A VIRTUAL UNIT OPERATIONS LABORATORY

Patrick J. Fleming, Michael E. Paulaitis
Johns Hopkins University • Baltimore, MD 21218

Chemical engineering students typically take a unit operations laboratory course and a capstone design course in their senior year. Experiments in the unit operations laboratory might focus on a practical design problem, while the design course is often based on a case study drawn from the experience of a practicing engineer. These courses are intended to confront students with problems that are not well-defined; problems that will be encountered in the complex "real world" of chemical engineering practice. The capstone design course, in particular, requires integration of basic science and engineering facts, theory, and quantitative problem-solving skills learned in the earlier years of the curriculum. The scope of these "real world" problems is, in most cases, limited by the traditional classroom or laboratory settings in which they are taught. Moreover, laboratory experiences that complement classroom instruction in other courses are the exception rather than the rule. A major constraint to developing new, innovative teaching laboratories that offer more practical engineering experiences to undergraduates is that operating and maintaining them is expensive in terms of manpower, space, and equipment.

In this paper, we describe a virtual laboratory now being created in the Department of Chemical Engineering at Johns Hopkins that features real-time dynamic simulations of each experiment in our undergraduate unit operations laboratory course. The overall goal of this virtual laboratory project is to enable our students to experience a broad range of design, scale-up (and even start-up) problems, normal and unusual operating conditions, and safety issues going well beyond the scope of experiences that could ever be contemplated in a traditional chemical engineering unit operations laboratory.

__Michael Paulaitis__ is Chair of the Department of Chemical Engineering at Johns Hopkins University. He holds degrees from Princeton University (BS, 1968), Stanford University (MS, 1970), and the University of Illinois (PhD, 1976). His research interests include chemical engineering thermodynamics, statistical/molecular thermodynamics, and molecular simulations.

__Patrick Fleming__ is Principal Research Scientist in the Department of Chemical Engineering at Johns Hopkins University. His BA (1969) is from Kalamazoo College and his PhD (1975) is from the University of Michigan. His research interests include simulation of protein interactions and solvation and protein folding.

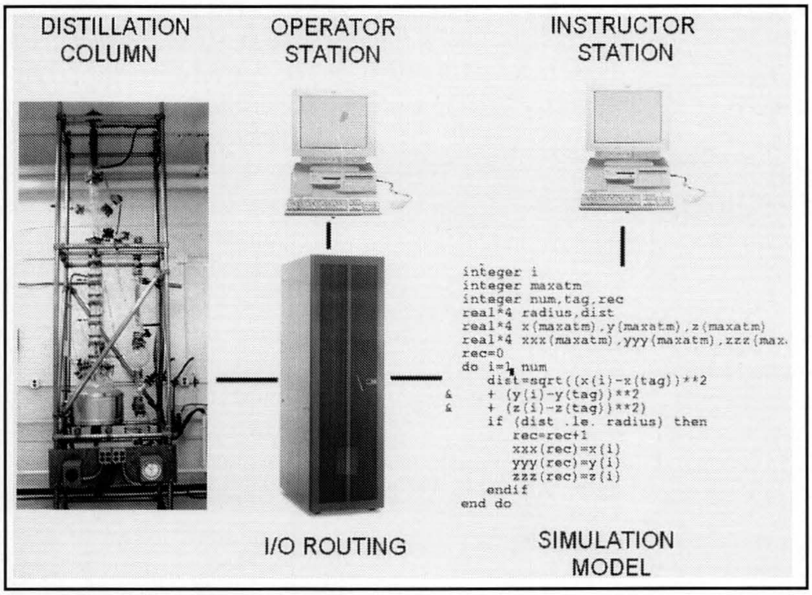
THE VIRTUAL LABORATORY

We have so far built, parameterized, and in-house tested a batch distillation column simulation model as the first experiment in the virtual laboratory. The simulation and process control software, provided by GSE Systems, Inc.,[1] is that used in the chemical, pharmaceutical, energy, process, and manufacturing industries (see Figure 1).

The software comprises a D/3 distributed control system (D/3 DCS™) with SimSuite Pro™ simulation software and runs on PC-level computers. The D/3 distributed control software permits display and control of any process communicating via analog or digital signal. SimSuite Pro is stand-alone software that is used to build, test, and run process simulation models dynamically and in real time. Additional Active X™-based software donated by GSE enables display of variable output, control panel, and process graphics inside a web browser. With these software modules we are able to control the pilot-scale distillation column now used in our chemical engineering unit operations laboratory, collect data from the column during an experiment, or simulate it in real time.

