TEACHING TIP: ELEVATOR TALKS

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Both industry and ABET require that engineering graduates can communicate. Clearly the best way to achieve this is to have frequent assignments throughout the curriculum requiring writing and oral presentations. Unfortunately, oral presentations tend to require a significant amount of class time. An alternative oral presentation is the “elevator talk.” The scenario: a student steps into an elevator with someone she needs to persuade or sell. For example, the student may want to convince the person to hire her. She has from one to two minutes to do this.

I assigned the topic to the students (ask for a job), gave them the time (two minutes), gave them a copy of the scoring rubric (Table 1), and told them to prepare a talk that they will present extemporaneously, without visuals. There was no written assignment. In class, I assigned the “boss” for each person. Students were told to assume that they knew the boss well enough to talk to. Presenters and bosses went to the front of the room and stood in the elevator. Talks were timed for a strict two minutes. Since two minutes is actually fairly long, most students finished early and had to do something—perhaps just stand there—for the remaining time. If they weren’t finished at two

minutes, the elevator door opened anyway and they had to summarize very quickly.

The students saw the relevance of elevator talks and were well prepared. Grading the talks with the scoring rubric was straightforward and I was able to finish the grading while the next pair walked to the front. Since it takes less than 30 seconds to change speakers, 20 two-minute talks can be done in a 50-minute period.

While not eliminating the need for more formal presentations, elevator talks can provide an easy way to include oral communication in courses that normally would not have time. Grading all of the talks with the scoring rubric and then saving copies provides evidence for ABET that all students have been assessed and can do oral presentations, at least at the barely acceptable level.

REFERENCES

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Author Guidelines for the LABORATORY Feature

The laboratory experience in chemical engineering education has long been an integral part of our curricula. CEE encourages the submission of manuscripts describing innovations in the laboratory ranging from large-scale unit operations experiments to demonstrations appropriate for the classroom. The following guidelines are offered to assist authors in the preparation of manuscripts that are informative to our readership. These are only suggestions, based on the comments of previous reviewers; authors should use their own judgment in presenting their experiences. A set of general guidelines and advice to the author can be found at our Web site: <http://che.ufl.edu/~ceei>.

- Manuscripts should describe the results of original and laboratory-tested ideas. The ideas should be broadly applicable and described in sufficient detail to allow and motivate others to adapt the ideas to their own curricula. It is noted that the readership of CEE is largely faculty and instructors. Manuscripts must contain an abstract and often include an Introduction, Laboratory Description, Data Analysis, Summary of Experiences, Conclusions, and References.

- An Introduction should establish the context of the laboratory experience (e.g., relation to curriculum, review of literature), state the learning objectives, and describe the rationale and approach.

- The Laboratory Description section should describe the experiment in sufficient detail to allow the reader to judge the scope of effort required to implement a similar experiment on his or her campus. Schematic diagrams or photos, cost information, and references to previous publications and Web sites, etc., are usually of benefit. Issues related to safety should be addressed as well as any special operating procedures.

- If appropriate, a Data Analysis section should be included that concisely describes the method of data analysis. Recognizing that the audience is primarily faculty, the description of the underlying theory should be referenced or brief. The purpose of this section is to communicate to the reader specific student-learning opportunities (e.g., treatment of reaction-rate data in a temperature range that includes two mechanisms).

- The purpose of the Summary of Experiences section is to convey the results of laboratory or classroom testing. The section can enumerate, for example, best practices, pitfalls, student survey results, or anecdotal material.

- A concise statement of the Conclusions (as opposed to a summary) of your experiences should be the last section of the paper prior to listing References.
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Chemical Engineering at
the University of Sherbrooke

J. Peter Jones, Bernard Marcos, and Gervais Soucy

The University of Sherbrooke is a French-language university in the city of Sherbrooke, Quebec. It is 100 miles east of Montreal, about 30 miles from the Vermont border, and approximately due north of Boston, Mass. The Main Campus, which houses the university administration and eight faculties, and the separate Health Campus—with the Faculty of Medicine and Health Sciences, and forming part of the Sherbrooke University Hospital Centre Complex—are all located in Sherbrooke, at the heart of the beautiful Eastern Townships region of southern Quebec. The area is well known for its many rivers, lakes, and mountains. Part of the Northern Appalachian chain of mountains, it is a favored cottage, skiing, and recreation area for Montrealers, among others.

THE UNIVERSITY

The university includes nine faculties and offers more than 260 study programs, at both the undergraduate and graduate levels.

The university has been experiencing unprecedented development: Since 2001, 650 people have been hired. In fact, more than 40% of its currently employed professionals joined the university within the last four years. In keeping with this growth, the university is presently investing some $310 million to renovate and make additions to existing buildings. Close to 35,000 students attend courses at the University of Sherbrooke, some 85% coming from outside the region; more than 1,300 international students are enrolled on a yearly basis.

A study, published annually for the past three years in The Globe and Mail national newspaper, reveals that the University of Sherbrooke has consistently been the most appreciated university in Quebec and is among the three top-ranked universities in Canada. According to MacLean magazine's annual study, the University of Sherbrooke enjoys the best overall reputation in Quebec. The university is first in Canada for the excellence of its cooperative system, which allows students to alternate between study terms and paid-work terms, and for the high quality of services offered to its students. The co-op education system provides a large number of students with paid-work terms, giving them an opportunity to combine the theoretical notions acquired in the formal classroom with their practical experiences as received in the workplace. Students
involved in Sherbrooke’s cooperative education system earn more than $30 million in salaries annually, for more than 4,000 paid-work terms.

A LEADER IN RESEARCH AND CREATION

The University of Sherbrooke has identified the fields of expertise it intends to develop, in both teaching and research, to meet tomorrow’s requirements both nationally and internationally. As well, the university is addressing increasing numbers of requests for “partnerships” from institutions in Europe, Latin America, North Africa, and Asia concerning its master’s and doctoral degree programs, especially in the fields of education, administration, cooperative management, and applied ethics. It also receives the most royalties of any Canadian university from past inventions by professors and researchers. Thus, it has received more than $79 million royalties to date, including $14.3 million in the 2002-2003 academic year alone. In addition, some 22 spinoff companies have been created by the University of Sherbrooke over the past 20 years.

In fact, the university holds title to 300 patents (both established and pending)—51% having been transferred to businesses. Notable among these innovations is the ACELP technology, developed at the University of Sherbrooke, which has become the standard in mobile telephony (with more than a billion users) and on the Internet (with more than 500 million users).

RECENT EARLY HISTORY

Sherbrooke’s Department of Chemical Engineering started its existence as a process engineering section in the Department of Mechanical Engineering. Originally, there were three professors: Bernard Coupal, André Marsan, and a French military co-operant, Bernard Koehret. They were later joined by Maurice Ruel, Esteban Chornet, and Normand Thérien. In December 1971, under the determined leadership of Coupal, the department was established as a full department in its own right, with a distinct program of studies in chemical engineering.

The battle to become a separate department was difficult as other departments were wary they would lose scarce resources, but Coupal advised them that the establishment of a Department of Chemical Engineering could be done at “zero cost.” Some of the older professors from other departments long remembered his statement, and used it liberally when later the department was fighting for an increased share of resources.

The department continues to be the only one in a Quebec university to have a fully cooperative program.
Sherbrooke’s Chemical Engineering Faculty

Nicolas Abatzoglou’s activities are in the areas of thermo-catalytic chemical reactors and the behavior of particulate systems in reactive and nonreactive industrial processes. His work is being used by companies for the gasification process commercialization, for conditioning of industrial gases, and for pharmaceutical product formulation. He has extensive scientific and industrial R&D experience in fields at the “juncture” of energy and environment as well as in dry formulation of pharmaceutical products, and has initiated a substantial program on Process Analytical Technology for the pharmaceutical industry. He teaches various courses including the capstone design course, reaction engineering, pharmaceutical engineering processes, and separation and purification in biotechnology.

Maher Boulos is a leading figure in the thermal plasma field, along with colleagues in Minnesota, France, Switzerland, and Japan. His work through the Sherbrooke Plasma Research Center has been broadly based and includes many novel experimental studies, but it has also included industrial scale development studies, modeling, and—with collaborators—more “in depth” theoretical work.

Esteban Chornet is a leading international figure in research whose work has led to the production of chemicals and energy values from biomaterials and organic wastes. The first chemical engineer in Canada to obtain the prestigious Steacie Fellowship for research, he is the founder of the research center on the transformation of biological materials. Much of his recent work has been applied to environmental concerns (e.g., “green” chemical engineering, biomaterials recycling, and environmental concerns). He has initiated a number of high-tech spinoffs in Quebec and has also developed spinoffs in his native Catalonia.

Nathalie Faucheur, a biochemist with a Ph.D. in biomedical engineering, plans to determine how biomaterials and cells can share information with one another. She is one of the few researchers in the world working to gain a deeper understanding of how biochemical signals, triggered by contact with a biomaterial, activate a cell’s capacity to survive, multiply, and function. The cutting-edge materials she is using are based on grafts of small molecules called peptides, which, among other things, promote cell adhesion. She holds a Tier 2 Canada Research Chair.

François Gitzhofer was recruited for his expertise in materials engineering from the University of Limoges, France. He has become director of the department’s Plasma Research Group, which is continuously evolving toward a broader role in fuel cell development and other energy-intensive applications. His focus is on creating new ways of making coatings on various substrates, using both established and newly emerging plasma technologies.

Denis Gravelle, one of the earliest professors to join the department, is an expert in the application of thermodynamics to thermal plasma systems and in the use of spectroscopic methods/techniques for a fuller understanding of plasma torch dynamics. A key teacher of thermodynamics at both the graduate and undergraduate levels, he is also involved in the lab courses, aiming at the integration of basic engineering concepts of thermodynamics, transport phenomena, and reaction kinetics.

Michèle Heitz, the associate dean for students (Engineering Faculty) and a full professor, teaches introduction to chemical engineering, thermodynamics, and chemical thermodynamics. She is also in charge of integrating projects for both the chemical and the biotechnological first-year students. Since 2002, she has also taught air pollution control and design, introduction to biochemical engineering, and chemical kinetics and reactor engineering. Her current research projects include air treatments by biofiltration as well as biodiesel production and biomass and whey valorization—both topics involving various chemical and biotechnological approaches.

Peter Jones arrived at the Sherbrooke shortly after the department was created. He has developed a research area in industrial water treatment and the application of statistical methods to environmental problems, and more generally, to experimental research. A past chairman of the department, he was director of the environmental engineering and science master’s program and vice dean for research.

Jerzy Jurewicz is a specialist in the area of environmental engineering, using either direct or high-frequency AC currents. He applies his expertise to the development of new reactors for the synthesis of new products, especially for nanometric powders. Jerzy is responsible for courses in safety in the first year and also in process safety courses in the fourth year, and is a key member of the design course team.

Bernard Marcos has done much work in the field of expert systems and neural networks as well as pursuing educational research such as the use of a system of intelligent tutorials. He was the first director of the new program in biotechnological engineering.

Pierre Proulx has been involved in mathematical modeling of thermal plasmas since his graduate studies under the supervision of Maher Boulos in the Plasma Research Center. His current projects entail mathematical modeling of complex reactors. He teaches transport phenomena and process control.

Joel Sirois, the most recently hired professor, comes with a very strong background in biotechnology and was recently the chief technology officer at a start-up company in this field. His focus is in the areas of characterization, modeling, and optimization of cell metabolism and the design and scale-up of bioreactors.

Gervais Soucy is current chair of the department. His teaching is concentrated in unit operations. His research field is in the application of new technologies for various processes in the aluminum industry. He has also developed expertise in thermal plasma technology to produce carbon nanostructures.

Normand Thérien, recently retired from the department, is an expert in the application of mathematical techniques to environmental problems. His most important work has been in the area of modeling of hydroelectric reservoirs, where he has been an important figure in determining how mercury can accumulate in reservoirs and render fish unfit for human consumption.

Patrick Vermette is a researcher at the Research Centre on Aging and is an engineer and professor in the department, with a joint appointment in the Service of Orthopaedics. He has built a state-of-the-art laboratory for surface science and tissue engineering studies. He and co-workers are involved in fields including biomaterials, angiogenesis, colloids and interface science, drug delivery systems, bioreactors, tissue engineering, and haematopoietic stem cells.
THE COOPERATIVE PROGRAM

The Faculty of Engineering at the University of Sherbrooke was a very early adopter of the cooperative system of engineering in North America. The University of Waterloo had initially adopted the cooperative system in 1956, and the University of Sherbrooke followed in 1966, before the Department of Chemical Engineering was formed. The co-op system seeks to prepare students for their future career(s) by providing the practical experience that meets employer requirements in the workplace. Thus, the work term offers students the opportunity to acquire practical experience and to develop competencies (knowledge, skills, attitudes, values, etc.) relevant to their future careers. Cooperative education, a pedagogical approach whereby students spend alternate trimesters studying in the classroom and earning wages in the workplace, also offers many valuable features to potential employers. As a pioneer of cooperative education in Quebec, the University of Sherbrooke is proud to be a leader in this expanding field. A result is that the University of Sherbrooke now ranks second in Canada—and is among the top five advanced learning institutions in North America—for the importance given to its cooperative education system. In the Department of Chemical Engineering, students are able to achieve this gradual integration by switching alternate trimesters between their paid terms in the workplace and their study terms at the university. When students graduate, they will have served five work terms (15 weeks/term) in an industrial company (90%) or in a research laboratory (10%). Since there are eight academic sessions, the student obtains his B.Eng. degree after a period of 52 months.

