USING A COMMERCIAL SIMULATOR TO TEACH SORPTION SEPARATIONS

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S ince modern practice of chemical engineering uses specialized process simulators extensively $(e.g., \text{Aspen})$ Plus, CHEMCAD, HYSIM, and PROSIM), chemical engineering departments need to prepare students to use these tools. For example, distillation columns are designed almost exclusively using process simulators, and if the equilibrium data is deemed reliable, the column will be constructed without any laboratory or pilot data. Most chemical engineering departments now use one of the steady-state process simulators in separations and/or design courses. $[1, 2]$

The steady-state simulators do not include adsorption, chromatography, and ion exchange (collectively, sorption), which are normally operated as unsteady-state processes. Formerly, sorption systems were designed by a combination of data and rules of thumb. Recently, it has become more common to use a more fundamental design procedure based on solution of the partial differential equations governing the heat and mass transfer in the column and the algebraic equations for equilibrium and pressure drop. In industry, the detailed simulations are always accompanied by laboratory and often pilot plant data.

Chemical engineering graduates who understand the fundamentals of sorption processes and are familiar with sorption simulators will have a competitive advantage. This paper discusses the use of the commercially available Aspen Chromatography simulator to teach sorption separations. The

course outline, grading procedure, assignments, computer laboratory operation, and testing procedure are delineated. Student survey results and the author's opinion of the effectiveness of teaching with this simulator are presented.

THE COURSE

ChE 558, "Rate-Controlled Separation Processes," is a three-credit, dual-level elective course that has been taught off and on for almost 30 years.^[3] The topics covered always include sorption separations, and depending upon the professor, might also include crystallization, electrophoresis, or membrane separations. I have used *Rate Controlled Separations* [4 l although this book is currently difficult to obtain. This course has always been taught in a lecture style with homework and often a course project.

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Three considerations led me to change the teaching method. First, since I believe that the sorption separation processes will eventually be designed almost entirely using simulators, proper preparation of graduates will require teaching with simulators. Second, the understanding of an average ChE 558 student was too low. Since I had observed student improvement in a distillation course when a simulation lab was incorporated,^[2] I expected an increase in understanding if a similar change was made in ChE 558. Third, I had proposed in the educational part of two NSF proposals to teach ChE 558 with a simulator, and now I had to deliver on these promises.

In spring 2005 I changed ChE 558 to focus entirely on sorption separations. The nominal schedule had a one-and-a-halfhour lecture on Tuesdays and a one-and-a-half-hour computer laboratory using the Aspen Chromatography simulator on Thursdays (see Table 1). This schedule had fewer lectures on

sorption separations than in previous years, but tests covered the same amount of material on these topics. The total amount of material in the course was reduced by removing the membrane separation material, which is now often included in the required undergraduate course on separations. The course was taken by four undergraduates and three graduate students. Only one of the students had previous experience with an unsteady-state simulator, but all had previous experience with Aspen Plus, which has a somewhat similar graphical user interface to Aspen Chromatography.

The grading scheme used a straight scale $(85-100 = A$, $75-85 = B$, $60-75 = C$, $50-60 = D$) as guaranteed grades, but I reserved the right to use lower cut-offs if that was appropriate. The two regular tests were each 25% of the grade, the lab exam was 20%, lab attendance 9%, lab assignments 6%, homework 5%, and the group course project was 10%. Students were encouraged to work together on lab assignments

Figure 1. Screenshot of Aspen Chromatography Interface with flow sheet for a simple chromatography system.

and homework. The complete course syllabus is available from the author at <wankat@ecn.purdue.edu>.

Homework assignments were problems from the textbook plus one straightforward simulation. The textbook problems were similar to the test problems; of course, new problems were written for the tests. Since the students were all able to come to class early, they were given two hours for each test. Unfortunately, due to a mistake in solving an ion exchange problem on the second test, this problem, although solvable, was about an order of magnitude too difficult. I adjusted scores based on the performance of the second-best student in the class (the best student appeared to be an outlier whose performance was not representative of the class). The students appeared to be satisfied with the fairness (or generosity) of this procedure.

