Integrating best practice pedagogy with computer-aided modeling and simulation to improve undergraduate chemical engineering education

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Abstract

Chemical engineering graduates need to have problem-solving capabilities combined with experience in computer-aided modeling and simulation (CAMS). This need has been strongly emphasized by the chemical industry. CAMS provides tools to help students conceptualized problems, explore the influence of relevant parameters, and test fundamental engineering principles. The aim of our Course, Curriculum, and Laboratory Improvement project is to meld the problem-based learning pedagogy with CAMS to produce students with an in-depth understanding of the fundamentals of chemical engineering as well as the ability to use computer simulation packages effectively in the workplace. The approach used here is to integrate the use of CAMS throughout the entire chemical engineering curriculum. The Accreditation Board of Engineering and Technology's Engineering Criteria 2000 framework will be followed to evaluate the outcome of this project. This reform process will beneficially affect both Chemical Engineering teachers and students. Computer packages such as HYSYS, PRO/II, ASPEN Plus, POLYMATH, and Gaussian are employed in nine Chemical Engineering courses. POLYMATH is used in several undergraduate classes to permit students to obtain numerical solutions to problems that are difficult to solve analytically. For example, in Kinetics POLYMATH allows the students to calculate the effects of pressure drop and nonisothermal operation on the design of reactor. In Mass Transfer, HYSYS is utilized to simulate a flash vaporization and test the effects of pressure and preheating. Dynamics and control of a propylene glycol plant are analyzed by Process Control students using HYSYS, which has an integrated steady state and dynamic simulation environment. The dynamic performance of various control schemes is evaluated. In Process Design, a creative preliminary design for silane production utilizes CAMS packages including raw material requirements, energy requirements, list of major process equipment, and process economics. In addition, a computer-based problem-based learning (PBL) classroom with multiple white boards and virtual reality to maximize group learning is being developed. Finally, changes in the undergraduate Chemical Engineering curriculum at Lamar University are currently being implemented. These changes will enable the students to receive the maximum benefit of CAMS. Our progress to date will be outlined and will be discussed in terms of best practice pedagogy and cognitive science.

Problem-Based Learning

This paper discusses an adaptation and implementation project that involves an innovative use and extension of problem-based learning (PBL) in Chemical Engineering education at Lamar University that links industry, faculty and students. Lamar University is located within one-half mile of the ExxonMobil refinery (225,000 barrels/day) and at the center of Spindletop where the petrochemical industry began. The project focuses on the integration CAMS into the undergraduate chemical engineering courses and curriculum.

PBL, student centered learning, is undergoing a renaissance in engineering education[1] and precedents for incorporation of computer-aided learning have been established[2]. This is clearly illustrated by the problem-based freshmen course incorporating computer based modeling technology at the University of Minnesota[3]. The strategy at Lamar University is to adapt the extensive PBL program developed at McMaster University and implement it into the ChE Department at Lamar University where we have a unique position with industry and strong industrial interest in participating in the program.

McMaster University, under the leadership of Donald Woods, has been developing and implementing PBL for 25 years with well-documented success[4–7]. In addition, we are incorporating the work of Scott Fogler at the University of Michigan in selecting computer-aided software and interactive teaching methods using virtual reality[8]. The authors are fully aware of the difficulties involved in PBL implementation[9,10] but have the complete support of the chemical engineering faculty and associated curriculum faculty from chemistry and other engineering departments. The final product will be a chemical engineering university training program that graduates students with enhanced problem-solving skills, particularly with computer-aided modeling and simulation, and a better conceptual understanding of real-world problems based on enhanced understanding of fundamentals. This report outlines our progress to date.

In this project, a special PBL computer-assisted classroom is being established. The classroom will have several PBL group areas that are fitted with individual computers and white-boards. The instructor station will be networked to these group areas and will be able to monitor and capture for documentation and assessment the material being discussed and recorded by the whiteboards. In addition, these group areas will be designed to encourage group discussions of the classic blackboard style that has worked so well in the past in student-instructor "jam sessions". Digital video and sound recording at the workstations will be available to aid in student learning.

Example Problems from Courses

The following sections give example problems from the various chemical engineering courses. To solve these problems, the students must resort to using CAMS. Furthermore, these problems are all examples of PBL.

Kinetics

In the undergraduate Reaction Kinetics class, the students used POLYMATH[11] extensively to solve three types of problems. The first type asked the students to use linear, polynomial, and/or nonlinear regression to fit experimental data to rate laws to determine best-fit values for the rate law parameters. The second type required the students to solve systems of nonlinear equations to analyze multiple steady states and hysteresis in continuous stirred-tank reactors. The third type asked the students to solve systems of nonlinear ordinary differential equations to model two classes of systems: those containing multiple chemical reactions and those used to analyze nonisothermal gas-phase reactions in packed bed reactors.