THE UNDERGRADUATE PROGRAMS

Chemical Engineering

The Department of Chemical Engineering has always kept up to date with the needs of employers in Quebec and the rest of Canada.

The studies program in chemical engineering was completely overhauled for students set to begin in September 2001 and graduate in December 2005. Table 1 presents the curriculum of the reformed chemical engineering program. We have since initiated five cohorts, or graduating classes, to this new

<table>
<thead>
<tr>
<th>Session</th>
<th>Description</th>
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<tbody>
<tr>
<td>S-1</td>
<td>Introduction to chemical engineering</td>
</tr>
<tr>
<td></td>
<td>The role of the engineer, safety and risks, chemistry, communications</td>
</tr>
<tr>
<td>S-2</td>
<td>Measurement techniques for use in the laboratory and the factory/plant</td>
</tr>
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<td></td>
<td>Instrumentation, chemistry, chemical analysis techniques, reports, controls</td>
</tr>
<tr>
<td>T-1</td>
<td>Work term #1</td>
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<td></td>
<td>At the end of the first year, the student should be capable of describing the chemical engineer’s role and of undertaking control actions and performing analyses, both in the laboratory and at the plant; thereby displaying, at an early stage, a satisfactory competence level in performing the necessary tasks.</td>
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<tr>
<td>S-3</td>
<td>Transport and exchange in fluids</td>
</tr>
<tr>
<td></td>
<td>Fundamentals of chemical transport/transfers in processes</td>
</tr>
<tr>
<td>T-2</td>
<td>Work term #2</td>
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<tr>
<td>S-4</td>
<td>Design of the basic units employed for a chemical process</td>
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<td></td>
<td>Advanced chemical transfer/transport, chemical reactor and associated units calculations</td>
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<td></td>
<td>At the end of the second year, the student should be capable of modeling the operations of several parts of a functioning chemical process plant.</td>
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<tr>
<td>T-3</td>
<td>Work term #3</td>
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<tr>
<td>S-5</td>
<td>Industrial scale plant operations</td>
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<td></td>
<td>Control methods, techno-economics, process control laboratories</td>
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<tr>
<td>S-6</td>
<td>Design basics of industrial-scale chemical processes</td>
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<td></td>
<td>Types of processes, process simulation, environmental and safety aspects</td>
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<td></td>
<td>At the end of the third year, the student should be capable of designing the unit parts and creating the basic overall process concept for an industrial-scale process.</td>
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<tr>
<td>T-4</td>
<td>Work term #4</td>
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<tr>
<td>S-7</td>
<td>Combining process design skills and experiences – I</td>
</tr>
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<td></td>
<td>Integration of all aspects required to establish, modify, and operate a chemical industry installation at an important scale</td>
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<tr>
<td>T-5</td>
<td>Work term #5</td>
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<tr>
<td>S-8</td>
<td>Combining process design skills and experiences – II</td>
</tr>
<tr>
<td></td>
<td>Integration of all aspects required to establish, modify, and operate a chemical industry installation at an important scale</td>
</tr>
<tr>
<td></td>
<td>At the end of the fourth year, the student should be capable of designing the unit parts and creating the basic overall process, taking into account relevant aspects of process economics as well as social and environmental issues.</td>
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</table>
Sherbrooke students pitch in on a project in one of the university’s well-equipped labs.

regime. This overhaul was dictated by our knowledge of the companies that hire our graduates. We were also influenced by the tradition of innovation in pedagogical methods used in the university’s Faculty of Engineering. We have aligned our developments with the goal that engineering graduates of our programs will be responsible for the development of new products and processes. Most of these new products and processes are not even mentioned in traditional course materials for aspiring chemical engineers, yet our students must now develop ability to work creatively in these areas. We have therefore developed three distinct avenues for going forward:

- Students are responsible for their own development, which is central to the educational process. They must combine their technical development with the simultaneous improvement of their leadership skills, their entrepreneurship, their teamwork skills, and their respect for their profession.
- Students must now take full and early advantage of the new computing and information technologies at their disposal, especially the software products specific to their profession and their technical competence as chemical engineers.
- Courses cannot be approached separately. We and the students must find the commonalities through the sessional projects program, activated during each of the first, third, and fourth years.

The result has been an immersion in the practice of chemical engineering from the very first session. Students were often ill-prepared for some of the challenges they faced, but through their initiative and determination they were able, nevertheless, to produce very interesting results. The projects performed in those early sessions required a lot of “digging” to find pertinent information. This information was then applied to experimental setups, which they also had to design. They did, however, have considerable help from professors leading the course(s) for each session, along with assistance from departmental technicians. The project is a capstone design project, with which we have now had considerable success for a number of years. These projects are presented at the CSChE competitions. We have won the SNC–Lavalin prize a number of times.

The 40 courses offered in the program are distributed in the following manner:

- 11 courses as general engineering courses in mathematics, thermodynamics, and materials
- 17 courses in chemical engineering, transport phenomena, unit operations, and reactor design
- six courses in humanities and social science, law, ethics, and engineering economics
- six courses in the students’ chosen major

Students are mentored by their more-senior peers, who help them become accustomed to the range of department operations and also provide them with professional contacts at the very beginning of their professional careers. The unifying projects chosen for each session are an excellent initiation to the later work terms, following two sessions spent in the department. Through the projects students also learn about the human and societal aspects of their chosen profession.

Biotechnological Engineering

The numerous recent developments in biotechnology and in the medical sciences have led the Engineering Faculty to readapt its curricula under the belief that the most precious asset of a profession is its intellectual core. In an era of rapid evolution in biotechnology-based industry, it is imperative that the biotechnological engineering discipline define its own core. It must strengthen its core through scholarly activities and diverse applications. Considering that biotechnology constitutes a broad field, biotechnological engineers need to integrate skills in engineering principles, process engineering, and biological sciences, without being restricted to particular applications. Biotechnological engineering programs must take into account the complexity of living systems with their discrete and nonlinear relationships. The integration of complex engineering principles is not a simple task, and the biology-engineering barrier is an obstacle that has to be overcome. It is not sufficient to incorporate biological science courses into a chemical engineering curriculum hoping that students will be capable of integrating both concepts. Biotechnological engineers must eliminate the present gap and correct misunderstandings between traditional engineers and biologists. They must accept the fact that living organisms are not entirely predictable. Consequently, they must master basic knowledge of living organisms and bioproducts, and of the fundamental unit operations and simulation tools used
by engineers. They must understand the physiology of prokaryotes and eukaryotes as well as the engineering concepts used in bioprocesses. Biotechnological engineers must also be able to operate and control small- and large-scale culture systems of cells and microorganisms for the production of products of commercial potential (e.g., proteins, antibiotics) as well as the downstream processing, including separation and purification of biomacromolecules. Finally, they must be skilled in project management and quality control. Broadly speaking, biotechnological engineers will be called upon to solve problems through the development of bioproducts and bioprocesses that use living organisms or the products they synthesize.

The biotechnological engineering program at the University of Sherbrooke was originated by the departments of biology and chemical engineering. It took four years to build the program, which now offers an integrated training in biotechnological engineering. Table 2 presents the curriculum of the new Biotechnological Engineering program at Sherbrooke. The program is divided into eight terms that include laboratory studies, applied projects, and lectures.

Creating a new discipline may present some drawbacks for the employment of new graduates. Industry will need to learn what a biotechnological engineer is—just as it understands what chemical engineers and biologists are. That is why the biotechnological engineering program was developed with industrial partners. These industrial partners are regularly updated on the curriculum’s development. Another area of concern is that biotechnological engineers may be too narrowly trained and too application-oriented. As explained previously, the biotechnological engineering program is a science-based program that should ultimately alleviate a too-narrow perspective.

The goal of the training is to prepare a generalist engineer who is able to manage the evolution of the biotechnology industry. The wide breadth of knowledge of tomorrow’s biotechnological engineers will be an important advantage to them.

Several segments of the bio-industry are relevant to the employment of future biotechnological engineers: biopharmaceutical and drug companies; agribusiness and food companies; environmental biotechnology companies; biomedical instrumentation companies; biomaterials; and the tissue-engineering sector.

<table>
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<tr>
<th>Session</th>
<th>Description</th>
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</table>
| S-1     | Introduction to Biotechnological Engineering  
Role of the engineer, safety and risks, biochemistry, information technology |
| S-2     | Introduction to Biology  
Biology, cell biology, functional biology, microbiology, laboratory techniques |
| S-3     | Genetics and transport phenomena  
The fundamentals of genetics and chemical transport |
| T-1     | Work term #1 |
| S-4     | Design of basic units  
Advanced transport, unit operations, experimental protocols |
| T-2     | Work term #2 |
| S-5     | Operation of industrial unit processes  
Bioreactors, process control, engineering economics, biological polymers |
| T-3     | Work term #3 |
| S-6     | Downstream operations  
Separation and purification, materials and biomaterials, biomolecular engineering |
| T-4     | Work term #4 |
| S-7     | Design of biotechnological processes  
GMP-GLP standards, process simulation, design |
| S-8     | Integration of the abilities required to design a chemical process  
Integrate all the aspects related to the building, the modification, and the operation of a large biotechnological industrial installation |

At the end of the fourth year, the student should be able to design a process to include all of the economic, environmental, safety, and societal aspects for functioning in today’s marketplace.
Double Degree Program with Bishop’s University

Sherbrooke students may choose to earn a double degree in engineering and liberal arts in a joint program with Bishop’s University. The engineering program includes four, four-month, paid-work internships. The remainder of the liberal arts program is undertaken by taking selected courses at Bishop’s University, located a few kilometers away from the University of Sherbrooke.

The liberal arts degree provides for a broad education in the social and human sciences, allowing students to develop fully as individuals in a chosen humanities specialty: history, literature, philosophy, fine arts, or theater.

This exclusive program is the result of close cooperation between the University of Sherbrooke and Bishop’s University. It allows students to study in both of Canada’s official languages while also experiencing the two unique and distinct university cultures.

Project-Based Learning Approach

The project-based learning approach is used to integrate coursework within an academic session in first-year projects and the third-year and final-year design project. Project-based learning is a new approach in the educational field. It was chosen by the department to fill new professional and industrial requirements. The main features of our approach are:

- The project involves solution of a problem taken from a “real world” case. For instance, the last-year design project was an oil sands exploitation situation; the first-year project was the design of a process for the valorization of lactoserum.
- The student is responsible for this “on the job” learning and the initiative is to be taken by the students. The class is divided into small teams and collaborative learning principles are used to find and share new knowledge. At the end of these projects, teachers have often noted that their students have improved appreciably in the application of self-learning skills.
- The project results in a “deliverable” (i.e., a process, product, flow sheet, report). In the last year, the deliverable (for the last-year project) was the design and specifications for the oil sands plant; the end product (for the first-year project) was the design and monitoring of a pilot plant for lactoserum valorization.
- The work lasts for a realistic amount of time. Each project is spread over two sessions.
- Professors involved are considered an advisory committee and the approach is student-centered. The teacher team performs the “follow-up” each week and provides advice, if necessary. The team realizes the assessment of the project. The project is also evaluated by other students.

Students subsequently present the project at public conferences and the annual Canadian Chemical Engineering Congress. During the last 10 years, Sherbrooke students have won many awards at the Congress of the Canadian Society for Chemical Engineering for the quality of their first-year and final-year project presentations. These projects enable students to substantially improve their mastery of both oral and written communications.

RESEARCH

Research has been a very significant part of the department’s activities from its beginning. The department received funding of more than 4,000,000 CAD last year. This funding is primarily in the form of grants, so there are fewer overhead charges than American schools are likely to bear. This funding has been principally used to support graduate students and researchers, as well as to build and maintain very well-equipped laboratories.

Research in the department is conducted in a number of areas, including aluminium production technology, biomass conversion, biotechnology, environmental engineering, fuel cell technology, flow modeling, and plasma technology.

The research has evolved over the years as a result of recruitment of professors and substantial research funding. In 1973, Bernard Coupal obtained a very substantial grant to develop applications for peat moss during the first year of the department’s existence as an independent entity. This grant provided a very important impetus to work in the department and led to a very substantial and lasting work program on biomass transformation.

Environmental engineering developed because we started a master’s degree program in environmental engineering and science. Biotechnology research was developed as we recognized the need for specialists in our new biotechnological engineering program. The interest in this research has progressed hand in hand with the hiring of new professors working in the field.

Thermal plasma technology was not common in chemical engineering departments before the 1970s but the arrival of Maher Boulos led to very substantial growth in this area at Sherbrooke. The need to model gas/plasma flows in plasma torches led to general interest in the modeling of flow, heat transfer and kinetics, and particle behavior in a variety of systems.

Fuel cell research evolved because of our specialized knowledge, which already existed in the plasma research center for materials, especially deposition on surfaces using thermal plasmas.

Other research “specialities” were taken up because of their importance to certain industrial sectors existing in the Quebec economy, notably in aluminium production. The pharmaceutical industry is very developed in Quebec, and we are consequently developing very active research in this area, including PAT (Process Analytical Technology).
Testimonial of a doctoral student's experience in a joint program with a university in Europe

“The Department of Chemical Engineering at the University of Sherbrooke provided me with an opportunity to do my doctoral research in collaboration with a Belgian laboratory at the Catholic University of Louvain (UCL). This collaboration lies within the scope of an agreement of joint direction established between the two universities.

