SIMULATION IN THE CHEMICAL ENGINEERING CLASSROOM

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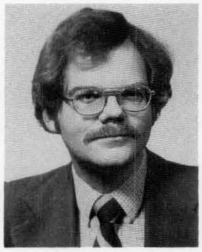

Wallace B. Whiting, *P.E., is Associate Professor of chemical engineering at West Virginia University, where he has taught for the past decade. He is active in ASEE and AIChE, and his research and teaching interests range from thermodynamics to process safety and process design. He welcomes dialogue on this and all of his articles.*

Many educators have found that active learning strategies can help students develop the higher level thinking skills of analysis, synthesis, and evaluation that are the essence of engineering.[1,2] Simulation is an effective technique for creating a classroom environment that is conducive to such learning. Whether we simulate a process on a computer or the work of an engineering team in a design project, the simulation experience brings a sense of reality to an assignment.[3,4] Students become more active, more interested. Few faculty who have engaged their students in simulation doubt its effectiveness.

Can we use simulation in all our courses? Should we? Through the following examples, I hope to show that the answer to both of these questions is "yes."

ROOT-FINDING ALGORITHMS

On the first day of a course in numerical methods for chemical engineers, I break the class into small groups of three to five students, and each group is told to find the largest positive real root of a function. The students don't know, however, that each group is given the *same* function, but in a *different* form. One group must find the solution by querying a computer program set up on a PC that accepts their guess and gives a value of the function, while another group is given an algebraic form of the function, which is a cubic. A third group is given a different form of the function, and yet another group is given the problem behind the assignment: to solve the van der Waals equation for the vapor molar volume given the constants a and b, the temperature, and the pressure. Each group is told to find the solution to the problem and to carefully keep track of how they solved it so that they can explain their technique to the rest of the class.

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The results of this exercise are amazing. My sophomore students (who have had no previous courses in numerical methods) independently develop all the root-finding algorithms in the text within thirty minutes, in addition to some other more sophisticated algorithms. (It should be noted that while the students have all brought the text to class, usually none of them has opened it yet!) As the groups go to the front of the class to explain their techniques, I tell them that this is called the bisection method, or Newton's method, or resubstitution with acceleration, or brute-force, or whatever. We discuss such topics as error propagation, accuracy criteria, advantages of solving the function analytically (for the groups that have the analytic form of the function), strategies for developing a good initial guess, and the risks and benefits of using a method that has already been programmed. Our discussion invariably broadens to include the roles of textbooks, computers, their own physical understanding, and their colleagues in solving numerical problems. We talk about why they are taking the course and what its relationship is to the rest of the curriculum and to their future careers.

Simulation? Yes, we simulated an engineer's attempt to solve a numerical (in this case, thermodynamics) problem. The students had a wide variety of experiences (guaranteed by the different versions of the problem) which they shared with each other in a structured way.

Through simulation the students develop new strategies for solving numerical problems. They learn quite a bit about specific numerical techniques (more than they could have learned in one traditional lecture), and they gain confidence in their abilities to solve new classes of problems. Perhaps most important—they learn the connection between numerical methods and the rest of chemical engineering. And, of course, they learn some thermo.

For larger classes, I use more groups rather than larger ones, and I choose one group of each type to lead the class discussion. If discussion lags (which is rare), another group is asked how its approach differed.

I have used the same kind of exercise with an optimization problem, with similar results.

THE LEVEE PROBLEM

I have used the "levee problem" several times—in senior design courses at two different universities and at a conference where most of the participants were chemical engineering faculty.[5] The kernel of the simulation comes from a homework problem, the source of which has been lost over the years. As originally stated, the problem appears to be a single-answer economics problem in which the student compares building a flood-control levee to not building it. Students are given a scenario in an expanded version of the problem (see Figure 1). They must write a memo, detailing their recommendations, to a specific person who has a specific technical background.

Responses to the assignment are wide ranging. Some students focus solely on the economics, concluding that the levee is a terrible alternative. Others ignore the costs and make what they feel to be the ethically correct recommendation (to build the levee at any cost). Many other solutions are presented, but few students attempt to tie the various aspects of the problem together.

But, what have they learned? . . . They knew what to do next; they knew how to learn on their own; they gave themselves the next assignment; they were good problem solvers. Heady stuff. And they learned that statistics can be useful—all within the confines of one class period.

