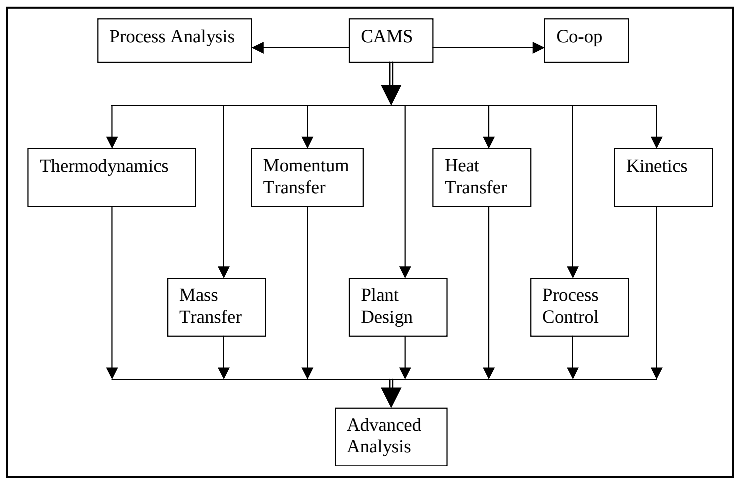
At Lamar University, as part of a National Science Foundation Course, Curriculum, and Laboratory Improvement Adaptation and Implementation (NSF CCLI-A&I) grant, we have been revising the undergraduate chemical engineering curriculum for the past few years. As part of this revision, each of the courses has been enhanced to include extensive computer applications, and a new course, CAMS, has been added to the sophomore year.

A. Computer-Aided Modeling and Simulation (CAMS) – A Path-finder Course

The NSF CCLI-A&I project has initiated a prototype course to integrate problem-based learning (PBL) pedagogy into the chemical engineering curriculum with an implementation of computer-aided modeling and simulation packages. It starts with a new course, CAMS (Computer Aided Modeling and Simulation), in the sophomore level and concludes at a senior course of Advanced Analysis. The course structure can be seen from the following chart.



In the CAMS class, the sophomore students are introduced to two types of computer packages: mathematical packages (MathCad, MATLAB, and POLYMATH) and simulation packages (Aspen and Pro/II). During the first six weeks of class, the students use the mathematical packages to solve math problems that typically arise in upper-level chemical engineering classes, including regression (both linear and nonlinear), nonlinear equations, and systems of ordinary differential equations. The remainder of the semester is devoted to familiarizing the students with the simulation packages. Since these sophomore students have not yet had any chemical engineering courses (except the material and energy balance class, which they take concurrently), some time is spent describing the theory behind such common unit operations as flash drums, heat exchangers, chemical reactors, distillation columns, etc., as well as the theory behind each package's solution algorithm. Of course, many of the details are left to later upper-level classes, after the students have been introduced to the required fundamental theory. However, typical problems that arise in several junior and senior courses are given in this class and solved by computer packages.

To start a Computer Aided Modeling and Simulation teaching at a stage as early as sophomore is quite new in the chemical engineering curriculum. However, after two and a half years experimenting, the NSF-CCLI implementation project finds that the advantages are quite obvious.

The first advantage is to help the students in co-op program and in Process Analysis (Material and Energy Balance). Most of our co-op students use a Computer Aided Modeling and Simulation package (such as ASPEN, Pro/II, and HYSYS) during the co-op time period. CAMS prepares them early enough that they will be able to move into the working situation quickly to solve practical problems in industry. When the co-op students come back to school to learn the fundamental principles in junior/senior engineering basic courses, they already have this "problem based learning" pedagogical mind-set. This helps to pave the way for the "problem based learning" pedagogy in chemical engineering curriculum.

The NSF-CCLI implementation project has found that the co-op students can learn the fundamental principles more effectively than the non-co-op students. This could be a difference between the learning pedagogies of science and engineering education. In other words, the engineering students feel the need to learn fundamental principles in order to solve problems.

The other advantage of CAMS is to prepare the students for the chemical engineering sophomore (Process Analysis), junior (Thermodynamics, Momentum Transfer, Heat Transfer, and Kinetics) and senior (Mass Transfer, Plant Design, and Process Control) courses in problem based learning with an implementation of computer aided modeling and simulation. CAMS teaches the students to do a process simulation for the units of Mixers, Separators, Heat Exchangers, Columns, Reactors, and Pressure Chargers. These units are the applications of Process Analysis, Momentum Transfer, Heat Transfer, Mass Transfer, and Kinetics. Besides, the selection of the thermodynamic models prepares the students to learn about the non-ideal mixtures of chemical compounds that will be studied in Thermodynamics.

With the preparation of CAMS the instructors should be able to assign homework closer to the real world problems. Furthermore the instructors can encourage the students to experiment with different operating variables to understand the fundamental principles. The purpose of this project is to develop the material in this prototype course, CAMS, so that the advantages of learning computer-aided modeling and simulation in the chemical engineering program can be realized.

Two typical CAMS problems are shown below: the first is related to Kinetics, while the second is related to Mass Transfer.

1) Kinetics: The problem given in the CAMS is a reactor design problem to model esterfication of acetic acid with ethanol to produce ethyl acetate. The temperature, the pressure, and the components of the feed stream are given, it is required to find the output concentration if the reactor type, size, and condition are specified. A description of this problem is given below.

