The Virtual Chemical Engineering Unit Operations Laboratory

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Abstract

There appears to be a growing trend in the chemical process industry (CPI) to reduce the dependency on pilot-plant studies by increasing the use of computer process modeling. For the CPI, this approach is reliable, safe, and cost effective. In the traditional pedagogy of unit operations laboratory, students are required to conduct experiments on lab-scale equipment. This practice may lead to a mismatch between the student's learning experience and later employment expectations. Therefore, while the traditional unit operations laboratory ought to remain an integral part of the chemical engineering curriculum, the instructional material should be modified to adapt to the increasing use of information technology in the chemical process industries. It is expected that with an increase in the authenticity and reliability of this form of pedagogy, student learning will be enhanced. A simultaneous benefit is a reduction in the financial burden associated with purchasing and maintaining expensive physical laboratory equipment and supplies.

To address this adaptation, we are developing a *virtual unit operations laboratory*. The pedagogical format includes the following.

(1)The partial replacement of selected lab-scale physical unit operations experiments with computer visualization of data from full-scale, industrial chemical processes. Using the process simulator, *CHEMCAD™*, which contains both steady state and dynamic unit operations models, we demonstrate the separation of mixture of organic acids using multiple distillation columns in series. The module simulates an actual separation train at the Celanese plant in Pampa, TX. We obtain excellent agreement with the archival data donated by Celanese. We also explore process conditions and alternative designs with the module, as would be done in an industrial process engineering department.

(2)Virtual analogs to the lab scale unit operations experiments of heat exchange, mass transfer, and humidification. Using *LabVIEW* software, we have developed a realistic control room interface overlaying a mathematical model of the unit operation. The student conducts the virtual experiment in the same fashion as the physical experiment.

In the fall of 2002, we conducted an experiment in the Unit Operations class designed to elucidate the impact of virtual experiments upon student learning. The TTU College of Education is now conducting the assessment. In this presentation, we demonstrate our virtual experiments and results of the assessment. We then recommend to what extent physical experiments can be replaced with virtual experiments without compromising student learning.

Introduction

The unit operations laboratory Texas Tech University is employed to reinforce to senior chemical engineering students the basic chemical engineering principles associated with various pieces of equipment. The unit operations laboratory is also used to familiarize the students with the safety concerns regarding each piece of equipment and about operational issues. The equipment used is comparable to pilot-scale units of industrial laboratories. The major pieces of equipment used in this project include a double-pipe heat exchanger, an ammonia gas-absorber packed column, and a cooling tower.

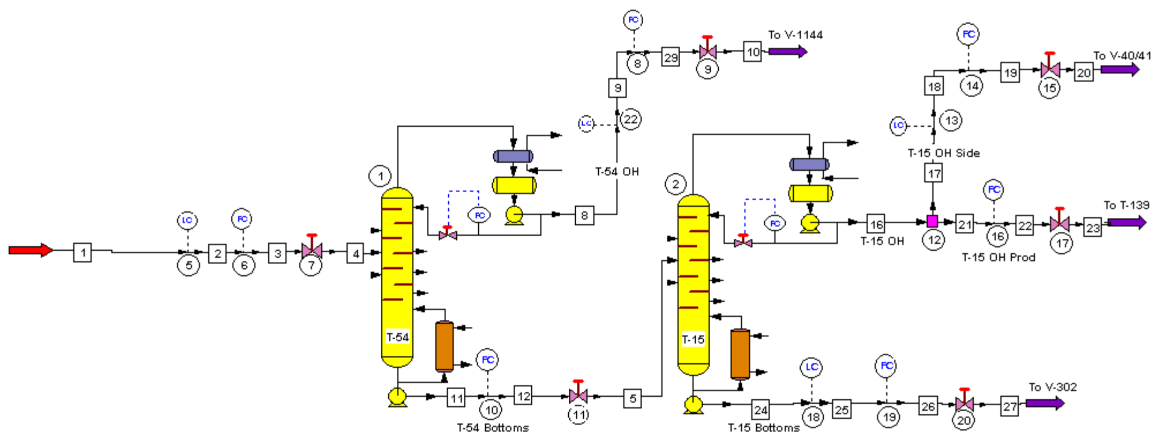

Figure 1 Flowsheet Simulation of Celanese Towers T-54 and T-15.