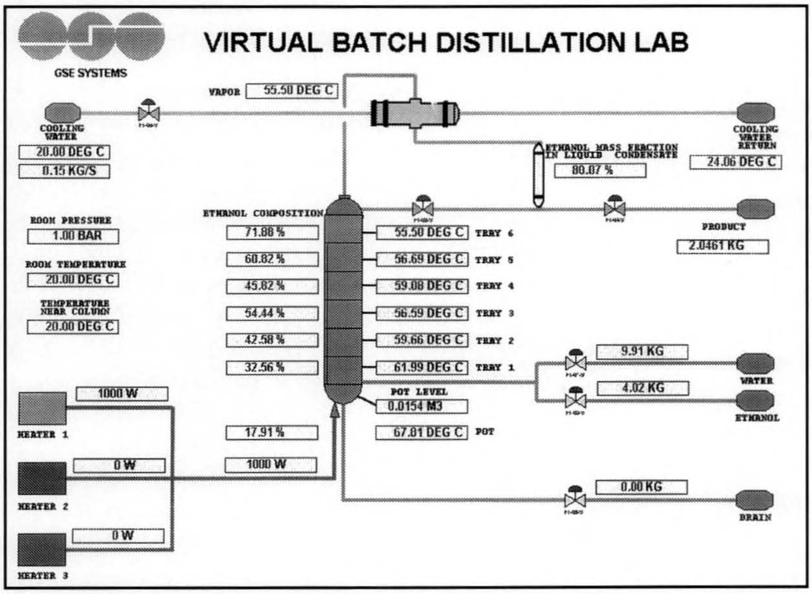
The actual column consists of six identical bubble cap trays, each fitted with a liquid sampling port and a copper-constantan thermocouple to measure the temperature of the entering vapor. The reboiler is a 20-liter vessel with variable electric heating. The total condenser at the top of the column is supplied with cooling water at 25°C and 30 psig. Reflux to the column is controlled by an electrically operated solenoid valve. During normal operations, this valve is in the "open" position when energized, and the liquid condensate is collected as product. In the event of electrical failure, gravity causes the valve to close such that all liquid condensate is returned to the column. The reflux ratio is controlled by a timer on the solenoid that periodically opens and closes the valve.

The distillation column simulation model is a computer program with graphic displays on an instructor's workstation and on an operator's console. It performs stagewise vapor-liquid equilibrium calculations based on tray pressure, mixture composition and enthalpy, and vapor-liquid traffic in the column. The model considers tray holdup, external heat transfer, and column geometry. It calculates in real time the temperature, vapor and liquid flow rates, enthalpies, and compositions for each tray. During equilibrium staged operations, the column is modeled by solving simultaneously component material and energy balances, and vapor-liquid equilibrium relationships using Wilson equation activity coefficients to account for thermodynamic non-idealities in the liquid phase.



```
integer i
integer maxatm
integer num,tag,rec
real*4 radius,dist
real*4 x(maxatm),y(maxatm),z(maxatm)
real*4 xxx(maxatm),yyy(maxatm),zzz(max.
rec=0
do i=1, num
   dist=sqrt((x(i)-x(tag))**2
&  + (y(i)-y(tag))**2
&  + (z(i)-z(tag))**2)
   if (dist .le. radius) then
      rec=rec+1
      xxx(rec)=x(i)
      yyy(rec)=y(i)
      zzz(rec)=z(i)
   endif
end do
```

Figure 1. *Configuration of process control and simulation modules for the distillation column experiment. The operator's station communicates with the simulator by means of a process control module that translates input/output signals to the appropriate format and display. The actual distillation column (or any other unit operations equipment) may also be controlled from the same operator's station by using a similar active display that is connected to the input/output addresses of components on the real equipment. The instructor's station may also control the simulation model or initiate malfunctions during the experiment.*