“This European collaboration enabled me to work for some two-and-a-half years within the Bioengineering Unit at UCL. I discovered innovative enzymatic methods for the elimination of recalcitrant phenolic compounds. This experiment also allowed me to establish a network with other European laboratories working in fields related to my research task.”

GRADUATE EDUCATION

The department has provided a strong graduate program from its earliest days. Professors who were in the process section of the mechanical engineering department had large contingents of graduate students. Upon creation of the chemical engineering department, we were accorded, in addition to our existing undergraduate programs, the master’s and doctoral programs.

There are presently approximately 50 post-graduate students working in the department. We graduate about eight master’s degrees and five Ph.D. degrees per year.

INFLUENCE OF OUR PROFESSORS IN CREATING HIGH-TECH SPINOFFS

The University of Sherbrooke generally and the Department of Chemical Engineering in particular have been very successful in obtaining licensing fees and creating spinoff companies. Esteban Chomet, with the contribution of Nicolas Abatzoglou, has created a number of companies, many very successful in the tasks of coproducing useful products and energy from biomass and organic wastes. Maher Boulos has created a company, based in Sherbrooke (Tekna), with more than 40 full-time employees, specializing in the area of thermal plasma technologies. This company exports its products all over the world, achieving particularly strong results in Japan.

THE FUTURE

The future is bright. We are recruiting large numbers of students into the biotechnological engineering program. The incoming class recruitment in chemical engineering is stable, with approximately 35 new admissions per year. We are in the process of recruiting additional professors for both chemical and biotechnological engineering.

The University of Sherbrooke provides a distinctive educational experience because of its “French” character. We encourage those predominantly English-speaking students who also have knowledge of “basic French” to come to Sherbrooke to simultaneously “perfect” both their chemical engineering and their French language skills for use in their future careers—in Canada, and beyond!

Winter visitors to Sherbrooke will see some of the prettiest scenery snowy climes have to offer, such as this view of nearby St. Benoit-du-Lac Monastery.
Susan Montgomery
of the University of Michigan

SCOTT FOGLER AND LARA ZIELIN
The University of Michigan • Ann Arbor, MI 48109

Undergraduate program advisor Susan Montgomery was three years into a tenure track position at the University of Michigan (UM) in education research when she realized that teaching and advising were her true passions. Driven by those passions, Susan did the unconventional thing and became a lecturer in 1999. Since then, she has been a “mom” for over 1,000 ChE students, who appreciate the warm and supportive community she helps create within a big university atmosphere.

“Susan Montgomery literally holds together the undergraduate curriculum at UM,” says Ron Larson, chair of UM’s chemical engineering department. “She is the most appreciated faculty member among the undergrads. The key element that makes her successful is her singular focus on the students and their needs. While other faculty members also care deeply about students, their research and administrative portfolios limit the extent to which they can involve themselves in the concerns of the students. There is simply no substitute for having a member of the faculty who is devoted exclusively to the students.”

This is no small feat in a ChE program as large as UM’s. Total enrollment hovers around 350 students. “UM can be daunting,” explains Larson. “Even within the ‘community’ of a department, students can get lost.” Susan works hard to combat this by maintaining a connection with each chemical engineering class. “Not only does she know every undergraduate that comes up through the program, she keeps track of them as they move on to their future careers,” says Larson.

While she loves the classroom and has taught a wide range of undergraduate classes—from introduction to engineering to process design—Susan has a hard time choosing a favorite topic. “The real fun is seeing students transition from one phase of their careers to the next,” she says. “The thrill is watching students blossom.”

Susan works tirelessly to make students’ growth and advancement a reality. In addition to her advising and lecturing, Susan is the principal author of the Visual Encyclopedia of Chemical Engineering Equipment, a CD-ROM designed to help beginning ChE students understand how chemical engineering equipment works.

The CD-ROM stemmed from her research in the Multimedia Educational Laboratory (MEL) at UM, which focused on studying the diverse learning styles of chemical engineering students, and developing multimedia educational software to address those learning styles. Susan then analyzed student use of this software to discern what types of interactions were preferred by what students. The goal was to help future educational software developers better understand the role that different interactions could play in addressing the needs of a variety of learners.

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Chemical Engineering Education
The CD-ROM includes animations and pictures of real equipment as well as examples of applications of the equipment. From the main menu, the user can branch into a variety of different topics and operations, such as the corresponding pieces of equipment for processes including heat transfer, reactors, materials handling, and more.

The CD-ROM encyclopedia has been extremely well received both in academia and industry. Figure 1 shows a screen capture from the CD illustrating a sample introductory overview of an item of equipment—cyclones and hydrocyclones in this instance. The possibilities for illustrating chemical engineering practice are almost endless, and many of the screens in the CD show dynamic operation of the equipment, as in the case of bubble-cap distillation columns, screw extruders, filters, and cyclones, to mention just a few. When a visit to a chemical plant or refinery cannot be made, the Visual Encyclopedia is an excellent substitute for illustrating various operations that might otherwise have to be described more passively. It has been used for numerous industrial training courses. The CD is also included in two of the most popular textbooks in the field: Rich Felder’s Elementary Principles of Chemical Processes, and Scott Fogler’s Elements of Chemical Reaction Engineering.

In addition to the Encyclopedia CD-ROM, Susan and her colleagues have developed two other CDs. The first, titled Engineering Fundamentals in Biological Systems, provides real-world applications in fundamental processes, such as material balances on an artificial kidney. The second CD, Material and Energy Balances, provides interactive problem solving in real-world environments including the car preprocessing system in Ford Motor Company’s Wixom Assembly Plant, and Ann Arbor’s wastewater treatment plant. The CD also includes tutorials on Pxy-Txy diagrams, psychrometric charts, and enthalpy-concentration diagrams. The CDs are distributed through the CACHE Corporation.

**FAMILY TIES**

Susan’s background and upbringing have much to do with her success in the field. She was born in Peru, of a Peruvian father and an American mother. Her father is a civil engineer who shared his passion for engineering with his daughters. He used to take Susan and her sister to job sites, showing them how things worked. Susan recalls going for a walk with her dad when they chanced upon a street replacement project. Her dad showed her all the layers that made up a street, and they met the construction workers.

Susan and her family lived for a year and a half in Nicaragua, where her father was an Agency for International Development consultant with their ministry of public works. Forced to leave suddenly in 1978 when a civil war broke out, Susan, her sister, and her mother moved to Ann Arbor, Mich., where her American grandmother lived.

The summer after her junior year in high school, Susan attended a Women in Science and Engineering program at Carnegie Mellon University and came home announcing that she intended to be a chemist. Her father corrected her, “reminding” her that she would be an engineer.

Susan graduated from high school at age 15, a feat she attributes to an excellent kindergarten that allowed her to complete first, second, and third grades in one year. She completed her undergraduate work at UM, then went on to Princeton University for her graduate work. Susan’s advisor at Princeton was Professor Ludwig Rebenfeld, of the textile Research Institute, where her research focused on flow through porous media. But her passion was in teaching, and her goal was a faculty position.

Susan had doubts, however, about her ability to complete the Ph.D. Thrice during her time at Princeton, she announced to Prof. Rebenfeld that she was quitting the program. Prof. Rebenfeld offered unwavering support, but two other factors

![Figure 1. A screenshot from Susan’s encyclopedia CD-ROM showing an oversize view of equipment, left, and the main navigation page, right.](image-url)
made her tough it out and complete the program. The first factor was knowing that without a Ph.D., she would not be able to fulfill her goal of becoming a faculty member. The second was the scolding of her grandmother, Margaret Hampshire, an independent woman with whom she lived while an undergraduate at UM. Where others, upon hearing that she was considering dropping out, offered condolences, her grandmother replied with comments such as, “We didn’t work this hard for you to drop it all now. You get back there and get that Ph.D.!”

Perhaps this is why Susan can now speak so well to the number of women students who are struggling to find their place in the ChE program. “After a month, they may come to me feeling like maybe they’re not good enough,” she says. “I encourage them not to focus on whether or not they’re ‘good enough’ but on whether or not this path is taking them where they want to go.” The approach seems to work. Susan says a number of alumni have thanked her for the advice she offered early on in their academic careers. “They’re out there doing what they love now, so they can look back and be glad they stuck with the program,” she says.

Susan has the strength to help many, but when she needs someone at her side she calls on her sister, Betsy Vera. Susan says Betsy has stood by her continuously. They remain best friends and stay close, even though Betsy now lives in Chicago.

“I have learned so much from my family,” says Susan. For example, she recalls watching her mother complete her undergraduate studies in her 40s, and then go on to earn a master’s degree in Latin American Studies from Georgetown University. “Now that I am in my 40s, too, I appreciate having my mother as a role model for living the life you are meant to live,” she says. Susan also says her mother’s death at the young age of 52 solidified the importance of living your life now, versus waiting until retirement to do things you’ve always dreamed of.

ENTERING THE FIELD

Susan got her first job on a fluke. Like many undergraduate students, she was struggling to find funding for spring semester of her third year. She was just leaving the dean’s office, disappointed, when she ran into Scott Fogler, a UM professor of engineering, whose class she had just finished taking, and acing—she had been the top student. He inquired about how things were going and, upon learning of her situation, he immediately offered her a summer job working in his laboratory and helping him with his textbook. This marked the beginning of more than 20 years of collaboration in various educational projects.

Susan’s first teaching position was as a TA for the junior-level laboratory course at Princeton, where she caught the bug for education. “I could see the light bulb go off in students’ minds,” she says. An internship at a local community college teaching pre-algebra at night made her intrigued about learning styles, and the de-
velopment of learners through their college careers. She was quite intimidated when asked to be responsible for the whole laboratory course at Princeton the following year, but that experience only cemented her decision to become a faculty member.

During this time, Susan also recalls going to the engineering library at Princeton to search for a research article in Chemical Engineering Science. Instead, she discovered Chemical Engineering Education, stacked right next to the journals she was supposed to be reading. All plans for the afternoon were scrapped as she spent long hours browsing through CEE instead.

Also during her time at Princeton, Prof. Rebenfeld supported her attendance at the 1990 ASEE National Conference in Toronto, back in the days when few graduate students attended the conference. Participants at that time stayed in college dorms, which really helped colleagues get to know one another better. “I always speak of this conference as the time in which I ‘found my people’,” she says. “Their dedication and passion for teaching matched my own.”

After graduate school at Princeton, Susan returned to UM to complete a two-year postdoctoral appointment developing educational software for chemical reaction engineering and problem solving. Once again, she collaborated with her former professor, Scott Fogler, along with two dozen outstanding chemical engineering students. It was these students who taught her how energizing it can be to supervise teams of undergrads.

Again, Susan experienced a sea change. “At the time, my plans were to teach at a small undergraduate institution, or community college,” she says. “But my love of UM and Ann Arbor meant I eventually accepted a tenure-track faculty position focusing on academic research, the first in a chemical engineering department.” Susan’s research focused on the use of multimedia to address diverse learning styles, and once again she supervised teams of undergraduate students in developing educational software.

Susan has a long list of accomplishments to her name. In addition to those already mentioned, in 1994 she started a student chapter of ASEE at UM, the third such chapter and one of the few long-standing active chapters. The chapter has remained strong through the years, creating real change in the culture and appreciation of teaching through activities such as workshops and panels on engineering education issues.

“I strongly feel that the ASEE student chapter changed the culture of teaching and graduate student training at the College of Engineering,” she says. “Many of the activities we organized, which centered around preparing students for faculty positions, have been adopted by the college.” These activities include academic job-search workshops and panel discussions on working toward tenure.

To further prepare students, Susan regularly teaches a graduate course, “Teaching Engineering,” that draws 50 graduate students and trains them for academic positions. The students learn to develop syllabi and course materials, practice presentation and teaching skills, and are introduced to different learning styles. They also learn to deal with student issues that may arise. “This has become
an invaluable class for would-be future faculty members,” says Sharon Glotzer, UM professor of chemical engineering. “It attracts students from around the College of Engineering, including postdoctoral students.”

Susan’s concern for the well-being of graduate students and staff extends beyond the academic arena. Susan works to assist students with both academic disabilities and psychological issues. “Many times these issues manifest themselves during college years,” she explains, “and bad grades are some of the early warning signs.” To aid students, Susan says she tries to remove any stigmas around the topic of mental illness by sending out e-mail messages to students about depression, educating faculty about the issue, and encouraging those who need assistance to seek professional help. Her important work has not gone unnoticed: Recently she was asked to take part in a video titled “Depression on College Campuses.”

In this sense, many faculty think of Susan as a pioneer. “She forges new ideas and utilizes new resources to make the curriculum more effective,” says chemical engineering lecturer Barry Barkel. And it’s not just students who benefit from her tireless work — so, too, do alumni. “Susan occupies the unique position of being the primary focal point of the department for both undergraduate students and alumni,” says Barkel. “She is the face of the department for many people.”

BEYOND RESEARCH AND TEACHING

Susan’s family members likely think of her as a pioneer, too. She and ex-husband Sean Montgomery, whom she met when they were both undergraduates at UM, have two boys — Ian, 12, and Nicky, 7, — whom she has taken on summer excursions to places such as the Grand Canyon and the Canadian Rockies, in keeping with her philosophy to take adventures now and not wait until retirement. This summer, they will embark on a trip to Peru with Susan’s sister, Betsy, where they will visit family members as well as journey to Machu Picchu.

Even when not traveling, life with two boys — and two cats, Smokey and Aten — is understandably very active. Both boys are involved with karate and Ian plays on various team sports. “We also enjoy going for walks and bike rides, and going canoeing down the Huron River,” Susan says.