With greater computational power, more costly pilot scale equipment, safety concerns and human resource allocation, the chemical process industries (CPI) are leading toward computer-based simulations rather than the traditional pilot-scale experiments. With this in mind, the unit operations laboratory at Texas Tech University is emulating the industrial switch, by producing computer-generated simulations based upon mathematical models for the pieces of equipment in the laboratory as well as a simulation for distillation columns found at the Celanese plant in Pampa, TX. This new Virtual Unit Operations Laboratory (VUOL) will be used to complement the existing laboratory in order to give the students realistic experience of industrial operations. Most of the time, the engineer will be working from a control room, or at least from behind a computer screen, very rarely will an engineer be out in the field adjusting valves and flow rates and temperatures, etc.; all of that is done using the computer interfaces of distributed control systems. The computer interfaces of the VUOL will give the students experience of controlling the equipment via the computer in addition to physically turning valves and checking temperatures.

Methods

For the distillation column experiment, the towers were simulated in CHEMCAD™ software (figure 1). Each tower initially had the parameters supplied by Celanese in Pampa, TX (figure 2).

Figure 2 – Organic Acid Separation Train, Celanese, Pampa, TX

Modification of these parameters was performed until the tower outputs matched the output expected according to the data provided by Celanese. The students used the benchmarked simulator to investigate the control of distillation towers. They tuned PI controllers based upon steady state, open loop, and closed loop responses.

With regard to the pilot-scale experiments (heat exchangers, cooling tower, and gas absorber), interfaces were created in LabVIEW resembling those interfaces used in industry for pieces of equipment are used for the virtual unit-operations laboratory. i.e. the double-pipe heat exchanger, the ammonia gas absorber, and the cooling tower. The pictures are drawn in AutoCAD 2002 and show an actual portrayal of the pieces of equipment. However, they are not drawn to scale.

The interface for the double-pipe heat exchanger is illustrated in figure 3. It is completely interactive. The user is able to alter the hot and cold-water flow rates, as well as the temperatures of those streams. When actually conducting the physical experiment, these parameters are adjustable. Another parameter that can be changed is the direction of flow, meaning the flow mode can be either countercurrent or cocurrent.