VAPOR 55.50 DEG C
COOLING WATER 20.00 DEG C
0.15 KG/S
ETHANOL MASS FRACTION IN LIQUID CONDENSATE 80.07 %
COOLING WATER RETURN 24.06 DEG C
ROOM PRESSURE 1.00 BAR
ROOM TEMPERATURE 20.00 DEG C
TEMPERATURE NEAR COLUMN 20.00 DEG C
ETHANOL COMPOSITION
71.88 %
60.82 %
45.82 %
54.44 %
42.58 %
32.56 %
17.91 %
1000 W
55.50 DEG C TRAY 6
56.69 DEG C TRAY 5
59.08 DEG C TRAY 4
56.59 DEG C TRAY 3
59.66 DEG C TRAY 2
61.99 DEG C TRAY 1
POT LEVEL 0.0154 M3
67.81 DEG C POT
PRODUCT 2.0461 KG
9.91 KG WATER
4.02 KG ETHANOL
0.00 KG DRAIN
HEATER 1 1000 W
HEATER 2 0 W
HEATER 3 0 W

Figure 2. *Active computer display seen by students during simulated operation of the distillation column.*

The simulation model was validated using temperature and composition data collected at each tray for ethanol-water mixtures in the actual distillation column. During transient regimes, it is modeled by allowing the stage efficiencies, Wilson equation parameters, and column heat losses to be functions of time. These functions were determined by tuning the model using data collected for ethanol-water mixtures in the actual column during transient operations. All the measurements were made by a team of Hopkins undergraduate chemical engineers as a summer project.

Flooding in the column, loss of cooling water, failed valves, or other malfunctions can be simulated from the instructor's station of the virtual laboratory. During development, the station is used to tune the running model, and during a virtual distillation experiment, it is used to set initial conditions, control model execution, and insert interventions, such as malfunctions. The system is capable of maintaining up to 100 different initial conditions: values for all process variables, remote functions, and malfunctions.

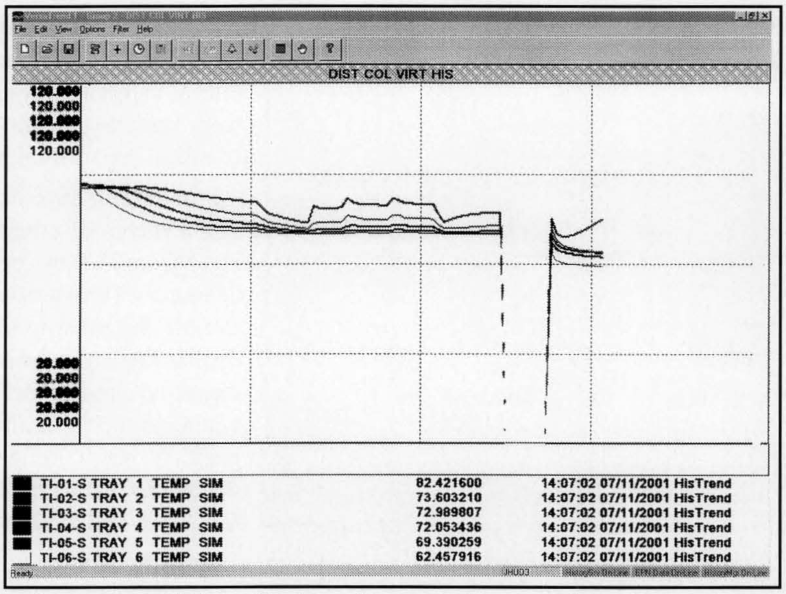
The simulation model exists not only as a computer program running in the background but is also experienced by the students as an on-screen graphic image depicting a distillation apparatus. Stream flows, temperatures, liquid compositions, and volumes are displayed in real time (see Figure 2). Operation of the distillation process is controlled by students from the screen by mouse-clicking on the various components. Students enter their choice of operating parameters such as heating current or valve openings or closings. The same graphic image may be used to monitor and control the actual distillation column. In principal, the student need not know if the virtual or actual distillation process is connected to the display, although in practice the virtual process provides more on-screen information such as tray compositions.

Data on many process variables is continuously collected and may be viewed in real time (see Figure 3) or downloaded to a spreadsheet program for later analysis.

CURRICULUM IMPLEMENTATION

The distillation simulation model was used for the first time during the 2000/01 academic year in two chemical engineering courses: Chemical Engineering Process Design and Separations Processes. The latter is a junior-year chemical engineering core course taught in the Spring semester. Chemical Engineering Process Design is taken by seniors in the same semester. In the previous (Fall) semester the seniors normally have taken Unit Operations laboratory. Batch distillation is a required experiment in this laboratory course, and the students are required to design and then carry out experiments to characterize the actual batch distillation column.