A good example of this last class of problem is Fogler's Problem 8-7[12], which asks the students to plot the temperature, conversion, and pressure versus weight of catalyst down the length of the reactor. The reaction in question is the elementary, irreversible, exothermic, gas-phase decomposition $A \rightarrow B + C$, which occurs in an adiabatic reactor packed with catalyst. To solve the problem, the students first obtained two coupled nonlinear ordinary differential equations: one for conversion as a function of catalyst weight derived from the design equation of a packed bed reactor, the other for pressure as a function of catalyst weight derived from the Ergun equation[13]. They next combined these two differential equations with algebraic equations derived from the energy balance (which relates the temperature in the reactor to the conversion), the rate law, and stoichiometry. Finally, they used the ordinary differential equation solver in POLYMATH to obtain the requested plots.

The three types of problems mentioned above can be divided into two categories: those that cannot be solved analytically, and those that can. For the first category, the advantage of using a computer is manifest: the students cannot otherwise obtain a solution. For the second category, allowing the students to use a computer still presents one main advantage: they can focus on getting the solution rather than on learning the sometimes arcane techniques required to obtain the analytic solution. One quintessential example of this is the problem of finding the roots of a cubic equation. The general analytic solution has been known since the 16th Century[14], but it is rarely used to solve the problem unless the emphasis is on the method rather than the solution. Thus, in the undergraduate Reaction Kinetics class the students made extensive use of POLYMATH to solve problems both on the homework and on the exams.

Mass Transfer

The Mass Transfer class at Lamar spends one-third of its time on fundamental principles and two-thirds on applications such as distillation, absorption, and extraction for both binary and multi-component systems. Although learning the binary system is important conceptually, learning the multi-component system is a must in the real world.

In this paper, we would like to use a simple example given in the textbook of Henley and Seader[15] (Examples 7.2 and 7.5), for which the flow diagram is shown in Figure 1. The high-pressure, high-temperature thermal hydrodealkylation of toluene to benzene uses excess hydrogen to minimize the cracking of aromatics. The conversion of toluene is only 70%. To separate and recycle hydrogen, hot reactor effluent vapor is partially condensed with cooling water. When the feed compositions are given and the pressure and temperature of the system are fixed, the amounts and the compositions of both liquid and vapor streams can be calculated. The
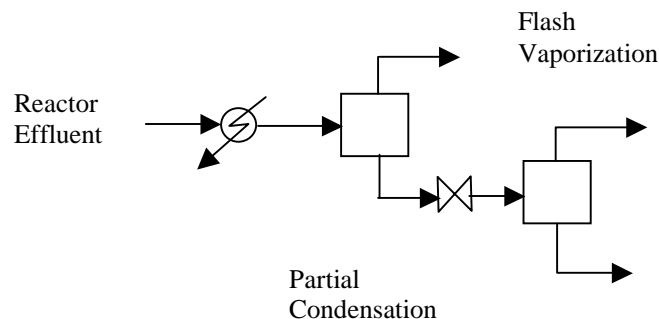
Figure 1: Thermal Hydrodealkylation of Toluene to Benzene.

hydrogen and methane contents in the liquid stream can be reduced further by using a simple adiabatic flash vaporization.

In the past, the students had to write their own computer programs to solve the MESH (mass balance, equilibrium, summation, and enthalpy) equations. Combining the calculation methodology with the thermodynamic properties predictions made this type of computation very tedious and time-consuming. Quite often, the students had to spend several days in programming and debugging; therefore, they did not have time to interpret the results. Now, using computer packages such as HYSYS, ASPEN, and PRO/II, the students can obtain the solution within a few hours (if not minutes). The students even have time to change the pressure of the flash drum or add a preheater to the feed stream to see their effects on separation of a key component.

By using the computer package, the students learn the fundamental principles through exploring the following questions:

1. What is the effect of condenser temperature on the amount and composition of the liquid stream?
2. What is the effect of condenser pressure on the amount and composition of the liquid stream?
3. What is the effect of pressure drop on the recovery of hydrogen during the flash vaporization?
4. What thermodynamic models should be used for this chemical system?

After this exploration and discussion, we, as educators, will not be afraid to use the computer packages and will not worry about students losing the opportunity to learn fundamental principles.