For Ian, watching his mom forge her own path in engineering may have inspired him. He has aspirations to one day be a robotics engineer. Nicky thinks that might suit him as well — if he doesn’t make it as an NBA player first.

Susan has not forgotten her Hispanic heritage, and has instilled this pride in her sons. Ian and Nicky’s friends have come to look forward to her alfajores — Peruvian treats she prepares for any and all occasions. She also serves as faculty advisor to the Society of Hispanic Professional Engineers, participates in numerous sessions organized by the Minority Engineering Program Office (MEPO), and recently started “Ingenieros,” an informal Spanish conversation group.

“Dr. Montgomery has been an integral part of the diversity effort here in the College of Engineering,” says MEPO program director Derrick Scott. “She rarely turns down a request to participate in our initiatives to attract and retain underrepresented minority engineering students.”

Susan is careful, however, not to get too busy. “My boys are the loves of my life and I want to share in every aspect of their growing up,” she says. After missing Ian’s first soccer goal while out of town to be an ABET observer, Susan was determined that she would travel for business for a few years. “Ron Larson, the department chair, supported my efforts to create a balance between my academic position and my family life,” she says. Despite this, Ian loves to point out that Susan missed his second soccer goal, which he scored while she was videotaping Nicky and his friends playing on the sidelines.

She did bend her own rules and take one business trip in 2002 to the ChE division Summer School for ChE faculty in Boulder, Colo. As Susan told the participants at the welcoming session: “It doesn’t matter what city you are in, if you are surrounded by your friends and colleagues of the ASEE ChE division, you’ll always feel at home.”

It’s hard not to feel at home around Susan, whether in Colorado, Michigan, or Peru. Her excellence, determination, and love for people translates into every activity she performs. “In short, every department needs a Susan Montgomery on its faculty,” says Ron Larson. “But they can’t have ours.”

Susan, right, with sons Ian, 12, and Nicky, 7, on a vacation to the Canadian Rockies.
AN AGITATION EXPERIMENT WITH MULTIPLE ASPECTS

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Agitation and mixing are important in a wide variety of areas in both the traditional and modern process industries,[1] and it is appropriate that chemical engineering students see related experiments in the unit operations laboratory. This paper describes a teaching experiment involving both agitation and mixing that illustrates—using a quite simple and relatively inexpensive apparatus—a number of aspects of this field. In particular the experiment involves not only simple and direct measurements, for example of torque and power as functions of stirring speed, but also more sophisticated data-acquisition and processing methods, for example indirect measurement involving the use of a model and a parameter estimation method.

APPARATUS

The apparatus is shown schematically in Figure 1 (next page). The major components of the apparatus are:

- A torque table, consisting of a 12-inch-diameter aluminum circle mounted on a tapered roller bearing set in a 12-inch-square aluminum base plate. Even with a load of about 20 kg, the torque needed to set the upper plate in motion is less than 0.00706 N m (1 oz inch). An arm attached to the upper plate bears a load cell (Omega Engineering, Model LCGC) connected to a panel meter (Omega Engineering). The data are acquired by a LabView program at 0.2-second intervals.
- A variable speed DC motor (Cole-Parmer) with speed controller and torque indication. The speed can be varied from 60 to 2400 RPM, and the maximum torque is 45 oz-in (0.318 N m).
- Two six-bladed turbines (of diameter 14.4 and 7.5 cm and blade width 3.32 and 1.83 cm), and two three-bladed propellers of diameter 14.4 and 7.5 cm. All are mounted on 3/8-inch glass-epoxy shafts inserted in a chuck on the motor shaft.
- A polycarbonate tank of ID 29.2 cm and volume about 18 L. This tank is equipped with four removable stainless baffles of width 2.43 cm, mounted on an acrylic top plate. A stainless funnel is mounted near the top of the tank, to be used for adding a conductive tracer, for example NaCl or KCl at 30 g/L. A platinum electrode conductivity cell is mounted near the bottom of the tank 180 degrees from the funnel. The cell is connected to a conductivity meter (Amber Sciences) that sends a 0- to

[1] Jordan L. Spencer is emeritus professor of chemical engineering at Columbia University. He received his B.S. in 1953 and his Ph.D. in 1961, both from the University of Pennsylvania and both in chemical engineering. His research and teaching interests involve control and optimal control, and the development of chemical engineering teaching experiments, including Web-operable experiments.
RESULTS

Presented below are some typical results, with comments related to what the results illustrate for the student.

Torque and Power

The 18-liter tank was filled with water to a depth of 25 cm. With the baffles in place and the 7.5-cm-diameter turbine mounted in the motor, the stirring speed was varied over a range of RPMs. The torque was measured by the load cell and averaged by a LabView program. Typical results are shown in Figure 2, where the torque (N m) is plotted as a function of RPM. Also shown is a curve of the form Torque = k RPM^2, which fits the data almost perfectly, as expected.

Since the torque signal was found to vary with time (with an amplitude about 10% of the average torque), especially at high RPM where the flow in the tank is quite turbulent, it was of interest to look at the power spectra of the data. A typical spectrum (Figure 3) shows that most of the power is at low frequencies, less than 0.15 cycles/sec. It is probable that the fluctuations reflect the presence of eddies or vortices generated by the impeller.

Non-Newtonian and High Viscosity Fluids

In order to examine the behavior of a non-Newtonian liquid, the 4-liter tank (with baffles) was filled to a depth of 15 cm with commercial ketchup. The 7.5-cm-diameter flat-bladed turbine was used to stir the ketchup. At 200 RPM the surface of the ketchup was stationary, clearly a non-Newtonian behavior. At 400 and 800 RPM the ketchup flowed smoothly at the surface. The data were well, but not perfectly, fitted by a curve of the form Torque = k RPM^2. Data were also collected under the same conditions using corn syrup (Karo), a Newtonian fluid with a viscosity about 2,500 times that of water. For these runs the torque was a linear function of the RPM, as expected.
Tracer Studies of Mixing Times—Modeling and Parameter Estimation

Mixing times have been estimated\(^1,2\) by visual observation following the addition of a dye or conductive tracer to the agitated liquid. This method, while satisfactory in some cases, has the disadvantage that it is inherently subjective, and cannot be used with cloudy or opaque fluids. A more objective method is based on acquiring and processing conductivity data following the addition of a conductive tracer (e.g., NaCl solution) to the agitated fluid in the baffled or un baffled 18-liter tank. The data are acquired by a LabView program, typically 100 baseline points in 20 seconds, followed by 400 conductivity points in 40 seconds. The tracer data are saved from Excel as a space-delimited (.pm) file readable by a QuickBASIC parameter estimation program.

The model used to fit the data, shown in Figure 4, consists of six well-mixed tanks. Three, of equal volume, correspond to downward-moving fluid in the core of the tank. The other three tanks (all of the same volume) correspond to the fluid moving upward along the walls of the tank. Symmetry around the propeller shaft is assumed, so that only three shell tanks are shown. Salt solution injection is assumed to take place at the upper right, and a conductivity probe is located at the lower left. The model contains two undetermined parameters, denoted \(b_1\) and \(b_2\), with \(b_1\) the fraction of the known tank volume in the three core tanks, and \(b_2\) the volumetric flow rate (L/s) downward through the core tanks and upward through the shell tanks. The volume of a core tank is \(b_1 V/3\), and the volume of a shell tank is \((1 - b_1)V/3\). An objective mixing time is three times the tank volume, denoted \(V\), divided by \(b_2\).

Figure 5 shows the normalized conductivity vs. time data for salt solution injection into the 18 L tank, with agitation provided by a 7.5-cm-diameter downward-driving propeller rotating at 60 RPM. Also shown is the best-fit curve corresponding to the model discussed above. The best-fit parameter values were \(b_1 = 0.484\) and \(b_2 = 1.368\) L/s. The conductivity does not rise for about five seconds, corresponding to the time needed for the salt solution to move from the wall of the tank to the center, down to the bottom of the tank, and then over to the conductivity probe located opposite the injection point. Then the conductivity rises and drops rapidly as the bolus of salt solution passes the probe. After some further oscillations the conductivity reaches a constant value. The curve based on the six-pool model fits the data fairly well, but certainly not perfectly. This is because

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**Figure 4.** Six-pool model of the flow pattern in the tank, used for analysis of conductive tracer-injection data. The core pools (tanks) represent the downward-flowing liquid in the center of the tank, the shell pools represent the upward-flowing fluid near the tank wall. Parameter \(b_1\) is the fraction of the tank volume \(V\) in the core, and \(b_2\) is the volumetric flow rate (L/s) through the array of well-mixed tanks. The state variables are the tracer concentrations in the six tanks.

**Figure 5.** Conductivity data vs. time, and best-fit response from model, for tracer injection into 18-liter baffled tank at 60 RPM using 7.5 cm propeller. Parameters: \(b_1 = 0.484\), \(b_2 = 1.368\) L/s.
At high Reynolds numbers the flow in the tank is, at least in some sense, strongly turbulent. This implies that particles suspended in the tank move in a chaotic and uncorrelated way, and thus move independently.

the model is much too simple to correspond exactly to the highly turbulent, three-dimensional, and complex flow pattern actually existing in the baffled tank, even at low RPM. The parameter $b_1$ (the fraction of tank volume) was 0.484, and $b_2$ (the circulation rate) was 1.368 L/s. When the stirring speed was doubled to 120 RPM the conductivity rose much earlier, overshot less, and settled out about three times more rapidly—corresponding to more vigorous mixing. The value for the circulation rate parameter $b_2$ was 2.765, more than double that for the 60 RPM run.

Similitude

In theory, for tanks that are geometrically similar, at the same Reynolds number the power numbers should also be equal. As a test of this theory, the torque is measured at 600 RPM using water and a flat-bladed turbine in the 4-liter baffled tank, and the Reynolds number is calculated. Then the torque is measured in the geometrically similar 18-liter tank, at an RPM corresponding to the same Reynolds number. When the experiments were performed, the calculated and measured torques typically agreed within 20%.

Heat Transfer Coefficient

It is well documented\(^1, 2\) that heat transfer coefficients in agitated tanks depend strongly on the intensity of agitation. In order to demonstrate this, the heat transfer probe was immersed in water in the baffled 18 L tank. The power to the probe was turned on, the stirring speed was set, and the probe temperature was allowed to come to steady state, which occurred in a few minutes. The difference between the probe and water temperature was plotted as a function of RPM. As expected, the temperature difference was highest at 0 RPM, dropped monotonically as RPM increased, and approached a nonzero constant as the RPM approached high values. This reflects the fact that the resistance to heat transfer is the sum of a constant resistance due to the aluminum wall of the probe, and a film resistance at the probe surface that varies with the $2/3$ power of RPM. From the high RPM asymptote the first resistance can be calculated, and from a second point the heat transfer coefficient can be found as a function of RPM. In general the results were consistent with Eq. (1):

$$k = a N^{0.67} = a N^{2/3}$$  \hspace{1cm} (1)

where $k$ is the heat transfer coefficient (Wm\(^2/\)°C), $a$ is a constant, and $N$ is the stirring speed (s\(^{-1}\)).

Figure 6. Optical sensor voltage for beads in 18-liter tank at 400 RPM. Each drop in voltage corresponds to the entry of a bead into the field of view of the phototransistor. Only drops below a selected voltage are counted as events.

Figure 7. Semilog plot of distribution of bead arrival intervals. The straight line corresponds to a Poisson distribution.
Note that all real-world measurements involve both signal and noise. In most cases the information is contained in the signal and we attempt to minimize the noise. But in some cases the noise also contains useful information. The results . . . illustrate this.

Particle Dynamics

At high Reynolds numbers the flow in the tank is, at least in some sense, strongly turbulent. This implies that particles suspended in the tank move in a chaotic and uncorrelated way, and thus move independently. In order to test this prediction about 200 plastic toroidal beads of approximate diameter 0.9 cm were added to the tank. The 7.5-cm turbine was run at 400 and 800 RPM. A typical sensor signal is shown in Figure 6, corresponding to a sample rate of 100 per second. Each drop in voltage represents the entries of one or more beads into the illuminated region. The program that acquired the data also used simple logic to identify close-bead approaches, to calculate the time interval between entry, and to construct an interval distribution function. If the beads in fact move independently, this is expected to be a Poisson distribution. Typical results, shown in Figure 7 in a semilog plot, correspond reasonably well to a straight line and thus to a Poisson distribution. The slope of the line is related to the average frequency of bead events, but also depends on the efficiency of detection of bead approaches, which is not easily known. The lower values at low time intervals probably correspond to the fact that the data acquisition program is not able to differentiate between two or more bead entries that occur at almost the same time.

Note that all real-world measurements involve both signal and noise. In most cases the information is contained in the signal and we attempt to minimize the noise. But in some cases the noise also contains useful information. The results above illustrate this.

Salt Crystal Dissolution

When a crystal of a soluble salt, for example NaCl, sits in water that is not moving, it dissolves relatively slowly. But the opposite holds for a crystal suspended in strongly turbulent water. Approximately one gram of a coarse (about 150 crystals per gram, the crystals being of variable size) kitchen salt was added to water in the baffled 18 L tank. At 0 RPM full dissolution required more than 60 minutes. The signal from the conductivity probe recorded by a LabView program is shown in Figure 8. Using the 7.5-cm-diameter turbine, dissolution was almost twice as fast at 800 RPM as at 400 RPM. These results demonstrate that the apparatus described above can be used in a wide variety of studies of the effect of stirring speed, impeller design, and other parameters on the rate of dissolution of (or extraction from) solids, as long as the solids release a conductive tracer.