The elementary and reversible reaction equation can be described by

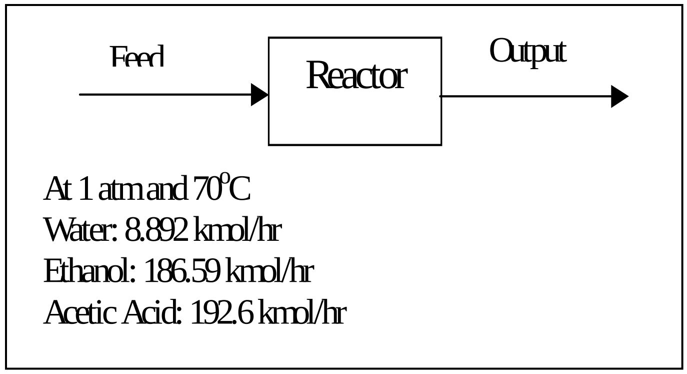
$$\text{Ethanol + Acetic Acid} \underset{k_r}{\overset{k_f}{\longleftrightarrow}} \text{Ethyl Acetate + Water}$$

where the reaction rate constants are given as

$$k_f = 1.9 * 10^8 \exp[(-5.95*10^7 \text{ J/kmol})/RT]$$

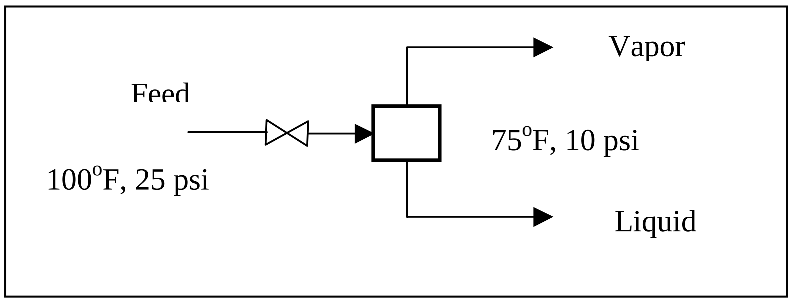
$$k_r = 5.0 *1\ 0^7 \exp[(-5.95*10^7 \text{ J/kmol})/RT]$$

What will be the output concentrations for a Continuous Stirred Tank Reactor (CSTR) with a reactor holdup V=0.14 m^3 at 70°C and 1atm?



The students will learn quickly that there are several different reactor types available in the simulation packages. It is fairly easy to explore the performance of different types of reactors, but the learning of the fundamental principles has to wait until the junior-level Kinetics class.

2) Mass Transfer: The problem given in the class is an equilibrium flash vaporization. A feed stream flowing at 1000 lb/hr contains an equimolar mixture of n-butane, n-pentane, n-hexane, and n-heptane at 100°F, 25 psi. The feed enters a flash drum maintained at 75°F and 10 psi. What is the flow rate and composition of the vapor and liquid streams leaving the flash drum?



What students can learn from this example are (1) equilibrium versus non-equilibrium flash vaporization, (2) isothermal versus adiabatic flash vaporization, and (3) pre-heat versus reduced pressure flash vaporization. This is a good example that should pave the way for students to learn thermodynamics, mass balance, and energy balance.

B. Advanced Analysis

Finally, in a last semester senior course, Advanced Analysis, the CCLI laboratory will be used fully to implement the CAMS and the problem based learning pedagogy. In Advanced Analysis, chemical engineering problems are given to the students at least one week ahead for the students to study and understand. In the class students have to use the fundamental principles learned from the courses as shown in the above chart to set up the system equations or the inputs for the CAMS packages. The instructor may initiate the questions and when the students answer the questions the others may challenge that answer. The instructor may give minimum necessary corrections in order to encourage the discussions. Through this problem based learning pedagogy, students can concentrate more than they typical do for the traditional teaching method because of the participation. We are expecting that the PBL pedagogy can be used effectively in the last semester Advanced Analysis class because all the basic principle courses have been taught.

To fully use the PBL pedagogy, a description of the problem must be distributed to the students days or even one week before the class discussion. This gives time for the students to understand the problem, search for references, and prepare for the class discussion. A simple problem selected from Jenson and Jeffreys (17) is shown below:

A tank contains 2 m^3 of water. A stream of brine containing 20 kg/m^3 of salt is fed into the tank at a rate of 0.02 m^3/s. Liquid flows from the tank at a rate of 0.01 m^3/s. What is the salt concentration in the tank when the tank contains 4 m^3 of brine? Plot the salt concentration and the volume versus time.

Students are encouraged to participate in the modeling of the system. The modeling process usually starts with the first principle, i.e. material and energy balance. To make modeling possible, assumptions are required. Typical assumptions for discussion are:

1. Will the liquid volume be changed after mixing?
2. Will the temperature be the same after mixing?
3. Will the brine concentration in the outlet be the same as that in the tank?

Because of the electronic white boards present in the CCLI laboratory, the students do not have to worry about taking notes. Instead, they can concentrate on the discussion of the modeling process. The instructor gives only guidance but not the "solution". Both sides of an assumption should be explored and discussed, and a reasonable assumption can be recognized but not assigned. Because of participation, the students have better understanding of the problem than the traditional one-way lecture.

To solve the system equations, we split the class into two groups. One group of student uses computer packages such as POLYMATH while the other one uses analytical method. Both numerical and analytical solutions can be presented and compared. A question about truncation error and round-off error initiated a discussion and the instructor had better be prepared to give guidance or even answer questions if the students are not familiar with the Runge-Kutta numerical method.

The students can present their results through a computer network with the LCD projector. Now, again, the interpretation is open to the discussion. For this example, the solutions are simple: the brine concentration increases exponentially and then gradually approaches the inlet concentration while the volume increases linearly with time. For other more complicated system, the discussions of the results are very involved. Most of the students find that it is very helpful to understand the system behavior through the discussion of the result. This part is called the interpretation of the results.