Process Control

The CHEN 4330 process control class covers fundamentals of process dynamics, PID feedback control, and advanced control (model-based, multivariable control)[16–18]. The CHEN 4150 Process Control Laboratory at Lamar University consists of three analog units for level, flow, and temperature control (donated by Fisher/Scallon Controls), a pH adaptive control unit, a Schweitzer Heat Exchanger/Thermal Mixing unit, an Atlantic Distillation Process Simulator (sponsored by Dow chemical), an ISA PID Tuning software, and a HYSYS dynamic process simulator[19,20]. An all-digital DeltaV control station donated by Fisher-Rosemont will be added in Spring 2001 to the lab class to upgrade the analog units. The Process Control Laboratory class

provides an indispensable learning experience to our senior students. Lamar University has been awarded a grant from CCLI to integrate simulation software into all ChE courses. For process control, these resources will be allocated to purchasing more up-to-date process dynamics and control software: ASPEN Dynamics , ASPEN Custom Modeler, and Aspen DMC Plus[21–24].

At this point, we have used HYSYS in our Process Control Laboratory as a lab unit for learning process dynamics and basic/enhanced PID control. HYSYS is widely used in the chemical process and natural gas industries. Familiarity with HYSYS is a valuable, marketable skill for chemical engineering graduates. The package has the distinct advantage of integrating the dynamic simulation and the steady state simulation into one program. As a result, students can run the propylene glycol steady state flowsheet and use the results as the initial conditions for the dynamic simulation when a disturbance is encountered. This process simulator helps students gain insight into how the controllers work by examining responses from the strip charts, just as engineers and operators can see from the console in a plant control room. In this exercise, a flowsheet for the production of propylene glycol is presented, as shown in Figure 2. The propylene oxide is combined with water to produce propylene glycol in a CSTR. The reactor products are then fed to a distillation tower, where essentially all the glycol is recovered in the tower bottoms.
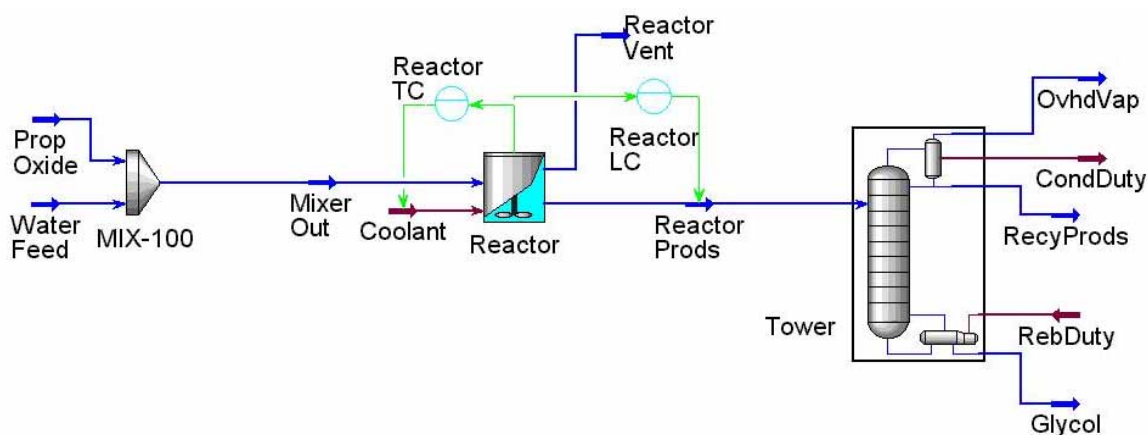

Figure 2: Process Flowsheet for Propylene Glycol Process.

The students are asked to install a PID to maintain the process at the desired operating conditions. Two dynamic simulations are studied including a drop of the reactor set point from 140 to 125 F and a return to the original set point using the controller ramp feature. As mentioned earlier, historical data can be viewed in the strip charts (as shown in Figure 3) and stored as a data file. The strip charts allow students to monitor the response of the reactor itself, as well as how the change propagates downstream to the distillation tower. All actions required can be completed within a reasonable time period (3 hours each week for two weeks). Students are required to submit a lab report a week after the lab is completed.

Figure 3: Strip Chart for Propylene Glycol Process.

Process Design

For process design, the students are asked to design a plant to produce 2.6 million pounds per year of silane from a mixture of hydrogen, silicon tetrachloride, and silicon. Given a preliminary process flow diagram consisting of a hydrogenation reactor, a stripper, three distillation columns, and two redistribution reactors (see Figure 4), the students must design (size and other specifications) and cost all of the equipment required to produce the silane as economically as possible[25–33]. To solve this problem, the students need to make extensive use of process modeling software such as HYSYS or Aspen both to obtain the material balances and to model and design (size) the equipment.