The context and motivation for the experiment is to train personnel with limited technical backgrounds to separate several liquid solvent mixtures using the actual pilot-scale batch distillation column to accomplish the task. The first objective is to decide what data needs to be collected to accurately characterize the column. As a team, the students identify tray efficiencies as the key information they need and carry out McCabe-Thiele analyses to get this information from the measured tray temperatures and compositions. The students are also required to select a suitable "model" system (ethanol/water is selected in the end), specify the operating conditions for the distillation of this mixture, determine startup and shutdown procedures, etc. They also consider safety, cost, and environmental impact.



```
TI-01-S TRAY 1 TEMP SIM     82.421600     14:07:02 07/11/2001 HisTrend
TI-02-S TRAY 2 TEMP SIM     73.603210     14:07:02 07/11/2001 HisTrend
TI-03-S TRAY 3 TEMP SIM     72.989807     14:07:02 07/11/2001 HisTrend
TI-04-S TRAY 4 TEMP SIM     72.053436     14:07:02 07/11/2001 HisTrend
TI-05-S TRAY 5 TEMP SIM     69.390259     14:07:02 07/11/2001 HisTrend
TI-06-S TRAY 6 TEMP SIM     62.457916     14:07:02 07/11/2001 HisTrend
```

Figure 3. *Real-time display of tray temperature data during simulated operation of the distillation column. Note the abrupt changes in temperature in all trays signifying a recharging of the reboiler.*

Once the actual distillation column has been characterized, the students move on to another experiment in the unit operations laboratory. The stated overall objective to train unskilled personnel to use the equipment to separate other solvent mixtures is never met or even considered beyond motivating the original experiments. With the ability to carry out essentially an unlimited variety of separations using the virtual distillation column, it is now straightforward to ask the students to run the virtual column to complete the overall objective of the experiment.

We implemented this "mini-design" project in Chemical Engineering Process Design using a problem-based learning approach.[2] Teams of senior chemical engineers who were now familiar with operating the actual distillation column were given the assignment of repeating the experiment using the simulation model. Each team of three seniors was introduced to the distillation simulation model during an initial two-hour session in which they operated the simulation according to prescribed instructions contained in a tutorial developed for the mini-design project of one of the authors (PJF).

During the second session, the students operated the virtual column independently. They charged the column pot with an ethanol/water mixture, brought the column to equilibration, and gathered data on the temperature and composition of each tray. For the third session, each team was given a virtual column with a different binary mixture, listed in Table 1. Their task was to determine the optimal operating parameters for performing a single batch distillation enrichment of the mixture and to prepare a training program and manual to teach inexperienced operators how to carry out the specific separation. Although guidelines on size and format were provided, each team could decide what the best content of such a training manual would be.

The juniors in the Separations Processes course served as the untrained personnel in this project. The timing of their involvement was coordinated such that they were just completing course work on the fundamentals of distillation. Teams of three juniors were paired with the senior teams for this training session. After a short oral presentation by the seniors, the junior operators carried out the batch distillation of their particular binary mixture according to the training manual written by the senior team. After the juniors became familiar with the column operation, the seniors were encouraged to introduce various malfunctions and the juniors were prompted to analyze the problem from displayed process variables and perform corrective actions in real time. One typical malfunction was a failure of the cooling water flow. This failure could be announced by an alarm (if desired by the instructor) or observed on the graphic display as a change in the flow rate of cooling water or an increase in the temperature of the cooling water return. The students usually come to the conclusion that the best corrective procedure is to turn off the heating coils immediately. Malfunctions were also introduced inadvertently. For example, one team accidentally opened the drain valve on the reboiler and quickly drained all of a noxious mixture out of the pot! The versatility of the virtual laboratory allowed us to explore the safety ramifications of this virtual accident, thus providing an educational opportunity that never would have occurred in the actual laboratory experiment.

One of the great advantages of the virtual column is the ability to speed up process clock time by as much as a factor of 10. Thus, instead of waiting hours for the column to reach steady state from a cold start, the start-up can be shortened to minutes. This accelerated process time encourages the students to carry out "what if" experiments that could never be contemplated with the actual distillation column.