CONCLUSIONS

The agitation and mixing experiment described above is based on a relatively simple and inexpensive apparatus. But it illustrates a number of aspects of the subject, including the
dependence of torque on stirrer speed, impeller design, baffle design, and nature of the fluid involved. The principle of similitude can be tested. The experiment also illustrates very general and more sophisticated concepts, including the use of modern data acquisition software and nonlinear regression methods to estimate the parameters of a model of the flow pattern in an agitated vessel. The apparatus is well adapted to studying the rate of dissolution of salt crystals, and the effect of agitation intensity on heat transfer from a solid surface.

Finally, students are able to acquire and process essentially stochastic data to obtain some information on the turbulent flow in the vessel.

REFERENCES
USING A COMMERCIAL SIMULATOR TO TEACH SORPTION SEPARATIONS

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Since modern practice of chemical engineering uses specialized process simulators extensively (e.g., Aspen Plus, CHEMCAD, HYSIM, and PROSIM), chemical engineering departments need to prepare students to use these tools. For example, distillation columns are designed almost exclusively using process simulators, and if the equilibrium data is deemed reliable, the column will be constructed without any laboratory or pilot data. Most chemical engineering departments now use one of the steady-state process simulators in separations and/or design courses. [1, 2]

The steady-state simulators do not include adsorption, chromatography, and ion exchange (collectively, sorption), which are normally operated as unsteady-state processes. Formerly, sorption systems were designed by a combination of data and rules of thumb. Recently, it has become more common to use a more fundamental design procedure based on solution of the partial differential equations governing the heat and mass transfer in the column and the algebraic equations for equilibrium and pressure drop. In industry, the detailed simulations are always accompanied by laboratory and often pilot plant data.

Chemical engineering graduates who understand the fundamentals of sorption processes and are familiar with sorption simulators will have a competitive advantage. This paper discusses the use of the commercially available Aspen Chromatography simulator to teach sorption separations. The course outline, grading procedure, assignments, computer laboratory operation, and testing procedure are delineated. Student survey results and the author’s opinion of the effectiveness of teaching with this simulator are presented.

THE COURSE

ChE 558, “Rate-Controlled Separation Processes,” is a three-credit, dual-level elective course that has been taught off and on for almost 30 years. [3] The topics covered always include sorption separations, and depending upon the professor, might also include crystallization, electrophoresis, or membrane separations. I have used Rate Controlled Separations [4] although this book is currently difficult to obtain. This course has always been taught in a lecture style with homework and often a course project.

Phil Wankat is a Distinguished Professor of chemical engineering at Purdue University who earned his degrees from Purdue and Princeton. His technical research is in separation processes, and he recently finished his textbook, Separation Process Engineering, 2nd Edition of Equilibrium Staged Separations, Prentice-Hall, 2006. He is also co-author of the book Teaching Engineering, available free at <https://engineering.purdue.edu/ChE/News_and_Events/publications/teaching_engineering>.

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Three considerations led me to change the teaching method. First, since I believe that the sorption separation processes will eventually be designed almost entirely using simulators, proper preparation of graduates will require teaching with simulators. Second, the understanding of an average ChE 558 student was too low. Since I had observed student improvement in a distillation course when a simulation lab was incorporated,[2] I expected an increase in understanding if a similar change was made in ChE 558. Third, I had proposed in the educational part of two NSF proposals to teach ChE 558 with a simulator, and now I had to deliver on these promises.

In spring 2005 I changed ChE 558 to focus entirely on sorption separations. The nominal schedule had a one-and-a-half-hour lecture on Tuesdays and a one-and-a-half-hour computer laboratory using the Aspen Chromatography simulator on Thursdays (see Table 1). This schedule had fewer lectures on sorption separations than in previous years, but tests covered the same amount of material on these topics. The total amount of material in the course was reduced by removing the membrane separation material, which is now often included in the required undergraduate course on separations. The course was taken by four undergraduates and three graduate students. Only one of the students had previous experience with an unsteady-state simulator, but all had previous experience with Aspen Plus, which has a somewhat similar graphical user interface to Aspen Chromatography.

The grading scheme used a straight scale (85-100 = A, 75-85 = B, 60-75 = C, 50-60 = D) as guaranteed grades, but I reserved the right to use lower cut-offs if that was appropriate. The two regular tests were each 25% of the grade, the lab exam was 20%, lab attendance 9%, lab assignments 6%, homework 5%, and the group course project was 10%. Students were encouraged to work together on lab assignments.

<table>
<thead>
<tr>
<th>Date</th>
<th>Class</th>
<th>Room</th>
<th>Subject</th>
<th>Reading</th>
</tr>
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<tbody>
<tr>
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<td>1</td>
<td>110</td>
<td>Intro. Adsorption &amp; Chromatography</td>
<td>207-228</td>
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<tr>
<td>Th, Jan 13</td>
<td>2</td>
<td>111</td>
<td>Lecture – Adsorption: thermo/phys. prop./flow; start solute movement</td>
<td>228-251</td>
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<tr>
<td>T, Jan 18</td>
<td>3</td>
<td>110</td>
<td>Lecture - Solute movement</td>
<td>239-251, 296-305</td>
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<td>Th, Jan 20</td>
<td>4</td>
<td>111</td>
<td>Lab 1 - Intro to Aspen Chromatography</td>
<td>Skim 268-274</td>
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<td>T, Jan 25</td>
<td>5</td>
<td>110</td>
<td>Solute movement/thermal effects-focusing</td>
<td>251-268</td>
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<td>Th, Jan 27</td>
<td>6</td>
<td>111</td>
<td>Lab 2 – Chromatography/adsorption basics</td>
<td>288-296</td>
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<tr>
<td>T, Feb 1</td>
<td>7</td>
<td>110</td>
<td>Heat &amp; Mass Transfer, local equilibrium solution</td>
<td>268-277, 296-305</td>
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<tr>
<td>Th, Feb 3</td>
<td>8</td>
<td>111</td>
<td>Lab 3 – Convergence</td>
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<tr>
<td>T, Feb 8</td>
<td>9</td>
<td>110</td>
<td>Chromatography – Linear solutions</td>
<td>305-316</td>
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<tr>
<td>Th, Feb 10</td>
<td>10</td>
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<td>Lab 4 – Chromatography</td>
<td>316-321, 336-347</td>
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<td>T, Feb 15</td>
<td>11</td>
<td>110</td>
<td>Chromatography – Linear solutions</td>
<td>316-331, 334</td>
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<td>111</td>
<td>Lecture – Constant pattern and scaling</td>
<td>365-393</td>
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<tr>
<td>T, Feb 22</td>
<td>13</td>
<td>110</td>
<td>Plateaus &amp; Nonlinear behavior, start MB and SMB</td>
<td>393-400, 521-533</td>
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<tr>
<td>Th, Feb 24</td>
<td>14</td>
<td>111</td>
<td>Lab 5 – Thermal effects</td>
<td>405-412</td>
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<tr>
<td>T, Mar 1</td>
<td>15</td>
<td>110</td>
<td>Test 1</td>
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<td>Th, Mar 3</td>
<td>16</td>
<td>111</td>
<td>Lab 6 – Flow reversal systems</td>
<td>405-418</td>
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<tr>
<td>T, Mar 8</td>
<td>17</td>
<td>110</td>
<td>Moving Beds and SMB; review test</td>
<td>499-537</td>
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<tr>
<td>Th, Mar 10</td>
<td>18</td>
<td>111</td>
<td>Lab 7 – TMB and SMB</td>
<td>521-533</td>
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<tr>
<td>T, Mar 22</td>
<td>19</td>
<td>110</td>
<td>Ion Exchange</td>
<td>452-484</td>
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<td>20</td>
<td>111</td>
<td>Lab 8 – Ion exchange</td>
<td>475-481</td>
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<tr>
<td>T, Mar 29</td>
<td>21</td>
<td>110</td>
<td>Ion exchange</td>
<td>475-491</td>
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<td>Th, Mar 31</td>
<td>22</td>
<td>111</td>
<td>Lab 9 – LAB EXAM</td>
<td></td>
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<tr>
<td>T, Apr 5</td>
<td>23</td>
<td>110</td>
<td>PSA/Gas separation</td>
<td>400-418, 421-438</td>
</tr>
<tr>
<td>Th, Apr 7</td>
<td>24</td>
<td>111</td>
<td>Lab 10 – Lab demo – ADSIM PSA Aspen Chromato. – obtaining data from article</td>
<td>Read article</td>
</tr>
<tr>
<td>T, Apr 12</td>
<td>25</td>
<td>110</td>
<td>PSA/Gas separation</td>
<td>421-431</td>
</tr>
<tr>
<td>Th, Apr 14</td>
<td>26</td>
<td>111</td>
<td>Lab 11 – Project</td>
<td></td>
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<tr>
<td>T, Apr 19</td>
<td>27</td>
<td>110</td>
<td>Lab 12 – Projects</td>
<td></td>
</tr>
<tr>
<td>Th, Apr 21</td>
<td>28</td>
<td>111</td>
<td>Test 2</td>
<td></td>
</tr>
<tr>
<td>T, Apr 26</td>
<td>29</td>
<td>110</td>
<td>Work on projects</td>
<td></td>
</tr>
<tr>
<td>T, Apr 28</td>
<td>30</td>
<td>111</td>
<td>Lab 13 – Project – reports and demos</td>
<td></td>
</tr>
</tbody>
</table>
and homework. The complete course syllabus is available from the author at <wankat@ecn.purdue.edu>.

Homework assignments were problems from the textbook plus one straightforward simulation. The textbook problems were similar to the test problems; of course, new problems were written for the tests. Since the students were all able to come to class early, they were given two hours for each test. Unfortunately, due to a mistake in solving an ion exchange problem on the second test, this problem, although solvable, was about an order of magnitude too difficult. I adjusted scores based on the performance of the second-best student in the class (the best student appeared to be an outlier whose performance was not representative of the class). The students appeared to be satisfied with the fairness (or generosity) of this procedure.

**ASPEN CHROMATOGRAPHY COMPUTER LABORATORY**

Aspen Chromatography is an algebraic-differential equation-solving program with a user interface for the solution of liquid adsorption and chromatography problems (see Figure 1). This simulator is very powerful and a trained user can often solve in a few hours a problem that used to take months. Aspen Chromatography uses the method of lines to solve the partial differential equations. The user can select both the differencing method to be used and the integration method to solve the resulting ordinary differential equations. Aspen Chromatography licenses are expensive for companies, but are reasonably priced for universities and can be bundled with other Aspen Technology programs. It cost $400 to add an Aspen Chromatography license for 60 users to Purdue's Aspen Technology order for University Lifecycle Package Bundle #1 (60 users) that cost $2,000. The current Version 12 is quite stable and reasonably user friendly, but not as user friendly as Aspen Plus. My experience with Aspen Plus is that 98-99% of the difficulties students have are due to operator error. With Aspen Chromatography about 80% of the students' difficulties are caused by operator error. As expected, the numerical integration routines, which use the method of lines to solve the partial differential equations, have difficulty converging when the profiles are steep and the isotherms are nonlinear. In general, the resources and expertise that have been developed for teaching with steady-state simulators are not available for sorption separations. More troubleshooting and more computer assistance will be needed.

Since much of my current research involves simulation of chromatography and simulated moving-bed systems with Aspen Chromatography, I am familiar with this simulator and my graduate students are very familiar with it. The graduate students and post-doc supported by the NSF grants were enlisted to help with the computer laboratory. With their aid, I developed 10 laboratory assignments including a laboratory
test. Each of the first eight laboratories showed how to build a flow sheet for a new aspect of Aspen Chromatography in a cookbook fashion, and then had the students solve simulation and design problems. Excerpts from the first laboratory assignment are presented in Table 2. All lab assignments are available from the author at <wankat@ecn.purdue.edu>.

As the semester progressed the amount of detail in the instructions was decreased. Most of the students stayed in the lab after the nominal closing time to finish the take-home assignments that accompanied the labs. The material covered in

**TABLE 2**

Excerpts from First Lab Assignment
A complete set of instructions for all labs is available from <wankat@ecn.purdue.edu>

The goal of this lab is to get you started in Aspen Chromatography. It consists of a cookbook on running Aspen Chromatography and some helpful hints. We will also simulate a real separation. Keep this lab assignment. You will want to refer back to it.

1. Log in to the computer. Go to Start, Programs, ChE Software, AspenTech, Aspen Engineering Suite, Aspen Chromatography 12.1, Aspen Chromatography. This opens a window if you are at a station that allows you to access the hard drive. Otherwise, you will get a message that essentially says, “The working folder is unavailable.” In this case, change working file to your N drive. Click on OK, and window should open. If not, run in circles, scream and shout, and ask for help.

2. We will first develop a simple chromatography (adsorption) column system. To do this, go to the menu bar and on the left side, File. Click on File and go to Templates, and in that window click on “Blank trace liquid batch flowsheet,” and click on Copy. It will ask for a file name. Use something like “column1.” This will be saved in your working folder. NOTE: In all file names and names for components, columns, streams, and so forth there must be NO spaces.

3. In the “Exploring simulation” box (LHS), click on “component list.” Then in box below (Contents) double click on Default. This lists A and B. Change these names to the names of the components to be separated (fructose and dextran T6). First, click “Remove all” button. Then in window below type in first component name (e.g., fructose) and click on “add” button. Do the same for all other components. Then click OK.