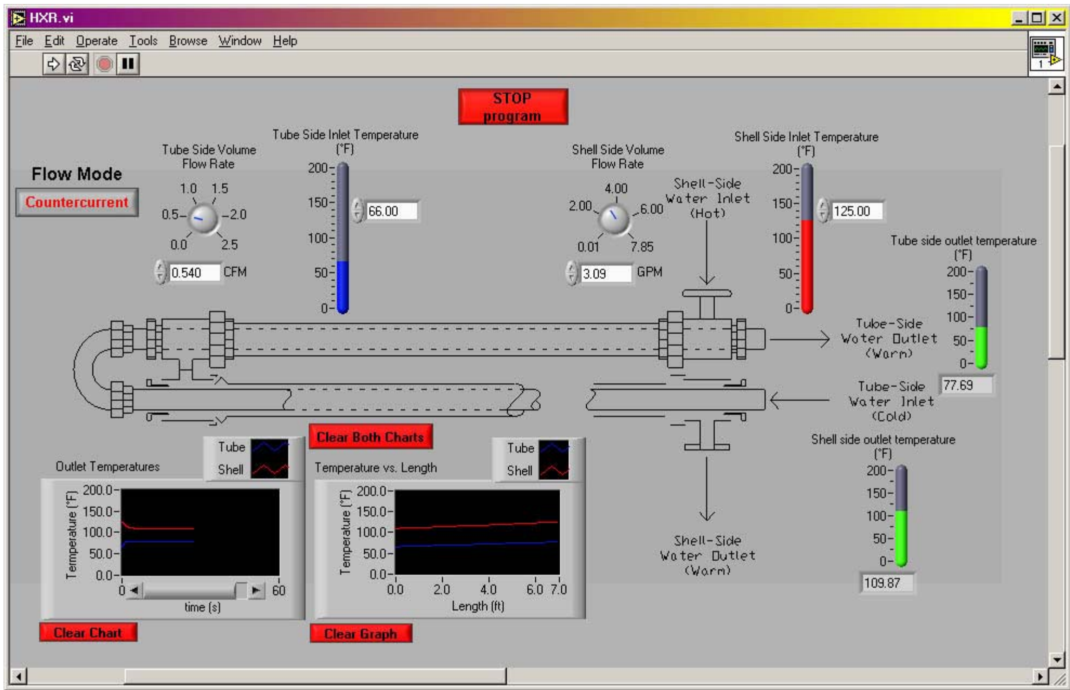

Figure 3 – Virtual Heat Exchanger Interface

To make the interface more accurate to the physical experiment, the shell-side flow rate is measured in cubic feet per minute (GPM) and the tube-side flow rate is measured in gallons per minute (CFM) since that is how they are measured physically. Also, either the shell or the tube-side can be used for the hot or cold water.

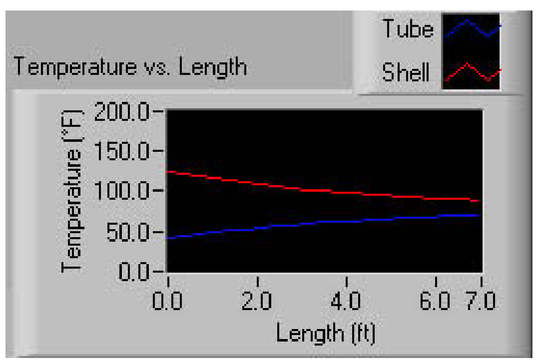

Figure 4 Steady State Temperature Profile in Virtual Heat Exchanger.

The interface also has one chart and one graph. The chart shows the outlet temperatures of both the shell and tube sides progressing with time. These values change until the system reaches a steady state, a change in an inlet temperature will affect both the outlet temperatures. The magnitude of the change is dependent on both the inlet temperatures and both the shell and tube-side flowrates. The graph, however, shows the temperature profile along the length of the exchanger for both tube and shell-side. With a countercurrent flow mode, this graph has two parallel lines, as in figure 3, along the length of the exchanger. In a cocurrent flow mode, this graph as two lines that converge toward the steady state temperature, as shown in figure 4. In both the physical and virtual versions of the heat exchanger, the students vary the shell-side flow rate, and compare the resulting Nusselt numbers as a function of Reynolds number with the Sieder-Tate correlation.

The ammonia gas absorber also has a completely interactive interface (figure 5). The user can change the flow parameters of the water flow as well as the ammonia and airflows. Using calibration data taken from the actual physical experiment, the dials on the interface match those of the actual rotameters found in the lab. This enables the student to emulate using the actual laboratory experiment. The gas absorber interface also has two graphs and a chart. The graphs show the ammonia compositions of the liquid and gas along the height of the column, and the chart shows the ammonia compositions in the exiting liquid and gas. As with the heat exchanger, the same experiment was conducted on both the virtual and physical versions of the gas absorber. The students determined the height of a transfer unit (*HTU*) the number of transfer units (*NTU*) the overall mass transfer coefficient based upon the vapor phase (K_ya), and the overall column efficiency (η) as functions of the liquid to gas ratio (*L/G*).