PART 1
Memo and Feedback

In class, the students are paired and asked to play the role of Chris E. Smyth as they read each other's memos. Chris is a very busy executive who has only three minutes to read the memo and to answer the following three feedback questions: (1) What is the recommendation? (2) Do you trust (or believe) the recommendation? (3) What will you do next? The students give immediate

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TO: Workshop Participants
FROM: W.B. Whiting, Vice President of Engineering *WBW*
DATE: 18 October 1990
SUBJECT: Economics Revisited
CC:

Please submit your answer to the following problem by noon, Wednesday, October 24, 1990. Someone will be chosen to present the problem to the group at 1:30 P.M., Thursday, October 25, in Room 449.

In your position as Director of Investment Planning at Technocats, you must make a specific recommendation for or against the capital expenditure described below. Write a memo to your boss, Chris E. Smyth, Executive Vice President, recommending and justifying appropriate action.

After a chemical plant was built on an island in a river, our geology/hydrology department discovered that the island was occasionally under water. U.S. Army Corps of Engineers data indicate that the chances of a flood are about one in seven each year. The likely flood damage would be $250,000, and we would need to lay off ten employees for three months during the repair, which would be a boon for a local construction firm.

A protective levee would cost $600,000 (total fixed capital investment), and our civil engineering department estimates its useful life as 28 years, with no salvage value. Our economics group has worked up an opportunity cost of 10% per annum, based on after-tax cash flows and no inflation. Other economic data are given below.

Remember, your boss is a former geologist who doesn't know much about time value of money, discounting, annuities, etc.

- Fixed costs other than maintenance: negligible
- Annual maintenance cost: 1% of fixed capital investment
- Effective income tax rate: 48%
- Depreciation: AMACRS, 15-year class life (ignore mid-year convention)
- Working capital: none
- Use end-of-year annualized costs.

Figure 1. Levee problem assignment memorandum

feedback to each other by answering these questions.

We then discuss the responses. With some classes I have already brought in engineering ethics, but with others I have not. Regardless of their background, however, the intensity of the discussion is always high.

PART 2
Engineering Presentation

The students are formed into small groups, and each group is given a role to play in the ensuing simulation (see Figure 2). The students are given fifteen to twenty minutes for preparation before the simulation begins. One member of a "Director of Investment Planning" group is chosen to present the results and recommendations to the vice president, chosen from a "Chris E. Smyth" group. Some groups prepare extensive overhead transparencies or "chalk talks," while others develop note cards or lists of questions. As before, more than one group may be given the task of preparing the Chris E. Smyth role, but only one member from one group is chosen for the simulation in front of the class. Thus, all students actively prepare for the simulation and all have an interest in the outcome, even though only one student will ultimately play the role. The other group members are anxious to see how their strategy works, and the groups that are not chosen have an opportunity later to compare their strategies to the ones demonstrated.

During the preparation time, no group knows what the other groups have been told. In particular, Chris E. Smyth and the Director of Investment Planning have no idea what will happen next. As a reporter enters the scene, with tape recorder running, the simulation heats up, and what you fear will happen usually does. The engineer talks to the reporter as if the reporter were an engineer, or an idiot. Outrageous one-liners (sound bites) are uttered. The reporter has a field day. Sometimes Chris E. Smyth brings things back under control, and sometimes not. You never know what is going to happen.

Next an observer group leads the class discussion. I initiate the first topic: *Why are we doing this?* Although they come up with various responses, none of the students has ever indicated any concern that time was wasted in this simulation exercise. They all know that it

Chris E. Smyth

You are the Executive Vice President of Technocats, Inc. As indicated on the assignment memorandum, you are a former geologist (not a chemical engineer) who doesn't know much about time value of money, discounting, annuities, etc. However, you are a good manager and have risen through the ranks at Technocats because of your ability to deal with people and to get things done. The Director of Investment Planning reports to you, and you really need to know what to do about this levee/flooding situation. You will make the final decision, but you will need to justify it to the President, to the CEO, and, perhaps, to the Board of Directors.

We have simulated your office, complete with desk, phone, etc. The Director of Investment Planning will come to your office to make a presentation.

Director of Investment Planning

You are a chemical engineer. As indicated in the assignment memorandum, you must make a specific recommendation for or against the capital expenditure described. You will go to Chris Smyth's office and give a presentation (you are expected). Chris will make the final decision, but you and your group have done all the analysis. Remember the background of Chris Smyth while preparing your presentation. You will have only about 5 minutes for the presentation.