4. Now draw the column. Click on the + to the left of “Chromatography” in the “Exploring Simulation” box to open other possibilities. Click on the word “chromatography.” This should give “Contents of Chromatography” in box below. Double click on the model you want to use (Reversible – since it is most up-to-date). Click and drag the specific model you want: in this case “column,” move to the center of the Process Flowsheet Window. This gives a column labeled B1. Left click on B1, then right click to open a menu. Click on Rename. Call the block something like “column.” Click on OK.

19. If you have time, do this next step. If not, save your file (remember the file name), exit Aspen and do this step outside of class. The two peaks are not completely separated. There are a number of ways they can be separated more completely. Double the value of L, to L = 50 cm. Click on Rewind, change L in the column dimensions table, and then rerun the one-minute pulse input. When you run pure solvent, a pause time greater than 10 minutes is needed since doubling column length will double time for material to exit. Do this run and look at the result. Separation is better, but still not complete. Print your plot and label it. This plot will be handed in with the lab assignment. Save your file (remember the file name) and exit Aspen.

**TABLE 3**

Handout on What to Expect in Lab Exam

The exam will be open book and open notes. You may not open or use any of your old Aspen Chromatography files.

**Part A.** (50 points) Generic Problem. This is a demonstration that you can do a basic Aspen Chromatography simulation. Open up Aspen chromatography and use a “Blank trace liquid flowsheet template.” Set up a chromatographic column with one feed, a column, and a product. Use specified models for the column, feed, product, and connecting streams. Set up the system to process compounds that will be specified in the test. Have Aspen do discretization with xyz procedure with NN nodes (these will be specified in the test). Use a model with convection plus a specified form of dispersion, constant pressure, and velocity. If needed, the dispersion coefficients will be supplied. Use a linear, lumped parameter model with a specified driving force and constant mass transfer coefficients (they will be given). The isotherms will be given and the units for q and c will be specified. Operation is isothermal. The column length and diameter will be given. The adsorbent has the following properties: ee = 0.aa, rp = 0.bb, KD = 1.0, qs = cc kg/m³. The following feed values will be specified: flow rate, pressure, and all component concentrations. Use a specified integrator with a specified fixed or variable time. Use default values of the tolerances. Develop a graph of the product concentrations (on the same scale) versus time.

1. Run a breakthrough curve for zz minutes. Print, label, and turn in your plot.
2. Input a dd-minute feed pulse and develop with pure solvent for a total time of zz minutes. Print your plot, label, and turn in.
3. Compare your solutions for problems 1 and 2 at the peak center time.

There should not be any convergence problems in Part A.

**Part B.** (50 points) The second part of the lab test will be a design problem for one of the other processes that we have studied (e.g., flow reversal, adiabatic operation, SMB, TMB, ion exchange).

**TABLE 4**

Homework Assignment 4

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Units</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>L</td>
<td>200.0</td>
<td>cm</td>
<td>Length of adsorbent layer in column</td>
</tr>
<tr>
<td>D</td>
<td>2.0</td>
<td>cm</td>
<td>Internal diameter of column</td>
</tr>
<tr>
<td>ee</td>
<td>0.4</td>
<td>m³ / (m³ x bed)</td>
<td>Inter-particle voidage</td>
</tr>
<tr>
<td>rp</td>
<td>0.0</td>
<td>m³ / m³</td>
<td>Intra-particle voidage</td>
</tr>
<tr>
<td>dp</td>
<td>0.01</td>
<td>cm</td>
<td>particle diameter (needed to find E_p,friction)</td>
</tr>
<tr>
<td>ED</td>
<td>0.15</td>
<td>cm² / min</td>
<td>Constant Dispersion Coefficient</td>
</tr>
<tr>
<td>k_m,a_p</td>
<td>5.52</td>
<td>1 / min</td>
<td>Constant mass transfer coefficient</td>
</tr>
<tr>
<td>Isotherm is linear</td>
<td></td>
<td></td>
<td>Isotherm parameter (q and c both in g fructose/liter)</td>
</tr>
<tr>
<td>K'</td>
<td>0.69</td>
<td>dimensionless</td>
<td>Isotherm parameter (q and c both in g fructose/liter)</td>
</tr>
<tr>
<td>Isotherm is linear</td>
<td></td>
<td></td>
<td>Isotherm parameter (q and c both in g fructose/liter)</td>
</tr>
</tbody>
</table>

1. Use the Lapidus and Amundson solution with E_p,friction, to predict the behavior of fructose in a column packed with silica gel. The feed is 50 g/liter, the feed pulse lasts for eight minutes, and then it is eluted with water. The flow rate is 20 ml/min. The other values are:

Value | Units | Description
--- | --- | ---
L = 200.0 | cm | Length of adsorbent layer in column
D = 2.0 | cm | Internal diameter of column
e = 0.4 | m³ / (m³ x bed) | Inter-particle voidage
rp = 0.0 | m³ / m³ | Intra-particle voidage
dp = 0.01 | cm | particle diameter (needed to find E_p,friction)
ED = 0.15 | cm² / min | Constant Dispersion Coefficient
k_m,a_p = 5.52 | 1 / min | Constant mass transfer coefficient
K' = 0.69 | dimensionless | Isotherm parameter (q and c both in g fructose/liter)

2. Solve problem 1 using Aspen Chromatography.
3. Compare your solutions for problems 1 and 2 at the peak center time predicted by the local equilibrium solution, peak center time minus four minutes and peak center time plus four minutes.
the laboratory was cumulative, and by the end of the semester the students were able to simulate rather difficult problems without detailed instructions.

Part A of the lab test was a demonstration by the students that they had learned how to use Aspen Chromatography for simple simulations. Two weeks before the test the students were given the generic form of part A (Table 3). They were encouraged to supply data and parameter values to generate their own form of the test and then practice solving it. Part B, a design problem, proved to be more difficult. The lab test was given during a normal lab period that was extended to two hours. Since there were only seven students in the class and I knew them all well, no special precautions beyond proctoring the exam were taken to ensure honesty. (When I gave an Aspen Plus lab test in a core junior class with 95 students, I wrote a different test for each of the five lab sections and disabled both e-mail and access to student files.)

During the 10th lab, students first watched a computer demonstration of the use of ADSIM for pressure swing adsorption. Gas separations can involve large changes in flow rates which are not modeled by Aspen Chromatography. Then the students did a simulation with Aspen Chromatography that required them to determine the parameters needed for the simulation from a literature paper. In the earlier labs the students had been given all the necessary parameters since that makes troubleshooting of student difficulties much easier. Students were told that the purpose of learning how to extract parameters from the literature was to prepare them for the course project.

The course project was to develop a new Aspen Chromatography problem and solution suitable for one lab period. This is a form of Felder’s generic quiz. Students were required to use equilibrium and mass transfer data from the literature and/or the Internet, not from the textbook or from Aspen Chromatography demonstrations. They were told that projects that considered operational methods not taught in the lab or that combined different operational methods would be most impressive. Student groups presented an oral report, including a computer demonstration, and turned in a written report. As a treat for the students, I ordered pizza to be delivered after the oral reports were presented. The student projects—nonisothermal ion exchange, ion-exchange with flow reversal, and SMB separation—were quite well thought out.

Since seven students do not divide evenly into groups, I divided the class into groups of 3, 3, and 1. I used this unusual procedure because one of the graduate students is doing his thesis research with me and during the course of the semester he had much more practice with Aspen Chromatography than the rest of the class. He agreed to be a group of one, and the class accepted my rationale when the groupings were presented. The other two groups were made as equal as possible based on grades in the course.

**EXAMPLE PROBLEM**

Students solved a number of chromatography and adsorption problems during the semester. The real strength of numerical analysis is it can solve problems with complicated nonlinear isotherms that cannot be solved analytically. To avoid the “black box” effect, benchmarking of numerical solutions with analytical solutions was done for linear problems where analytical solutions exist. One convenient analytical solution is the Lapidus and Amundson solution\(^4\) with an effective dispersion coefficient that includes the effects of dispersion and mass transfer.\(^5\) Homework assignment 4 (see Table 4) illustrates benchmarking of analytical solutions. This assignment requires students to solve a simple, single-component chromatography problem with a large pulse of feed by the Lapidus and Amundson method and numerically with Aspen Chromatography.

The effective dispersion coefficient that lumps all dispersive effects into axial dispersion and assumes negligible mass transfer resistance was estimated to be 8.062 cm\(^2\)/min. This is much greater than the axial dispersion coefficient value 0.15 cm\(^2\)/min because mass-transfer resistance controls dispersion. The Lapidus and Amundson solution requires the use of superposition as a step up followed by a step down eight minutes later.

The same problem was solved numerically with Aspen Chromatography using two of the higher-order differencing schemes, Buds (Biased Upwind Differencing Scheme, a 4th-order method) and QDS (Quadratic Differencing Scheme), and the default UDS1 (Upwind Differencing Scheme 1) with 50 nodes. The solutions all used the Gear method with a fixed time step for integration. The QDS solution was done first with the actual value of the mass transfer coefficient and axial dispersion coefficient, and then with a very high mass-transfer coefficient (essentially no resistance) and the effective dispersion coefficient.

A screenshot of the Aspen Chromatography solution using
Buds with 200 nodes is shown in Figure 2 and a screenshot of the solution using UDS1 with 50 nodes is in Figure 3. The Lapidus and Amundson solution and the higher-order numerical solutions were bell-shaped curves and looked almost identical. UDS1 with 50 nodes also produced a bell-shaped curve, but it is much more spread out and has a lower peak concentration than the other curves because of significant numerical dispersion. The curves are different enough that students can easily see the differences by comparing Figures 2 and 3. Thus, the use of UDS1 with 50 nodes is numerically inappropriate for this problem.

Since the Lapidus and Amundson and the higher-order numerical analysis curves are so similar, differences can only be ascertained by looking at exact values of concentrations and times (Table 5). The concentrations predicted by the Lapidus and Amundson solution are: \( t = 25.575 \), \( c = 25.0 \) g/liter; \( t = 29.575 \), \( c = 48.54 \) g/liter (peak maximum); and \( t = 33.575 \), \( c = 24.975 \) g/liter. The Lapidus and Amundson solution has its peak center at exactly the time predicted by the local equilibrium solution (29.575 minutes). The peak concentration, peak time, and the predicted times for concentrations of 25.0 and 24.975 g/liter are given in Table 5 for the five different solutions. Since the two QDS solutions are quite close to each other, the use of an effective dispersion coefficient is valid for this linear system. All of the reasonable solutions (excluding UDS1) are quite close, with a small shift in times. Although the Buds solution with 200 nodes is the best fit to the analytical solution, in practical terms it doesn’t matter which is used. One of the lessons students learn from this and other benchmarking exercises is that they must pay close attention to numerical convergence.

RESULTS

A survey on the computer laboratory was developed, and a research exemption was obtained from the Purdue Institutional Review Board for Human Subjects Research. The students all responded to the survey (Table 6) on the last day of class. To avoid biasing any of the responses, the survey was administered by the undergraduate secretary; I was not in the room while the students filled out the survey, and the process was completed before the students knew there would be a pizza delivery.

The students’ responses to the survey (Table 6) show that previous knowledge of different computer applications varied from no knowledge to comfortable. General comfort levels with computers were high. With the exception of the speed of the Distributed Academic Computing System (DACS), which allowed remote access to Aspen Chromatography, laboratory operation was rated as about right. The students thought that both the computer labs and the lectures helped them learn sorption separations and that combining lecture and lab was an appropriate way to teach this material. Most of the comments are positive and reinforce the advantage of

![Figure 2. Screenshot of Aspen Chromatography solution for problem 2 in Table 4 using Buds with 200 nodes.](image1)

![Figure 3. Screenshot of Aspen Chromatography solution for problem 2 in Table 4 using UDS1 with 50 nodes (an inappropriate choice).](image2)
TABLE 5
Comparison of Solutions for Problems in Table 4

<table>
<thead>
<tr>
<th>L &amp; A Soln.</th>
<th>Aspen Chromatography Solutions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Buds QDS QDS (100 nodes) UDS1</td>
</tr>
<tr>
<td></td>
<td>200 nodes 100 nodes [E=E$_a$ MTC=100,000] 100 nodes</td>
</tr>
<tr>
<td>Peak time</td>
<td>29.575 29.6 29.5 29.5 28.7</td>
</tr>
<tr>
<td>Peak conc.</td>
<td>48.54 48.63 47.84 47.87 34.30</td>
</tr>
<tr>
<td>Time, min  @ upward curve, c=25.0</td>
<td>25.575 25.47 25.43 25.38 24.90</td>
</tr>
<tr>
<td>Time, min  @ downward curve, c=24.975</td>
<td>33.575 33.44 33.43 33.38 32.46</td>
</tr>
</tbody>
</table>

TABLE 6
ChE 558 Computer Laboratory Survey
(The average values and comments in italics are based on student responses.)
I. Computer experience before taking ChE 558. Rate your experience with the following applications (name package used where asked) using the following scale:
1 = Never used it before 558. 2 = Knew a little about it before 558. 3 = Used it some before 558. 4 = Very comfortable with it before 558.