Curriculum Changes

The undergraduate chemical engineering curriculum at Lamar University is undergoing two changes this semester. First, since the ultimate goal of this project is to include CAMS in every undergraduate chemical engineering class, we have decided to teach the basics for many of these computer programs in a single required sophomore-level class, Computer-Aided Modeling and Simulation, which will be offered concurrently with our material and energy balance course. This class will be offered for the first time in the Spring 2001 semester. This one-credit class will consist of a weekly three-hour laboratory taught in our chemical engineering computer lab. We anticipate being able to introduce the students to several useful computer applications, including POLYMATH, Aspen, PRO/II, MathCad, and Matlab. The goal is to teach the basics of each of these programs to the students so that later, when they need to use these programs in their other chemical engineering courses, the instructors will not need to spend time covering the basic use of each program.
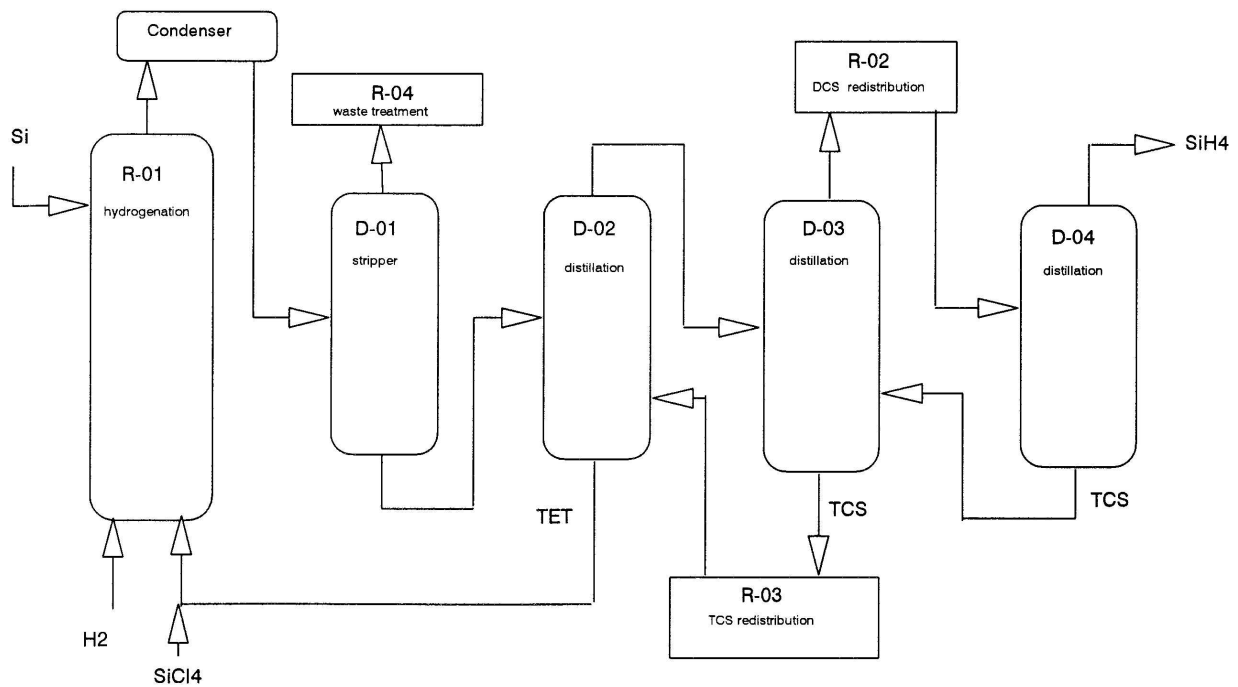
Figure 4: Silane Process Flowsheet

The other curriculum change is the addition of a second process control class to the undergraduate program. This proposal has been heartily endorsed by our departmental advisory council, which has said that industry has a great need for engineers with a command of process control. In addition, local industries have provided strong support for the training of advanced process control and dynamic simulation. Lamar has received a grant from ExxonMobil Oil Company to develop Process Simulation courses with Aspen and PRO/II. A renewed grant from ExxonMobil extends this cooperation to the training in the dynamic simulation and control areas by providing funding for instructor's training, software licensing (Dynsim, DMC Plus), and hardware maintenance. This Advanced Process Control course will cover topics that we usually don't have time to cover in our undergraduate process control class, including multiple-input multiple-output control, dynamic matrix control, real-time optimization, and other topics relevant to industrial process control. In the Spring 2001 semester this class will be offered by an adjunct faculty member who is an expert in industrial process control. To make room for this class, we will combine two upperclassman classes: Computer Applications and Advanced Analysis.

Conclusions

Since many of the proposals in this paper are to be carried out in the Spring 2001 semester, we will need to wait to see what transpires. However, the early returns are promising.

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