Each team (seniors and juniors separately) were required to give oral presentations of their results and to prepare written reports. The seniors were present for the junior team presentations to ask questions. In both oral presentations, the students were asked to describe what they learned during the training session from the perspective of either trainers or trainees. The combination of problem solving, group interaction and delegation of teaching/learning responsibility uses many of the elements described by Wankat for efficient effective teaching.[3]

TABLE 1
Binary Mixtures for Distillation Experiments

Mixture	*Boiling Points (°C)*	*MSDS Remarks*
Acetone/Water	56/100	Extremely Flammable
Acetone/Isopropanol	56/82	Extremely Flammable
Benzene/Ethanol	80/79	Carcinogenic, Azeotrope
Heptane/Toluene	98/110	Extremely Flammable
Isopropanol/Water	80/100	Flammable, Azeotrope
Methanol/Water	65/100	Flammable
Methylene Chloride /Ethylene Chloride	40/83	Flammable, Extremely Toxic

In their written evaluations of the project, the seniors were unanimous in their opinion that the opportunity to separate different mixtures and to explore various operating conditions in the virtual column, which they could not do in the unit operations laboratory, allowed them to gain a deeper understanding of distillation. The juniors, in their written evaluations, indicated that the project provided them with a perspective of distillation that went well beyond the fundamentals they learned in the classroom.

To evaluate the continuing impact of this junior-level exposure to virtual distillation experiment, we gave a written survey to the juniors after they had taken the senior unit operations laboratory course and performed the actual distillation experiment. This survey was designed in the format of the Student Assessment of Learning Gains instrument available at the National Institute for Science Education.[4] We asked the students to rank a list of classroom aspects on a five-category scale from "No Help" (1) to "Very Much Help" (5). The questions addressed the value of: a) working in groups; b) hands-on control of simulation; c) the written lab manual; d) verbal instruction by seniors; e) final presentation report; f) impact of virtual lab on real lab. The average scores for the first five aspects (a through e) of the virtual lab were between 2.8 and 3.0 (a little to moderate help); the average score for the last question on the impact of the virtual lab was 3.4 (moderate to much help). Verbal comments from the students that correlate with this high level of impact indicated that their virtual experience instilled more confidence in performing the actual experiment.

It is important to point out that computer simulations such as those described here are not meant to supplant existing real laboratory experiments, but rather to complement them. As stated previously,[5] neither the virtual nor the real laboratory format is "better"—rather, they have different roles in the curriculum. We have used the virtual experiment as a tool to integrate efficient, effective teaching elements[3] into our curriculum. In designing the virtual laboratory experiments, we recognize a key responsibility is to ensure that students continue to have actual hands-on experience with an actual process or device.

FUTURE

A major goal for the coming year is to make the virtual distillation experiment web-accessible and to create and evaluate virtual laboratory experiments in partnership with several other universities. We also plan to introduce the virtual laboratory in a local high school. We intend to design and evaluate several specific experiments and educational modules around the virtual batch distillation column simulation and use them as templates for a much larger effort to develop a variety of virtual experiments maintained by faculty at other universities. Web-accessibility of virtual experiments has the potential to give chemical engineering students at many educational institutions access to specialized virtual experiments that can complement existing laboratory curricula. Our "mini-design" project demonstrated the important element vertical integration to other courses in the undergraduate chemical engineering curriculum.

ACKNOWLEDGMENTS

The authors gratefully acknowledge support from the Special Grant Program in the Chemical Sciences, the Camille and Henry Dreyfus Foundation, and computer software, hardware, and training from GSE Systems, Inc., Columbia, Maryland 21045. The efforts of undergraduate students Robin Cohen, Elizabeth Chambers, Gabe Farkas, and Austin Lin are also greatly appreciated. We thank Professor Joseph Katz for help with the actual distillation column operation.

REFERENCES

1. <www.gses.com> GSE Systems, Inc., is a leading global provider of dynamic simulation and process control systems to the chemical, pharmaceutical, energy, process, and manufacturing industries
2. Woods, D.R., *Problem-Based Learning: How to Gain the Most from Problem-Based Learning,* Hamilton, Ontario, Canada (1994)
3. Wankat, P.C., "Effective, Efficient Teaching," *Chem. Eng. Ed.,* **35**(2), p. 92 (2001)
4. <www.wcer.wisc.edu/nise/>
5. White, S.R., and G.M. Bodner, "Evaluation of Computer-Simulation Experiments in a Senior-Level Capstone ChE Course," *Chem. Eng. Ed.,* **35**(1), p. 34 (1999) ❐