ASPEN CHROMATOGRAPHY COMPUTER LABORATORY

Aspen Chromatography is an algebraic-differential equation-solving program with a user interface for the solution of liquid adsorption and chromatography problems (see Figure **1).** This simulator is very powerful and a trained user can often solve in a few hours a problem that used to take months. Aspen Chromatography uses the method of lines to solve the partial differential equations. The user can select both the differencing method to be used and the integration method *Summer 2006*

to solve the resulting ordinary differential equations. Aspen Chromatography licenses are expensive for companies, but are reasonably priced for universities and can be bundled with other Aspen Technology programs. It cost \$400 to add an Aspen Chromatography license for 60 users to Purdue's Aspen Technology order for University Lifecycle Package Bundle **#1** (60users) that cost \$2,000. The current Version 12 is quite stable and reasonably user friendly, but not as user friendly as Aspen Plus. My experience with Aspen Plus is that 98-99% of the difficulties students have are due to operator error. With Aspen Chromatography about 80% of the students' difficulties are caused by operator error. As expected, the numerical integration routines, which use the method of lines to solve the partial differential equations, have difficulty converging when the profiles are steep and the isotherms are nonlinear. In general, the resources and expertise that have been developed for teaching with steady-state simulators $[1, 2, 5]$ are not available for sorption separations. More troubleshooting and more computer assistance will be needed.

Since much of my current research involves simulation of chromatography and simulated moving-bed systems with Aspen Chromatography, I am familiar with this simulator and my graduate students are very familiar with it. The graduate students and post-doc supported by the NSF grants were enlisted to help with the computer laboratory. With their aid, I developed 10 laboratory assignments including a laboratory

test. Each of the first eight laboratories showed how to build a flow sheet for a new aspect of Aspen Chromatography in a cookbook fashion, and then had the students solve simulation and design problems. Excerpts from the first laboratory assignment are presented in Table 2. All lab assignments are available from the author at <wankat@ecn.purdue.edU>.

As the semester progressed the amount of detail in the instructions was decreased. Most of the students stayed in the lab after the nominal closing time to finish the take-home assignments that accompanied the labs. The material covered in

TABLE2 Excerpts from First Lab Assignment A complete set of instructions for all labs is available from <wankat@ecn.purdue.edu>.

The goal of this lab is to get you started in Aspen Chromatography. It consists of a cookbook on running Aspen Chromatography and some helpful hints. We will also simulate a real separation. Keep this lab assignment. You will want to refer back to it.

1. Log in to the computer. Go to Start, Programs, ChE Software, AspenTech, Aspen Engineering Suite, Aspen Chromatography 12.1, Aspen Chromatography. This opens a window if you are at a station that allows you to access the hard drive. Otherwise, you will get a message that essentially says, 'The working folder is unavailable." In this case, change working file to your N drive. Click on OK, and window should open. If not, run in circles, scream and shout, and ask for help.

2. We will first develop a simple chromatography (or adsorption) column system. To do this, go to the menu bar and on the left side, File. Click on File and go to Templates, and in that window click on "Blank trace liquid batch flowsheet," and click on Copy. It will ask for a file name. Use something like "columnl." This will be saved in your working file. NOTE: In all file names and names for components, columns, steams, and so forth there must be NO spaces.

3. In the "Exploring simulation" box (LHS), click on "component list." Then in box below (Contents) double click on Default. This lists A and B. Change these names to the names of the components to be separated (fructose and dextran T6). First, click "Remove all" button. Then in window below type in first component name (e.g., fructose) and click on "add" button. Do the same for all other components. Then click OK.

4. Now draw the column. Click on the+ to the left of "Chromatography" in the "Exploring Simulation"box to open other possibilities. Click on the word "chromatography. "This should give "Contents of Chromatography" in box below. Double click on the model you want to use (Reversible - since it is most up-to-date). Click and drag the specific model you want: in this case "chrom_r_column," and move to the center of the Process Flowsheet Window. This gives a column labeled B1. Left click on B1, then right click to open a menu. Click on Rename. Call the block something like "column." Click on OK.