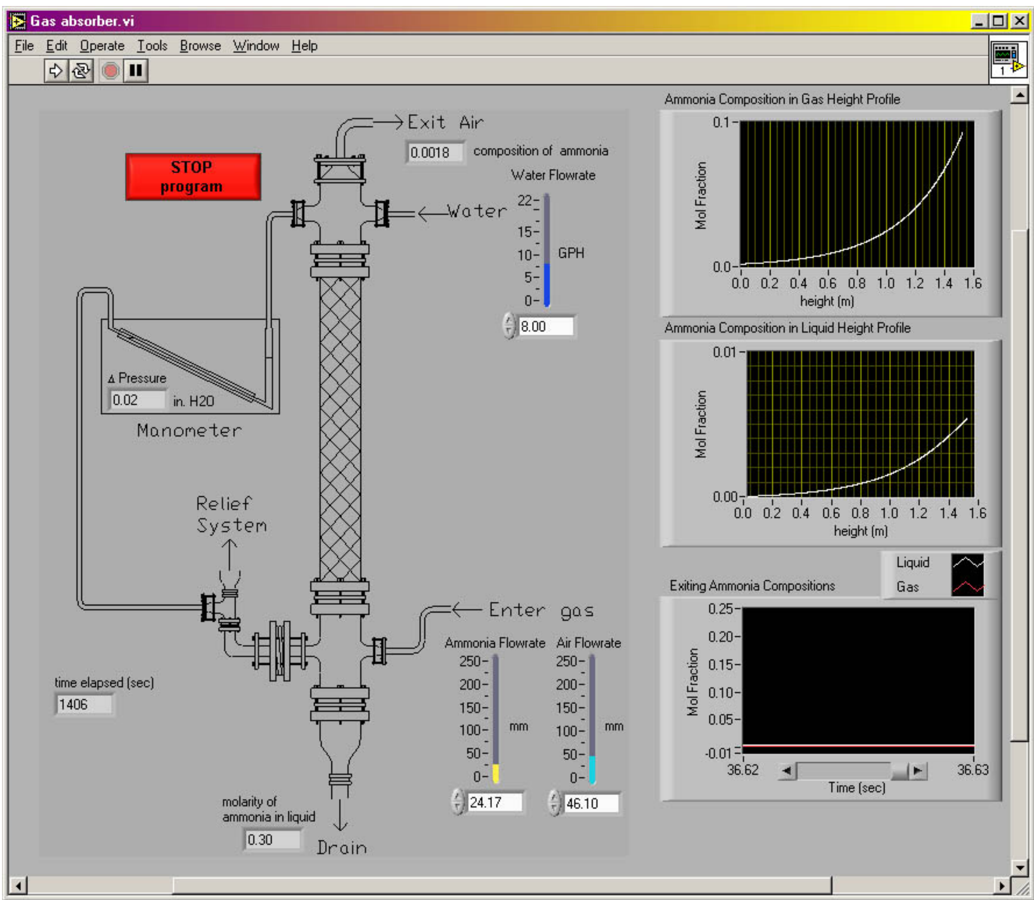

Figure 5 – Virtual Gas Absorber Interface

The cooling tower interface (figure 6), similar to the heat exchanger and the gas absorber, is also completely interactive. This interface uses the inlet air wet and dry bulb temperatures, fan speed, and the temperature and flow of inlet water, to determine the outlet temperatures of the water and air. The students determined the heat transfer coefficient, mass transfer coefficient, and the height of a transfer unit, as a function of inlet liquid flow rate

