**237c Using a Commercial Simulator to Teach Adsorption and Chromatography**

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Since modern practice of chemical engineering uses spreadsheets, mathematical software (e.g., Mathcad, Maple, Mathematica, MATLAB), CFD software (e.g., FEMLAB, Fluent) and specialized process simulators (e.g., Aspen Plus, CHEMCAD, HYSIM, PROSIM, and VMGSim) extensively, chemical engineering departments need to prepare students to use these tools. Most chemical engineering departments use one of the steady state process simulators in separations and/or design courses, and Prof. Benny Freeman has developed a membrane simulator that he has made available on the web.

This paper discusses the use of the commercially available Aspen Chromatography simulator in a dual level elective course, ChE 558, "Rate-Controlled Separation Processes," to teach adsorption and chromatography. Aspen Chromatography licenses are expensive for companies, but are reasonably priced for universities and can be bundled with other Aspen Technology programs. I have taught ChE 558 as a straight lecture course previously. In spring 2005 I taught the course with 1 ½ hours of lecture and nominally 1 ½ hours of computer laboratory every week. The course outline, grading procedure, assignments, and testing procedure are delineated in the paper. 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 the steady state Aspen Plus simulator, which has a somewhat similar graphical user interface.

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. Because teaching adsorption and chromatography with commercial simulators was the educational part of two NSF research grants, I enlisted my graduate students and post-doc to help with the computer laboratory. With their aid, I developed ten laboratory assignments including a laboratory test. Each of the first eight laboratories introduced a new aspect of Aspen Chromatography in a cookbook fashion, and then had the students develop a flow sheet and solve a simulation or design problem. 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 the laboratory assignments was cumulative and by the end of the semester the students were able to simulate rather difficult problems without detailed instructions. The ninth lab was a lab test. The tenth lab, which lasted for several periods, was a group course project to develop a new assignment for the 558 lab. The lab test and course project are discussed in detail in the paper. The lab assignments are available free from the author .

Comparing the students' understanding of adsorption and chromatography in spring 2005 to previous years, my belief is they learned the material in more depth in 2005. This seemed to be true across the spectrum of student abilities. Since in previous years the course also covered membrane separations, the breadth of coverage of separation methods was less in 2005; however, the students learned sorption operations better despite less lecture time spent on this topic in 2005. The students' responses to a survey showed that they agreed that the computer labs helped them learn adsorption and chromatography and that combining lecture and lab was an appropriate way to teach this material.

Aspen Chromatography is an algebraic-differential equation solving program with a user interface that was developed for the solution of liquid adsorption and chromatography problems. 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 98-99 % of the problems students have are due to operator error. With Aspen Chromatography about 80 % of the students' problems are caused by operator error while the remaining problems are due to simulator difficulties. 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 are not available for adsorption and chromatography. Thus, professors and teaching assistants will need to do more trouble shooting. A good relationship with the computer gurus in the department is absolutely necessary since their help will be needed.

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