19. If you have time, do this next step. If not, save your file (remember the file name), exit Aspen and do this step outside of class. The two peaks are not completely separated. There are a number of ways they can be separated more completely. Double the value of L, to $L = 50$ cm. Click on Rewind, change L in the column dimensions table, and then rerun the one-minute pulse input. When you run pure solvent, a pause time greater than 10 minutes is needed since doubling column length will double time for material to exit. Do this run and look at the result. Separation is better, but still not complete. Print your plot and label it. This plot will be handed in with the lab assignment. Save your file (remember the file name) and exit Aspen.

TABLE3 Handout on What to Expect in Lab Exam

The exam will be open book and open notes. You may not open or use any of your old Aspen Chromatography files. Part A. (50 points) Generic Problem. This is a demonstration that you can do a basic Aspen Chromatography simulation. Open up Aspen chromatography and use a "Blank trace liquid flowsheet template." Set up a chromatographic column with one feed, a column, and a product. Use specified models for the column, feed, product, and connecting streams. Set up the system to process compounds that will be specified in the test. Have Aspen do discretization with xyz procedure with NN nodes (these will be specified in the test). Use a model with convection plus a specified form of dispersion, constant pressure, and velocity. If needed, the dispersion coefficients will

be supplied. Use a linear, lumped parameter model with a specified driving force and constant mass transfer coefficients (they will be given). The isotherms will be given and the units for q and c will be specified. Operation is isothermal. The column length and diameter will be given. The adsorbent has the following properties: $\epsilon e = 0$.aa, ε p = 0.bb, KD = 1.0, ρ s = cc kg/m³. The following feed values will be specified: flow rate, pressure, and all component concentrations. Use a specified integrator with a specified fixed or variable time. Use default values of the tolerances. Develop a graph of the product concentrations (on the same scale) versus time.

1. Run a breakthrough curve for zz minutes. Print, label, and turn in your plot. Use the history to accurately determine the center of the breakthrough curve and the t_{MTZ} for one of the components where t_{MTZ} is measured from 0.05 times the feed concentration to 0.95 times the feed concentration. These calculations should be shown on the plot.

2. Input a dd-minute feed pulse and develop with pure solvent for a total time of zz minutes. Print your plot, label, and turn in.

There should not be any convergence problems in Part A. Part B. (50 points) The second part of the lab test will be a design problem for one of the other processes that we have studied (e.g., flow reversal, adiabatic operation, SMB, TMB, ion exchange).

TABLE4 Homework Assignment 4

1. Use the Lapidus and Amundson solution with $E_{\text{effective}}$ to predict the behavior of fructose in a column packed with silica gel. The feed is 50 g/liter, the feed pulse lasts for eight minutes, and then it is eluted with water. The flow rate is 20 ml/min. The other values are:

time predicted by the local equilibrium solution, peak center time minus four minutes and peak center time plus four minutes.

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the laboratory was cumulative, and by the end of the semester the students were able to simulate rather difficult problems without detailed instructions.

Part A of the lab test was a demonstration by the students that they had learned how to use Aspen Chromatography for simple simulations. Two weeks before the test the students were given the generic form of part A (Table 3). They were encouraged to supply data and parameter values to generate their own form of the test and then practice solving it. Part B, a design problem, proved to be more difficult. The lab test was given during a normal lab period that was extended to Students solved a number of chromatography and adtwo hours. Since there were only seven students in the class sorption problems during the semester. The real strength of and I knew them all well, no special precautions beyond numerical analysis is it can solve problems with complicated proctoring the exam were taken to ensure honesty. (When nonlinear isotherms that cannot be solved analytically. To I gave an Aspen Plus lab test in a core

the use of ADSIM for pressure swing *for the solution* large changes in flow rates which are not $\begin{array}{c} \text{modeled by Asnen Chromatooranh} \\ \text{modeled by Asnen Chromatooranh} \end{array}$ ed for the simulation from a literature very powerful and and Amundson method and numerical interaction of the students had paper. In the earlier labs the students had α **trained user can often** been given all the necessary parameters since that makes troubleshooting of student difficulties much easier. Students were told that the purpose of learning how to extract parameters from the literature was to prepare them for the course project. *months.*