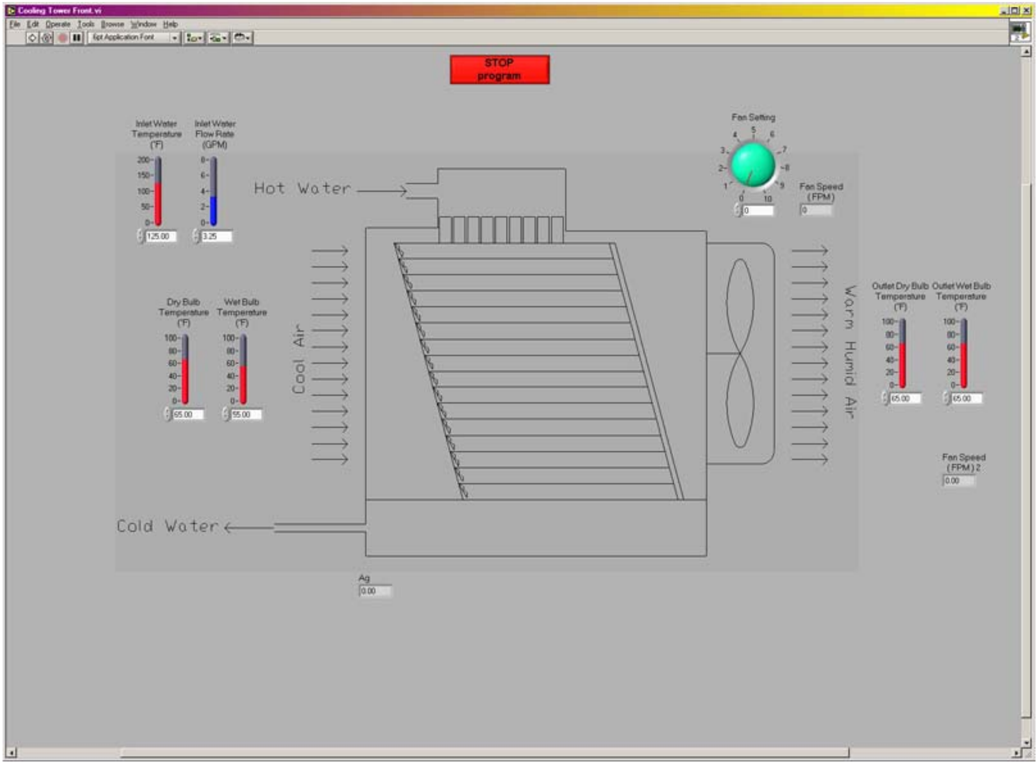

Figure 6- Virtual Cooling Tower Interface

The models for the pilot-scale experiments were developed from unsteady mass and energy balances. These were then discretized into recurrence formulae in the time dimension to provide and open-ended simulation. By way of example, we illustrate the mathematical treatment of the double pipe heat exchanger. The governing equations for this experiment are given in equations (1) and (2)[3].

$$\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial z} = \frac{4U}{\rho C_p D_1}\left(T_s - T\right) \qquad \text{(tube-side)} \qquad (1)$$

$$\frac{\partial T_s}{\partial t} + \operatorname{sgn} v_s \frac{\partial T_s}{\partial z} = \frac{4 D_1 U}{\rho_s C_{ps}\left(D_2^2 - D_1^2\right)}\left(T - T_s\right) \qquad \text{(shell-side)} \qquad (2)$$

The exchanger is subject to the following initial and boundary conditions.

$$\begin{aligned} &T(z,0) = T_0(z) \\ &T_s(z,0) = T_{s0}(z) \\ &T(0,t) = T_{inlet}(t) \\ &T_s(0,t) = T_{s,inlet}(t) \qquad \text{cocurrent} \\ &T_s(L,t) = T_{s,inlet}(t) \qquad \text{countercurrent} \end{aligned} \qquad (3)$$

T is the tube side temperature, *t* is time, and *v* is the tube side velocity averaged across the cross-section. *z* is the distance along the exchanger, *U* is the overall heat transfer coefficient, and D_1 is the diameter of the inner tube. T_s is the shell side temperature. ρ and C_p are the density and the heat capacity of the tube side fluid. The subscript *s* indicates properties of the shell side fluid. The subscript *0* indicates initial conditions. *sgn* = +1 or -1, indicating cocurrent or countercurrent flow respectively. *L* is the length of the exchanger.