<table>
<thead>
<tr>
<th>Application</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spreadsheets</td>
<td>2.0</td>
</tr>
<tr>
<td>Internet</td>
<td>3.7</td>
</tr>
<tr>
<td>DACS</td>
<td>1.4</td>
</tr>
<tr>
<td>Aspen Chromatography</td>
<td>1.1</td>
</tr>
<tr>
<td>Aspen Plus</td>
<td>3.1</td>
</tr>
<tr>
<td>Other steady-state simulator</td>
<td>3.1</td>
</tr>
<tr>
<td>(Mathlab, Mathcad, Maple, Mathematica)</td>
<td>3.1</td>
</tr>
<tr>
<td>DEQ-algebraic eqn solver</td>
<td>1.0</td>
</tr>
<tr>
<td>Data Base</td>
<td>2.0</td>
</tr>
<tr>
<td>Statistical package</td>
<td>2.9</td>
</tr>
<tr>
<td>Programming language(s)</td>
<td>2.1</td>
</tr>
<tr>
<td>Other</td>
<td>1.0</td>
</tr>
</tbody>
</table>

II. Computer comfort level. Rate your comfort level with the computer:
1 = Uncomfortable 2 = Neither comfortable nor uncomfortable 3 = Reasonably comfortable 4 = Very comfortable

<table>
<thead>
<tr>
<th>Comfort level</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>General comfort level using computer before class</td>
<td>3.7</td>
</tr>
<tr>
<td>General comfort level using computer now</td>
<td>3.7</td>
</tr>
<tr>
<td>Comfort level using Aspen Chromatography now</td>
<td>3.4</td>
</tr>
</tbody>
</table>

Comments:

III. Computer Laboratory Operation. Please circle the appropriate response.

<table>
<thead>
<tr>
<th>Question</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>The computer speed with direct installation (without DACS) was:</td>
<td>2.1</td>
</tr>
<tr>
<td>Computer speed using DACS was:</td>
<td>1.4</td>
</tr>
<tr>
<td>The laboratory assignments were:</td>
<td>2.0</td>
</tr>
<tr>
<td>Computer lab should be scheduled for:</td>
<td>2.0</td>
</tr>
<tr>
<td>The assistance available during lab from the graduate student and the professor was:</td>
<td>2.4</td>
</tr>
</tbody>
</table>

Comments: On one survey the term “graduate student” was underlined.

IV. Learning. Please answer these questions with the following scale:
1 = Strongly disagree 2 = (Between 1 & 3) 3 = Neither agree nor disagree 4 = (Between 3 & 5) 5 = Strongly agree.

<table>
<thead>
<tr>
<th>Learning question</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>The computer labs helped me learn adsorption and chromatography.</td>
<td>4.7</td>
</tr>
<tr>
<td>The lectures and homework on the theory helped me learn adsorption and chromatography.</td>
<td>4.9</td>
</tr>
<tr>
<td>The format of ChE 558 (combining lecture and computer laboratory) is appropriate for this subject.</td>
<td>4.6</td>
</tr>
</tbody>
</table>

Comments: “Because of the complexity of solving chromatographic problems, being able to see what actually happens in a column was quite nice.” • “Two-day Tues./Thurs. schedule worked great” • “Without lab a lot of material would be lost” • “More classroom time would be helpful to reinforce some material”

V. Suggestions for improving 558 computer lab:
“Run the simulations before the students run them.” • “More labs with more lab time, cover a little more material.”
the students thought this was a good course. I believe the students learned sorption separations in more depth in spring 2005 than in previous years. This seemed to be true across the spectrum of student abilities (good students learned more than good students previously, average students learned more than average students previously, and struggling students learned more than struggling students previously). Since in previous years the course also covered membrane separations, the breadth of coverage was less in 2005; however, the students learned sorption operations better despite less lecture time spent on this topic. Obviously, the 2005 students are also prepared to use the simulator.

DISCUSSION AND CONCLUSIONS

The students generally liked the format of lab and lecture and thought it helped them learn; however, these students all volunteered to take this elective knowing there would be a computer lab. Students who feel uncomfortable using the computer probably took other electives.

During the semester a faulty installation of Windows caused difficulties running Aspen Chromatography in the computer laboratory. For several weeks the students needed to log into DACS, which was slower than the direct installation. Once the problem was identified and Windows was reinstalled, we had no difficulties with the direct installation of the software. The comment in Table 6, “Run the simulations before the students run them,” probably referred to this difficulty running some of the labs on DACS. Lab 6, with flow reversal, ran without problems when I tested it using the direct installation of Aspen Chromatography in my office, but would not run on DACS. The student group that later did its course project with flow reversal had no difficulty following the original lab instructions and obtaining solutions with a direct connection. It is important to have reliable computer support before scheduling use of any simulator.

If there are transferable skills in learning how to use simulators, students who become skilled with, for example Aspen Plus, will learn to use another simulator faster. This appeared to be true for Aspen Chromatography. Thus, even if they never use simulators taught in the curriculum, the experience of learning to use these simulators will probably help graduates efficiently learn to use simulators on the job.

ACKNOWLEDGMENT

The assistance of Nadia Abunasser, Jin-Seok Hur, Weihua Jin, and Dr. Jeung-Kun Kim is gratefully acknowledged. The computer personnel in ChE—George Bailey and Eric Pratt—were extremely helpful in making the computer lab run smoothly. This project was partially supported by NSF grants CTS-02112008 and CTS-0327089. This paper was presented orally at the AIChE Annual Meeting, Cincinnati, November 2005.

REFERENCES

4. Wankat, P.C., Rate-Controlled Separations, Kluwer, Amsterdam (1990) (There were earlier printings by Elsevier and Blackie. Kluwer is now part of Springer.)
HOW TO TEACH (ALMOST) ANYBODY (ALMOST) ANYTHING

RICHARD M. FELDER AND REBECCA BRENT
North Carolina State University • Raleigh, NC 27695

It seems it’s no longer enough for you to teach about the Navier-Stokes equations and potential flow past submerged objects. The ABET coordinator says that students in the fluids course have to be taught oral communications too, and the department head got inspired at some workshop and now wants to teach critical thinking in every course, including fluids. You argued at the faculty meeting that it’s all you can do to get through fluids in the fluids course but got little sympathy, and it looks like there’s no way out of it.

You probably have some questions at this point, like, (a) Exactly what are those skills I’m supposed to teach? (b) Can they be taught (as opposed to you either have them or you don’t) and (c) How? For an answer to (a), we invite you to check out an article we wrote on learning objectives, teaching strategies, and assessment methods that address ABET Outcomes 3a–3k. The answer to (b) is, yes. This column suggests some answers to (c)—how do you enable students to develop and improve a targeted skill, whether ABET-related or not? While we don’t guarantee that the techniques we’ll recommend will always work for all students, we’re confident the results will be good enough to satisfy ABET and your department head, and—as long as your expectations are realistic—you.

1. R.M. Felder and R. Brent, “Designing and Teaching Courses to Satisfy the ABET Engineering Criteria,” J. Engr. Education, 92(1), 7-25 (2003), <www.ncsu.edu/felder-public/Papers/ABET_Paper_JEE.pdf>. If you’re not an engineering educator or you are one and just got back from the latest Mars expedition, let us explain that Outcomes 3a–3k are specified attributes engineering students in accredited programs should have by the time they graduate. They include the usual technical abilities but also such things as communication skills, the ability to work effectively in multidisciplinary teams, and an understanding of the professional and ethical responsibilities of an engineer.


► Write detailed learning objectives and let the students in on them

Learning objectives (or instructional objectives) are explicit statements of what students should be able to do to demonstrate that they have learned what you want them to learn. The objectives must specify directly observable actions (list, explain, calculate, derive, model, critique, design . . .). Verbs such as “learn,” “know,” “understand,” and “appreciate” are unacceptable. You can’t see students understanding something; to know whether or not they understand, you have to ask them to do something that you can see that demonstrates their understanding. For examples, see <www.ncsu.edu/felder-public/che205site/studyguide2.pdf>, a study guide containing a subset of the learning objectives for the introductory chemical engineering course. Even if you don’t know the course content, you should be able to convince yourself that if the students can do everything on those two pages, they have

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Rebecca Brent is an education consultant specializing in faculty development for effective university teaching, classroom and computer-based simulations in teacher education, and K-12 staff development in language arts and classroom management. She codirects the ASEE National Effective Teaching Institute and has published articles on a variety of topics including writing in undergraduate courses, cooperative learning, public school reform, and effective university teaching.

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probably learned what the instructor wants them to learn in that part of the course.

Our first recommendation is to write detailed learning objectives and give them to the students as study guides for exams and as guidelines for other assignments such as project reports and oral presentations. Make sure your objectives cover all the skills you would like students to master, especially high-level skills (such as critical and creative thinking) and the ABET-mandated outcomes that have not been traditionally addressed in engineering courses, such as communication and lifelong-learning skills. When you are explicit about your expectations, the likelihood that your students will meet them goes up dramatically, especially if the expectations involve difficult or unfamiliar material.

**Teach skills before you assess them**

Take problem formulation as an example—another one of those ABET outcomes few of us ever thought about before they showed up in the Engineering Criteria. Suppose an objective in your fluids course states that the students should be able to make up (and solve) fluid dynamics problems whose solutions call for creative thinking. If you simply expect the students to do that, most won’t get what you’re after and you’ll see mainly problems that look like, “Given X and Y, calculate Z.” That shouldn’t surprise or disappoint you, since nobody ever taught them how to do what you’re now asking them to do.

If, however, you first explain and illustrate what you’re looking for, then show several good and bad examples and have the students work in small groups in class to critique them, then give and grade two assignments that include the same task and perhaps show some submissions from students who got the idea, you’ll start seeing creative problems. Doing all that would allow you to check off both problem formulation and critical thinking on the list of outcomes addressed in your course. You can do the same thing for, say, writing technical memos (communication and critical thinking), analyzing workplace case studies (professional and ethical awareness), or critiquing an engineering-related article in the popular press (professional awareness, communication skills, understanding the societal impact of engineering solutions, knowledge of contemporary issues, and lifelong-learning skills).

**Use rubrics for grading**

Problem-solving and multiple-choice tests are relatively easy to grade, and if the grading system is rational, students should have no trouble understanding what they did wrong and why they got the grade they did. The same is not true of written project reports, essays, case study analyses, and oral presentations. When students just get grades and a few written comments as feedback, they may understand why they were marked down but may have little idea about how to do it better next time.

There’s a better way. Use a rubric to grade anything that involves subjective judgment on the part of the grader. Decide on criteria you will use to evaluate the memo, report, or presentation (e.g., technically accurate, complete, appropriately documented, well organized, well written, good visuals, sound theoretical analysis . . .); assign weights to each criterion; and—for a four-point rating scale—briefly summarize the attributes of a 1, 2, 3, and 4 for each criterion. Then, when you give students illustrative written products or oral presentations to critique in class, have them use the rubric individually and then compare their ratings, and then share your ratings with them. When you hand back their assignments, give them your completed rubric as well—and watch how they improve on the next assignment. As with learning objectives, when a grading system is clear, the students are more likely to meet expectations.

**If a skill is important to you, assess it**

Once you’ve communicated your learning objectives and assessment method for a particular skill, and you’ve provided examples and practice in applying the skill, then (and only then) is it legitimate to test the students’ mastery of the skill—and at that point, you definitely should. Engineering students barely have enough time to keep up with their assignments; they don’t have time to dig deeply into everything in all of their courses. If they are sure that something requiring effort on their part to learn won’t count toward their grade, most won’t bother to learn it. That’s not laziness—that’s rational behavior. The assessment drives the learning: if a skill is important to you, assess it.

Here’s our challenge to you: (a) Pick a problem-solving or professional (“soft”) skill that your students have always had trouble mastering; (b) write one or more learning objectives that list the things you might ask students to do to demonstrate mastery of that skill; (c) share the objectives with the students—if possible, as part of an exam study guide; (d) give your class examples of what you’re looking for and several opportunities to practice the skill, in and out of class; and (e) assess the students’ mastery of the skill (using a rubric if subjective judgment is involved) by asking them to do some of the things specified in the objectives. If you see better performance than you’ve ever seen (which we always have when we’ve done all that), consider making this strategy a permanent addition to your teaching toolkit.

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4. You can see an illustrative rubric for evaluating student presentations at <http://www.ncsu.edu/midlink/rub.pres.html>.

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All of the Random Thoughts columns are now available on the World Wide Web at http://www.ncsu.edu/effective_teaching and at http://che.ufl.edu/ccc/
HYPER-TVT: DEVELOPMENT AND IMPLEMENTATION OF AN INTERACTIVE LEARNING ENVIRONMENT

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ETH Swiss Federal Institute of Technology Zurich • CH-8092 Zurich, Switzerland

Rapid advances in information technology and easy access to the Web have motivated students and educators to use more and more Internet and multimedia technology for educational purposes. Educators and students are challenged by the great potential of the Internet for delivering and sharing a large amount of information among a greater public, and by the possibility of creating alternative and breakthrough ways of teaching and learning by using advanced software. Today, in almost every field of education, a broad range of e-learning material is available online. “Computer-based learning system” has been the catch phrase for the last few years to indicate a wide area of systems using the Web and multimedia technology for education.

These systems can be classified depending on the main functionality and research focus as: computer-aided education systems; multimedia/virtual laboratory; distance-learning systems; or intelligent tutoring systems.[1] This classification identifies different levels of e-education: from the simple integration of computer technologies into the traditional teaching system—where face-to-face meetings and personal relationships are still of primary importance—to the stage where the information transfer rate is no longer managed by a human tutor but it is adaptively controlled by an intelligent computer system.[1] In all cases the objective is always to use the technology not just for technology’s sake, but to enhance the quality of higher education. This contribution aims to present Hyper-TVT, a public interactive learning environment on separation process technology (<www.hyper-tvt.ethz.ch>). The name Hyper-TVT derives from the word “Hypertext” and the German acronym of the course name, i.e., “Thermische VerfahrensTechnik,” meaning thermal separation processes.