The course project was to develop a

new Aspen Chromatography problem and solution suitable for one lab period. This is a form of Felder's generic quiz.^[6] Students were required to use equilibrium and mass transfer data from the literature and/or the Internet, not from the textbook or from Aspen Chromatography demonstrations. They were told that projects that considered operational methods not taught in the lab or that combined different operational methods would be most impressive. Student groups presented an oral report, including a computer demonstration, and turned in a written report. As a treat for the students, I ordered pizza to be delivered after the oral reports were presented. The student projects-nonisothermal ion exchange, ion-exchange with flow reversal, and SMB separation-were quite well thought out.

Since seven students do not divide evenly into groups, I *Summer 2006*

divided the class into groups of 3, 3, and 1. I used this unusual procedure because one of the graduate students is doing his thesis research with me and during the course of the semester he had much more practice with Aspen Chromatography than the rest of the class. He agreed to be a group of one, and the class accepted my rationale when the groupings were presented. The other two groups were made as equal as possible based on grades in the course.

EXAMPLE PROBLEM

junior class with 95 students, I wrote **Aspen Chromatography** ing of numerical solutions with analytical a different test for each of the five lab $\left| \right|$ is an algebraic-differential solutions was done for linear problems sections and disabled both e-mail and *is an algebraic-alfferential* where analytical solutions exist. One access to student files.) **equation-solving program** convenient analytical solution is the During the 10th lab, students first **here here here h h** *x* **h** *x xith a <i>xser interface* **h** *x n s solution^[4] with a <i>xser interface x x n s s s s s s s s* with **with a user interface**
watched a computer demonstration of **an** effective dispersion coefficient that
for the solution **and** includes the effects of dispersion and adsorption. Gas separations can involve
large changes in flow rates which are not
large changes in flow rates which are not modeled by Aspen Chromatography.

Then the students did a simulation with

Then the students did a simulation with Then the students did a simulation with **reduces chromatography Aspen** Chromatography repulse component chromatography problem them to determine the parameters need-
 problems. This simulator is with a large pulse of feed by the Lapidus

and Amundson method and numerically

> The effective dispersion coefficient that lumps all dispersive effects into axial dispersion and assumes negligible mass transfer resistance was estimated to be 8.062 cm²/min. This is much greater than the axial dispersion coefficient value 0.15 cm2 /min because mass-transfer resistance controls dispersion. The Lapidus and Amundson solution requires the use

of superposition as a step up followed by a step down eight minutes later.

The same problem was solved numerically with Aspen Chromatography using two of the higher-order differencing schemes, Buds (Biased Upwind Differencing Scheme, a 4thorder method) and QDS (Quadratic Differencing Scheme), and the default UDSI (Upwind Differencing Scheme 1) with 50 nodes. The solutions all used the Gear method with a fixed time step for integration. The QDS solution was done first with the actual value of the mass transfer coefficient and axial dispersion coefficient, and then with a very high mass-transfer coefficient (essentially no resistance) and the effective dispersion coefficient.

A screenshot of the Aspen Chromatography solution using

solve in a few hours a problem that used to take

Buds with 200 nodes is shown in Figure 2 and a screenshot of the solution using UDS 1 with 50 nodes is in Figure 3. The Lapidus and Amundson solution and the higher-order numerical solutions were bell-shaped curves and looked almost identical. UDSI with 50 nodes also produced a bell-shaped curve, but it is much more spread out and has a lower peak concentration than the other curves because of significant numerical dispersion. The curves are different enough that students can easily see the differences by comparing Figures 2 and 3. Thus, the use of UDS 1 with 50 nodes is numerically inappropriate for this problem.