We now introduce the following dimensionless variables and multiply by *L/v*.

$$\text{dimensionless time} \quad \tau = \frac{tv}{L} \tag{4}$$

$$\text{dimensionless exchanger length} \quad Z = \frac{z}{L} \tag{5}$$

$$\text{dimensionless tube-side temperature} \quad \theta = \frac{T - T_{inlet}}{T_{s,inlet} - T_{inlet}} \tag{6}$$

$$\text{dimensionless shell-side temperature} \quad \theta_s = \frac{T_s - T_{inlet}}{T_{s,inlet} - T_{inlet}} \tag{7}$$

The non-dimensionalized energy balances produce a pair of partial differential equations (PDEs) (equations (8) and (9))

$$\frac{\partial \theta}{\partial \tau} + \frac{\partial \theta}{\partial Z} = a \cdot (\theta_s - \theta) \tag{8}$$

and

$$\frac{\partial \theta_s}{\partial \tau} \pm \gamma \cdot \frac{\partial \theta_s}{\partial Z} = a_s \cdot (\theta - \theta_s) \tag{9}$$

The dimensionless initial and boundary conditions become equations (10).

$$\begin{aligned} &\theta(Z,0) = \theta_0(Z) \\ &\theta_s(Z,0) = \theta_{s0}(Z) \\ &\theta(0,\tau) = 0 \\ &\theta_s(0,\tau) = 1 \qquad \text{cocurrent flow} \\ &\theta_s(1,\tau) = 1 \qquad \text{countercurrent flow} \end{aligned} \tag{10}$$

The quantities a, a_s, and γ are lumped parameters.

$$\begin{aligned} a &= \frac{4U}{\rho C_p D_1} \cdot \frac{L}{v} \\ a_s &= \frac{4 D_1 U}{\rho_s C_{ps} \left(D_2^2 - D_1^2 \right)} \cdot \frac{L}{v} \\ \gamma &= \frac{v_s}{v} \end{aligned} \tag{11}$$

We employ Lax's modification to the FTCS method (forward in time, centered in space) to numerically discretize and solve the system of PDEs [2].

$$\frac{\partial f}{\partial \tau} \cong \frac{f_{i+1,j} - \frac{1}{2}(f_{i,j+1} + f_{i,j-1})}{\Delta \tau} \tag{12}$$

$$\frac{\partial f}{\partial Z} \cong \frac{f_{i,j+1} - f_{i,j-1}}{2\Delta Z} \tag{13}$$

The index *i* denotes time, and *j* denotes space. Returning again to the heat exchanger example, the discretized forms of the PDEs become:

$$\theta_{i,j+1} \approx \frac{1}{2}(1+c)\cdot\theta_{i-1,j} + \frac{1}{2}(1-c)\cdot\theta_{i+1,j} + \alpha\cdot\left(\theta_{s_{i,j}} - \theta_{i,j}\right) \quad (14)$$

$$\theta_{s_{i,j+1}} \approx \frac{1}{2}(1+\text{sgn}\cdot c_s)\cdot\theta_{s_{i-1,j}} + \frac{1}{2}(1-\text{sgn}\cdot c_s)\cdot\theta_{s_{i+1,j}} + \alpha_s\cdot\left(\theta_{i,j} - \theta_{s_{i,j}}\right) \quad (15)$$

The quantities c and c_s are the Courant numbers for the two sides of the unit operation, and a and a_s are the dimensionless lumped parameters. The composition of these 4 quantities are given as follows.