Reporter

Neither Chris Smyth nor the Director of Investment Planning knows that you will show up. You are an investigative reporter for the *Washington Post.* You have heard a rumor that Technocats has a chemical plant that could be subject to a flood. As with most journalists, you have no scientific or engineering training, but you are bright and ambitious. You go to see Chris Smyth, Executive Vice President, without an appointment. You have a tape recorder to record everything. During the simulation, you will be announced by the secretary, but, before Chris has a chance to say no, you enter the office and begin asking questions.

Observer

Your job is to observe what is going on. The Director of Investment Planning will give a presentation to Chris Smyth (Executive Vice President). During the presentation, an investigative reporter from the *Washington Post* will show up and begin asking questions. Neither Chris nor the Director of Investment Planning has any idea that the reporter exists.

After the simulation, you will be called upon to give an analysis of the simulation and to lead the postmortem.

Figure 2. *Roles for the levee problem simulation*

can happen to them. They realize that the engineer's inability to say the "right things" to the reporter stems from the engineer's overly simplified analysis of the situation and a lack of understanding of the difference between engineers and the rest of the population which they serve. The ensuing discussion ranges from topics such as ethics, to net present value, to statistics.

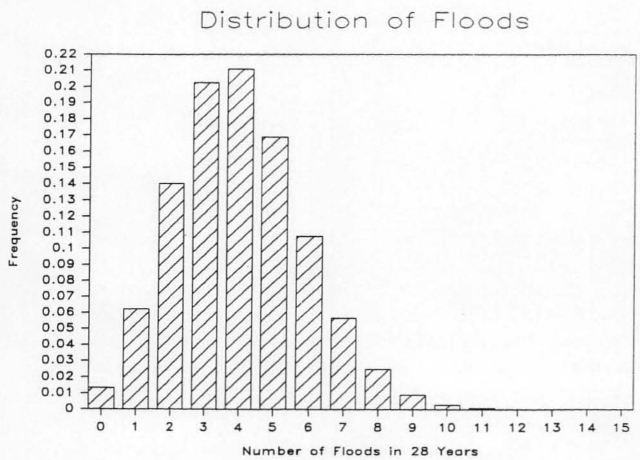

Figure 3. *Distribution of floods*

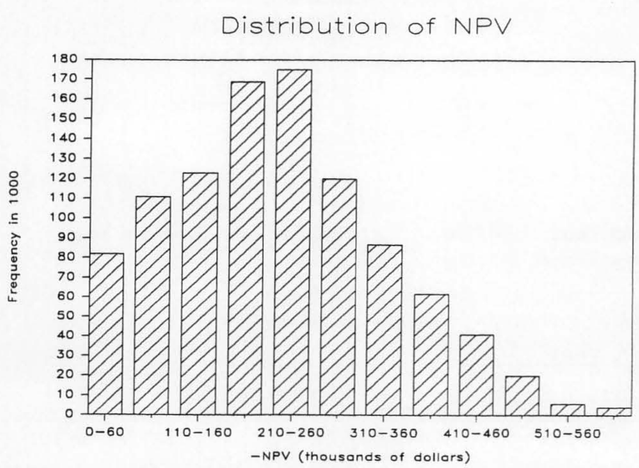

Figure 4. *Distribution of net present value*

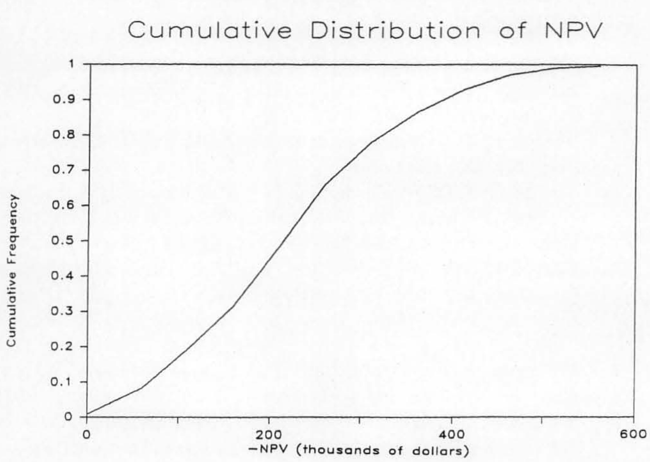

Figure 5. *Cumulative distribution of net present value*

PART 3
Monte Carlo Simulation

Yes, *statistics.* Students typically assume, for their calculations, that the interval between floods is exactly seven years. Some students assume that the first flood is in the first year while others assume that it occurs in the seventh year. The first time I used this simulation, my students asked how to quantify the chances that there would be a given number of floods in a given number of years and how the timing of such floods would affect the economics. They realized that they couldn't integrate the societal, technical, and financial aspects of the problem without such data. The *students* developed the next assignment: to do a Monte Carlo simulation to determine the frequency distribution of floods and the frequency distribution of the net-present-value comparison (essentially a probabilistic benefit-cost analysis[6]). Most of these students had taken no courses in probability or statistics, and none of them had heard of Monte Carlo simulation when I told them that that was what they were describing. Most students chose to use LOTUS 1-2-3 for the Monte Carlo simulation, but some wrote BASIC or FORTRAN programs. The results of their simulations are shown in Figures 3, 4, and 5. The same thing has happened with succeeding classes.

But, what have they learned? After years of diligently studying for what they *hoped* would be a rewarding career, they now know it's real. What engineers do is important (and difficult and scary). They are preparing for their career, and they know it. Realizing that their calculations can affect real people in serious ways is exciting. They knew what to do next; they knew how to learn on their own; they gave themselves the next assignment; they were good problem solvers. Heady stuff. And they learned that statistics can be useful—all within the confines of one class period.