Since the Lapidus and Amundson and the higher-order numerical analysis curves are so similar, differences can only be ascertained by looking at exact values of concentrations and times (Table 5). The concentrations predicted by the Lapidus and Amundson solution are: $t = 25.575$, $c = 25.0$ g/liter; $t = 29.575$, $c = 48.54$ g/liter (peak maximum); and $t = 33.575$, $c = 24.975$ g/liter. The Lapidus and Amundson solution has its peak center at exactly the time predicted by the local equilibrium solution (29.575 minutes). The peak concentration, peak time, and the predicted times for concentrations of 25.0 and 24.975 g/liter are given in Table 5 for the five different solutions. Since the two QDS solutions are quite close to each other, the use of an effective dispersion coefficient is valid for this linear system. All of the reasonable solutions (excluding UDS1) are quite close, with a small shift in times. Although the Buds solution with 200 nodes is the best

fit to the analytical solution, in practical terms it doesn't matter which is used. One of the lessons students learn from this and other benchmarking exercises is that they must pay close attention to numerical convergence.

RESULTS

A survey on the computer laboratory was developed, and a research exemption was obtained from the Purdue Institutional Review Board for Human Subjects Research. The students all responded to the survey (Table 6) on the last day of class. To avoid biasing any of the responses, the survey was administered by the undergraduate secretary; I was not in the room while the students filled out the survey, and the process was completed before the students knew there would be a pizza delivery.

The students' responses to the survey (Table 6) show that previous knowledge of different computer applications varied from no knowledge to comfortable. General comfort levels with computers were high. With the exception of the speed of the Distributed Academic Computing System (DACS), which allowed remote access to Aspen Chromatography, laboratory operation was rated as about right. The students thought that both the computer labs and the lectures helped them learn sorption separations and that combining lecture and lab was an appropriate way to teach this material. Most of the comments are positive and reinforce the advantage of

Figure **2.** *Screenshot of Aspen Chromatography solution for problem 2 in Table 4 using Buds with 200 nodes.*

Figure 3. Screenshot of Aspen Chromatography solution for problem 2 in Table 4 using UDS1 with 50 nodes (an inappropriate choice).

having a computer lab. At the same time they filled out the survey, the students responded to the standard course evaluation questionnaire required in all ChE courses. Course evaluation questions that ask for global ratings correlate positively with student learning.^[8] These core questions were, 1. "Overall, I would rate this course as:" and 2. "Overall, I would rate this instructor as:" The choices were: Excellent=5, Good=4, Fair=3, Poor=2, and Very Poor=l. The scores obtained for these questions-4.1 and 4.6, respectively-collaborate the impression that

the students thought this was a good course.

I believe the students learned sorption separations in more depth in spring 2005 than in previous years. This seemed to be true across the spectrum of student abilities (good students learned more than good students previously, average students learned more than average students previously, and struggling students learned more than struggling students previously). Since in previous years the course also covered membrane separations, the breadth of coverage was less in 2005; however, the students learned sorption operations better despite less lecture time spent on this topic. Obviously, the 2005 students are also prepared to use the simulator.

DISCUSSION AND CONCLUSIONS

The students generally liked the format of lab and lecture and thought it helped them learn; however, these students all volunteered to take this elective knowing there would be a computer lab. Students who feel uncomfortable using the computer probably took other electives.

During the semester a faulty installation of Windows caused difficulties running Aspen Chromatography in the computer laboratory. For several weeks the students needed to log into DACS, which was slower than the direct installation. Once the problem was identified and Windows was reinstalled, we had no difficulties with the direct installation of the software. The comment in Table 6, "Run the simulations before the students run them," probably referred to this difficulty running some of the labs on DACS. Lab 6, with flow reversal, ran without problems when I tested it using the direct installation of Aspen Chromatography in my office, but would not run on DACS. The student group that later did its course project with flow reversal had no difficulty following the original lab instructions and obtaining solutions with a direct connection. It is important to have reliable computer support before scheduling use of any simulator.

If there are transferable skills in learning how to use simulators, students who become skilled with, for example Aspen Plus, will learn to use another simulator faster. This appeared to be true for Aspen Chromatography. Thus, even if they never use simulators taught in the curriculum, the experience of learning to use these simulators will probably help graduates efficiently learn to use simulators on the job.

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