$$\begin{aligned} c &= \frac{v\Delta t}{\Delta z} = \frac{\Delta\tau}{\Delta Z}, \qquad c_s = \frac{v_s\Delta t}{\Delta z} = \frac{v_s}{v}\frac{v\Delta t/L}{\Delta z/L} = \frac{\gamma\Delta\tau}{\Delta Z} \\ \alpha &= \frac{4U\Delta\tau}{\rho C_p D_1}\frac{L}{v} = a\Delta\tau, \quad \alpha_s = \frac{4UD_1\Delta\tau}{\rho_s C_{ps}\left(D_2^2 - D_1^2\right)}\frac{L}{v} = a_s\Delta\tau \end{aligned} \quad (16)$$

We performed similar procedures utilizing ammonia balances on the gas and liquid phases of the gas absorber[3], and energy balances on the air and water phases of the cooling tower[1]. Interestingly and conveniently, the dimensionless models for all three experiments have the same generic form as equations (8) and (9). Thus we obtained recurrence formulae in the time dimension similar to equations (14) and (15) for the absorber and cooling tower as well.

Assessment

The knowledge and skills we expect the students to acquire in our unit operations laboratory are 1) the understanding and the ability to operate the unit operations of gas absorption, heat transfer, humidification, and distillation, 2) ability to conduct a Hazard and Operability Analysis (HAZOP), and 3) ability to scale pilot data to industrial levels. These are the specific chemical engineering skills we require, in addition to which we require competence in ABET criteria a)-k).

To acquire the aforementioned knowledge and skills, each student performed 2 physical and 2 virtual experiments. Which students performed the virtual versions of a particular experiment was varied systematically among the class so that we could assess the differential impact of virtual experiments upon student learning.

We are assessing the outcome of these experiments using 3 sources of information collected in the fall of 2002. The first source is the oral presentations each student had to make to the class as a whole. The presentations were jointly given by two students, one who had conducted the physical version of the experiment, and one who had conducted the virtual version of the experiment. The students were asked to assess the strengths and weaknesses of both types of experiments and recommend to what extent computer simulation should be used in the unit operations laboratory. The second source is a comprehensive exam over the course. On each experiment, 8 questions were asked regarding theory, safety, data collection, and data analysis. We will compare the scores obtained by those who conducted the virtual versions of the experiment with those obtained by those who performed the physical versions. The third source was a questionnaire anonymously answered by students regarding how the ABET a)-k) criteria were met. The assessment is being conducted by the Texas Tech University College of Education.

Preliminary Results

To date we have examined the two of the 3 data sources: 1) the recommendations of the students in their oral presentations, and 2) the results of the ABET questionnaire. Of 12 presentation teams, 9 recommended a combination of physical and virtual experiments, and 3 recommended a purely physical lab. No teams recommended a completely physical lab.

With regard to the effect of virtual learning upon ABET a-k criteria, we compared how the 2002 class as a whole perceived their learning in these areas to the perceptions of the 2001 class. The 2001 class did not conduct virtual experiments, while the 2002 class did conduct virtual experiments. Students were asked "To what degree did your education contribute to your learning and development in the following areas". The students then assigned a numerical value to each of 20 questions about ABET a-k criteria. The results are given below in Table 1.

Table 1: Student Perceptions of Meeting ABET Criteria-with and without Virtual Experiments.

