongly agree.

[Response key: R3(15) = 15 responses gave a rating of 3.]

A. Working in groups was appropriate in this lab.
R1(3), R2(2), R3(5), R4(21), R5(51). Wt. Avg. = 4.40
B. Having the TA available for the first hour was sufficient.
R1(6), R2(18), R3(21), R4(29), R5(8). Wt. Avg. = 3.18
C. Lab helped me understand the lecture material.
R1(2), R2(12), R3(29), R4(34), R5(4). Wt. Avg. = 3.32
D. The labs were well integrated into the course.
R1(0), R(9), R3(19), R4(42), R5(12). Wt. Avg. = 3.70
E. The labs were effective in learning how to use AspenPlus.
R1(0), R2(4), R3(8), R4(45), R5(25). Wt. Avg. = 4.11
F. My group was able to finish the labs that had to be turned in during the lab period (does not include writing the lab report).
R1(0), R2(5), R3(10), R4(38), R5(28). Wt. Avg. = 4.10
G. The portion of the course grade (10%) assigned to labs is appropriate.
R1(4), R2(13), R3(10), R4(42), R5(13). Wt. Avg. = 3.57
If you don't agree, should it be more or less?
More = 17, Less = 2
H. The grading of the lab reports was fair.
R1(0), R2(2), R3(8), R4(34), R5(38). Wt. Avg. = 4.32
I. The laboratory workload was reasonable.
R1(0), R2(3), R3(8), R4(55), R5(16). Wt. Avg. = 4.02
J. Labs should be retained as part of CHE 306.
R1(1), R2(3), R3(7.5), R4(27.5), R5(43). Wt. Avg. = 4.32
Please write any other COMMENTS (use the back for more room if necessary)

Table 4. Comments from Student Surveys

"I don't think we should miss 3 pts for grammar." [On lab reports]

"I think we should spend more time learning how to use the program rather than rushing through to finish the labs in time."

"It is valuable to learn Aspen."

"[Lab] gives a real-life, hand-on application of material learned in class."

"Getting the lab handout a little earlier would be a great help. Instead of getting a look at it and reading during lab, we could get familiarized with it."

"It would be better if the TA could be there the whole time."

"This lab is good because it actually shows how 306 does relate to real world "sorta" circumstances."

"Aspen is a big part of chemical industry, & it's important that we're exposed to it before entering a real job. Very pertinent to materials in class."

"I felt that we were thrown into Aspen w/o much background. Our group didn't work well together, which isn't anyone's problem or anything that could be fixed….Different levels of experience caused the problem. Background information or Aspen lectures may be helpful."

"If lab was gotten rid of, we would be screwed in the business world."

"The TA should stay longer than one hour."

"I think we should have learned to do more things in Aspen (since that is what is used in industry.)

"I guess its good to learn Aspen but other than that, I can imagine getting the same out of 306 without labs."

"The lab helped me to understand class concepts. Using Aspen the first time was a bit confusing, though. A little bit more time should be spent in the fist lab learning the menus, or perhaps an additional "intro" lab should be introduced."

"Labs really help to understand material. It shows you the real stuff going on."

"Learned a lot of AspenPlus."

"Works for me. I liked the opportunity to play with Aspen."

"I really enjoyed having a practical course application but when we wasted time in class about McCabe-Thiele that we will never use because we have Aspen. The course should be more practical applications like Aspen. Lab was good but the reports took too much time for only 10% of our grade."