But who was simulating what? The students were simulating a common engineering situation wherein after analysis, synthesis, and evaluation the engineer presents and defends a recommendation to technical and non-technical audiences, receives criticism, and decides what to do next.

For ease of use in different classroom settings, I have broken this levee problem simulation into three parts. The memo and feedback portion of the problem (Part 1) can be used to introduce students to simulation. The engineering presentation (Part 2) can be used with or without the reporter, or the full simulation, including the Monte Carlo assignment (Part 3) can be used. In each case, a postmortem discussion of the simulation, bringing in as many student viewpoints as possible, is essential.

OTHER SIMULATIONS

There are many other types of simulations, ranging from intricate ones to simple ones. At West Virginia University we have used an extended and involved simulation for the year-long senior design project for over fifty years.[4] An AIChE Student Contest Problem can also be adapted for individual or group simulation. A very simple simulation which I have used to introduce a guest lecturer in a course is shown in Figure 6. At first glance, it appears that nothing has changed. I have merely let the students know the topic for two lectures while I am out of town. The subtle simulation here introduces the students to the concept of professional development activities and to the role of government regulation in their profession. Their attitudes toward the lectures are modified, and their learning is enhanced.

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TO: Task Force 108A
FROM: W.B. Whiting, Vice President of Engineering
DATE: 26 February 1992
SUBJECT: Safety
CC:

Please read the attached article from the *Los Angeles Times* concerning new OSHA regulations. To prepare for these regulations, it is imperative that all Technocats engineers attend a special Professional Development Seminar on Monday, March 2, and Wednesday, March 4, 8:00—9:50 A.M., in Room 2444 of our headquarters. We have arranged for an outside expert in HAZOP (HAZard and OPerability study) to present these seminars. For Friday, March 6, you will perform a HAZOP on the reactor of our subsidiary XXX's Acrylic Acid Plant.

Our research department has found the attached article from *Plant Operations Progress* that should be of interest.

Attachments:

Los Angeles Times, "OSHA Issues Safety Rules to Avert Explosions at Petrochemical Plants," February 15, 1992, p. A5.

Kurland, J.J., and D.R. Bryant, "Shipboard Polymerization of Acrylic Acid," *Plant/Operations Progress,* **6**(4), 203 (1987).

Figure 6. *Announcement of guest lecturer*

I have sometimes videotaped more intricate simulations, with the class viewing and analyzing the simulation during the postmortem. Additional faculty, graduate students, and others (including our outside seminar speakers) are sometimes brought in to participate.

Design projects and laboratory experiments can easily be developed as simulations, but a good homework problem from any engineering course can be put into a real context. After preparation, students role-play the situation. Finally, class discussion can help students explore and understand the important relationships both within the subject matter and between it and the bigger picture.

CONCLUSIONS

Simulation is an ideal technique for improving student learning. These activities help students recognize connections between courses, the curriculum, and their profession. They exercise critical thinking skills and develop self-guided learning strategies. Simulation offers an opportunity to both broaden and deepen coverage while enhancing student learning.

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