		Fall 2001 (without VUOL)	Fall 2002 (with VUOL)
Question: To what degree did your education contribute to your learning and development in the following areas?	ABET a-k	Average Rating Mean ± SD N=25	Average Rating Mean ± SD N=24
Fundamental knowledge of ChE principles	a	4.7 ±1.0	4.6 ±0.6
Mathematical Skills	a	4.2 ±1.0	4.4 ±0.8
Ability to design and conduct experiments	b	4.7 ±0.7	4.6 ±0.7
Ability to analyze and interpret data	b	4.7 ±0.8	4.9 ±0.5
Ability to design systems and components as needed	c	4.3 ±0.8	4.0 ±1.1
Ability to work well in diverse or multidisciplinary teams	d	4.7 ±0.8	4.6 ±0.8
Leadership abilities	d	4.6 ±0.7	4.3 ±.06
Ability to work independently	e	3.3 ±1.0	3.7 ±1.1
Self confidence	e	4.0 ±0.9	4.1 ±0.7
Problem-solving Skills	e	4.5 ±1.0	4.7 ±0.6
Creative Thinking	e	4.1 ±1.1	4.6 ±0.7
Critical Judgment	e	4.3 ±0.8	4.6 ±0.7
Appreciation of professional behavior	f	4.5 ±0.9	3.4 ±0.7
Appreciation of ethical behavior in engineering	f	4.3 ±0.9	4.4 ±0.9
Writing Skills	g	4.8 ±0.7	4.8 ±0.5
Speaking Skills	g	2.6 ±1.1	4.3 ±0.7
Ability to learn on your own	i	3.6 ±0.7	4.0 ±1.0
Understanding of contemporary issues in science and technology	j	3.8 ±1.2	4.0 ±1.0
Awareness of the political and societal context of engineering	h	3.7 ±0.9	4.0 ±1.0
Computing Skills	k	4.4 ±0.9	4.8 ±0.5

The adjectival description of the numerical values is given in Table 2.

Table 2: Legend to Table 1

Key	Adjectival Description
0.0-1.9	Not at all
2.0-2.9	Somewhat
3.0-3.9	Considerably
4.0-5.0	A great deal

Two results are apparent from the results in Table 1. The first is that, in both terms, the students felt that the class contributed either a *great deal* or *considerably* in all areas of ABET criteria a-k. The second result is that there is no significant difference in the student perception to their learning in 18 out of 20 areas, either in the presence or absence of virtual unit operations experiments. The only 2 areas which display significant differences between the control and experimental groups are “Speaking Skills” and “Appreciation of Professional Behavior”. The perception without virtual experiments is lower in the former area. The difference is attributable to the fact that oral presentations were not required in the class in the Fall of 2001. The perception of learning in the area of professional behavior is lower in the presence of virtual experiments. The source of this difference is not known, but is likely attributable to differing emphases by the two different instructors for each term, and not to the mode in which the experiments were conducted.

As of this writing, the analysis and interpretation of the scores on the comprehensive exam is not complete. It will be interesting to see how learning of the concepts of unit operations is impacted by the use of virtual experiments.

Discussion

Although the assessment is not complete, it already seems apparent that a total virtual unit operations laboratory would not be welcome to the students. On the other hand, preliminary results indicate that the use of some virtual experimentation does not adversely affect student learning in generic engineering skill sets. Virtual and physical experiments could complement each other and thus could be done together to enhance student learning. With the physical portion of the lab, students will get a feel for what the equipment looks and feels like, as well as how it operates. With the virtual portion, the students will become familiar with the computer interfaces that are similar to industrial control rooms, and learn to manipulate the equipment via those controls instead of manually turning valves and knobs. They can also explore operating scenarios which are not easily or economically investigated with physical equipment. A powerful capability added by virtual experiments is the ability to use simulation to plan which laboratory experiments would be most useful to meet the goals of a lesson..

Summary

With the two labs complementing each other, the unit operations laboratory would be highly beneficial to the students by teaching both the physical and computer based portions. The students who graduate from these classes will have a better understanding of industry as well as the equipment used in industry.

Acknowledgments

This work is supported by a Special Grant in the Chemical Sciences from the Camille and Henry Dreyfus Foundation, fund number SG-01-090. And also, we would like to thank R.M. Bethea, Ph.D., P.E. for his work done in the unit operations laboratory during the fall of 2001.

References

1. Al Nimr MA. 1998. Dynamic thermal behaviour of cooling towers. *Energy Conversion and Management.* 39(7):631-636.

2. Pozrikidis C. 1998. *Numerical Computation in Science and Engineering.* New York. Oxford University Press. pp. 555-567.

3. Schiesser W, Silebi CA. 1997. *Computational Transport Phenomena.* Cambridge, UK. Cambridge University Press. pp. 289-329.