MOTIVATION

In recent years, the educational concept has been extended toward the integration of new generations of Internet- and computer-based courses intended to lower the gap between theoretical knowledge and practical experience in the modern curriculum for process and chemical engineering. This concept addresses the nowadays frequent request of students for continuous, adequate preparation (i.e., solving practical...
problems and facing real issues), thus allowing them to become better aware of the physical reality of the processes, the industrial world, and their future profession. Likewise, Lewin, et al., claimed that the “instruction of chemical engineers should reflect the challenges they face in industry.”[2] Indeed, teaching and learning in the field of chemical engineering can be enormously enhanced by the use of information technology and Web tools. In comparison to traditional textbooks, these new avenues can offer videos, animations, and interactivity that help students visualize the reality behind equations and diagrams, thus compensating for the lack of practical experience in common engineering curricula.

In that respect, a very good reference for an e-learning environment is, in our opinion, the one developed by Fogler and Gulmer in the field of chemical reaction engineering.[3] The Web site is offered by the University of Michigan and is freely accessible online. Besides texts, equations, and diagrams, this Web site provides interactive tools for self-assessment, videos, and audio descriptions to demonstrate the concepts of chemical engineering, helping users visualize the applications within the industrial world.

In the field of separation process technology as well, all top-ranking technical universities provide e-learning systems and online courses in an effort to extend traditional chemical engineering classes. Access to these modules, however, is very often restricted to enrolled students of the course or to faculty,[4, 5] and a lot of material is available only in closed environment via CD-ROM or password-protected LAN.[6] In other cases, the courses are freely accessible but a lot of the online material provides only course information and assignments,[7] or provides the course syllabus as pdf files or PowerPoint presentations. Although this static material is of high quality and has the benefit of being always available online, a very low degree of interactivity, or none at all, is offered and therefore this approach exhibits only minor advantages as compared to traditional textbooks.

A lot of interesting material covers only some specific topic of the separation processes, such as distillation. Comprehensive theory, pictures, schemes, diagrams, and videos are published online by research groups at universities and companies working in the field.[8, 11] Finally, other universities and organizations are active in the e-learning field, providing databases and links to facilitate searches for material, organizations, communities, journals, and publications about e-learning technology, such as ChemEngInfo,[12] World Lecture Hall,[13] EuPaCE.net,[14] and MERLOT.[15]

The class on separation process technology is compulsory in most curricula in process and chemical engineering. It demonstrates the application of chemical engineering principles within an industrial context for effective design of processes, particularly of multistage separation processes. Topics covered are: fundamentals of separation processes; absorption and stripping; flash evaporation; distillation; and liquid-liquid extraction. These subjects are particularly suited for the development of e-learning tools due to the synergy between theoretical issues and practical experience. Hyper-TVT is a freely accessible e-learning system for students of chemical and process engineering at the ETH Swiss Federal Institute of Technology Zurich, and also for all individuals and institutions involved or interested in process and chemical engineering education and practice. Its purpose is to complement the already existing tools, and, at the same time, to compensate for their limitations in access and scope, and to take full advantage of interactive and multimedia technology. Therefore Hyper-TVT is not comparable to commercial process simulators such as HYSYS, plant, CHEMCAD, or Aspen Plus, which have different scopes and purposes.

Hyper-TVT is a didactic support, which is complementary to, but not a replacement for, traditional lectures and textbooks. In fact, combining Hyper-TVT with conventional education elements—e.g., lecture, textbook study, and discussion with the teacher—contributes to enhancing teaching effectiveness and flexibility. The Web site offers both educators and students a number of tools such as videos, animations, simulations, and a self-assessment environment, thus creating a better balance between synchronous and asynchronous approaches in teaching and learning, as illustrated in Figure 1. The design concepts, the didactic content, and the technical features of Hyper-TVT will be discussed in detail in the following chapters.

**DESIGN CONCEPT**

**“Textbook” structure**

The structure of the Web site is organized in chapters and paragraphs, as it would be for a traditional textbook. Figure 2 is a screenshot of the page content of the “Contactors”
lesson as an example of page structure. The choice of minimizing any structural complexity has two purposes: to let students and educators focus better on the Web site content, and to make using the tool as easy as possible. Within each paragraph the topic is presented using explanatory text, images, and interactive diagrams and schemes. Every paragraph develops a certain concept independently and completely by integrating the multimedia material within the text and by providing logical links to other pages of the learning environment.

Navigability

Due to its simple structure and the implementation of a navigation system, the Hyper-TVT Web site is easy to browse. In every section of the Web site, menus help answer three fundamental questions: Where am I?; Where have I been?; Where can I go? Within every lesson, an interactive table of contents highlights the user’s current location within the lesson, helps to find other related content, and suggests the logical learning sequence, as shown in Figure 3.

Interactivity

The added value of a Web-based educational system is the interactivity offered to students and educators. The Hyper-TVT system stimulates interactivity through pictures, animations, a modeling and simulation environment, videos, and self-assessment tools, all of which are very consistent with the learning objectives in the domain of process and chemi-
cal engineering. Two examples of animations about distillation topics are shown in Figure 4.

Reusability

Hyper-TVT teaches some of the key separation processes technologies, i.e., a fundamental subject in the process and chemical engineering curriculum that is well established. For this reason, the content of Hyper-TVT is not expected to be subjected to revision in the near future, if ever.

Therefore the Hyper-TVT Web site is available, now and in the future, to students, educators, and practitioners of different institutions, countries, and educational sectors, e.g., higher education, vocational training, professional organizations, industry, and schools.

Outreach to other categories of users

The target users of Hyper-TVT consist of all individuals and institutions involved in process and chemical engineering education. Its simple structure, links, and interactive modules, however, make Hyper-TVT easy to be followed by others, who, though not chemical or process engineers, still need or want a quick and complete overview of the separation process technologies.

DIDACTIC CONTENT AND METHOD

Hyper-TVT consists of seven lessons presenting class material using text, images, animations, interactive tools, and simulation environments. These are:

1. Introduction of separation processes
2. Fundamentals of separation processes
3. Contactors
4. Absorption and stripping
5. Flash evaporation
6. Distillation
7. Liquid-liquid extraction

The first lesson is a presentation of the separation processes and their role and importance in the industrial context. In the second lesson, basics of thermodynamics and mass transfer are revisited; these are fundamental for further understanding of multistage separation technologies. Lesson number three, on contactors, presents an overview of the industrial equipment for gas-liquid and liquid-liquid separation. Lessons four, six, and seven cover the design of three of the most important multistage separation processes. The fifth lesson, on Flash evaporation, introduces many concepts useful to understanding distillation. The didactic approach first provides students with all basic concepts and tools needed. Then, students are challenged to use the new material to solve problems given as home assignments. Besides the lessons, three additional sections of the Web site contain videos that can be streamed, PowerPoint and pdf files that can be browsed, and tests that can be used for self-assessment. The videos focus on industrial equipment for separation processes (i.e., lesson three) and have been partly created for this use and partly provided by companies, e.g., Sulzer ChemTech, Kihmi, and FRI (Fractionation Research, Inc.). In the videos, an off-screen narrator guides the visitor into a virtual tour of the real equipment to observe directly and in detail phenomena that neither words nor photos alone would be able to clarify. A screenshot of a video about column internals is shown in Figure 2. Videos can have a great didactic value, and not just in the field of chemical and process engineering, because they overcome physical barriers and bring the world into the classroom. The PowerPoint and pdf files are a collection of mathematical derivations of the equations used in the lessons for process design. Their format allows students to use them interactively online or to download them for further reading. The test section provides multiple choice and descriptive questions. Students also have the option to submit completed questionnaires, receive support online, and access and print homework assignments as pdf files. Another important element of the Hyper-TVT Web site is its database. The database contains five specific search categories, e.g., text, notation, images, glossary, and bibliography. The "text" category provides links to pages where keywords are mentioned. "Notation" contains detailed explanation of all the symbols used in the Hyper-TVT Web site. "Images" is a collection of diagrams and graphics already present in the lessons, but it...
Feedback from the ETH Zurich students indicates 95% appreciated the learning environment and found it useful, both during lectures and outside the classroom.

The whole environment is continuously revised based on feedback collected in different ways. The ETH students attending the class are asked to fill out an evaluation form at the end of the semester, and an online evaluation form allows students and educators from other institutions to provide helpful comments. On one hand, these have been used for modifications, refinements, and improvements of some parts of the Web site. On the other hand, and more in general, feedback from ETH Zurich students indicates 95% appreciated the learning environment and found it useful, both during lectures and outside the classroom, as support material and in completing homework assignments. The Web site is used very intensively in preparation for the final exam. The major advantage, as indicated by students, is the interactive and audio-visual content, i.e., the flash animations, videos, diagrams, and pictures. As a further positive comment, students and practitioners underline the easy navigability offered by the Web site. Very positive reactions have been received from educators of other institutions and technical universities as well. The result, although possibly not yet statistically relevant, is very encouraging about the usefulness of the Web site.

Use of the Web site is not a requirement of the separation processes class for students at ETH Zurich. Rather, the Web site is presented at the beginning of class as additional support and its interactive material and videos are used during some of the lectures. In this way, students get a first impression of the real world of separation process technology while gaining familiarity with the Web site, thus making its use easier. The purpose of this approach is to increase student interest about the proposed subject with more motivating material and tools, thus stimulating their self-study skills and responsibility.

The most difficult issue we have experienced as instructors has been integration of the Web site during traditional lectures. In fact, this implies an allotment of time in the lecture plan for use of the computer-based didactic material. This is not a simple task since the traditional course has to be reorganized and restructured to implement a new hybrid methodology (traditional and computer-based lecture). It requires an additional effort and a lot of motivation by the instructor. For students as well the integration of the Web site into their traditional way of learning is challenging. Many studies have been conducted to determine what factors impact the perception and acceptance of new e-learning tools on students. Such tools generally require students to become more independent and
more responsible of their personal learning processes, and
to apply new technologies—an additional workload that is
not always well received at first. With the time and guided
assistance of the tutor, however, students usually recognize
and appreciate the benefits of the computer-integrated edu-
cational system. Typically, their learning efficiency and
performance improve, resulting in increased self-confi-
dence and greater motivation.

The Hyper-TVT system is available online (<www.hyper-
tvt.ethz.ch>) and can be accessed without restrictions
through the Web.

Hyper-TVT shows how dissimilar pedagogic methods—tra-
ditional and Web-based—can be implemented in parallel to
offer a more stimulating and productive learning environ-
ment. Students, in turn, gain tools for self-paced learning
and become more autonomous. Use of Hyper-TVT can foster
their skills in analysis, synthesis, and evaluation. Finally, the
lecture time with the instructor can be invested more effec-
tively to discuss advanced issues. Our experience in using
Hyper-TVT has been very positive so far, and we encourage
students, educators, and chemical and process engineers to
explore it as well.

ACKNOWLEDGMENTS

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of ETH Zurich, which the authors thank for funding and
support.

REFERENCES

Virtual Laboratory System for Unit Operations and Process System
5. <http://www.ucl.ac.uk/learningtechnology/webct/>
   <http://webct1.imperial.ac.uk/webct/public/home.pl>
   <http://www.kcl.ac.uk/learningteaching/e-learning>
7. <http://ocw.mit.edu/OcwWeb/Chemical-Engineering/10-32Spring-
2003/CourseHome/index.htm>
8. <http://www.eng.usf.edu/~bhethana/McTh/McTh.html>
   htm>
rowsecat=101>
   of the SVC Embryology Course,” Proceeding of the 5th International
INTEGRATING BIOLOGICAL SYSTEMS
in the Process Dynamics and Control Curriculum

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The discipline of chemical engineering is evolving, as evidenced by the recent wave of departmental name changes that reflect both the increasing number of chemical engineering faculty involved in research on biology-oriented topics, and the fact that the percentage of chemical engineering undergraduates obtaining initial employment with companies in the biotechnology and biomedical sectors increased from 4.6% in 1998 to 10.3% in 2001-02. A series of MIT-organized and NSF-sponsored workshops examined the current state of undergraduate chemical engineering education and recommended a sweeping set of changes. Foremost among the proposed changes were the introduction of biology as a core science, the importance of addressing complexity, and the expanded use of the systems approach. The present discussion focuses on these three elements within the context of the traditional process dynamics and control curriculum.

The dynamics and control course, typically taught late in the junior or senior year, is a natural point for including biological systems content along with chemical process material. Due to the focus on general principles rather than specific processes, biological systems can be integrated without detracting from the coverage of more traditional applications. This expanded vision of the system dynamics and control curriculum requires the following difficult issues to be addressed: (1) how can these complex systems be introduced in a meaningful way to undergraduate chemical engineers with little background in biology?; and (2) what changes are required to include biological content without sacrificing the traditional core of process dynamics and control? The objective of this paper is to provide some practical answers to these questions using the experiences of three courses taught at our respective institutions. The first two examples illustrate the introduction of biological content into the traditional process control course, while the third example focuses on the development of a new course in which the systems approach is applied to a diverse set of biological problems.
INTEGRATION OF BIOLOGICAL SYSTEMS CONTENT

A typical process dynamics and control course covers a broad range of new material at a rather brisk pace. To produce students who can apply traditional dynamic analysis and controller design techniques is a formidable challenge even when the focus is purely on chemical process systems. The addition of biological content along with the requisite modeling and analysis techniques requires a carefully crafted course to avoid leaving students overwhelmed. A possible structure for a semester-long course is illustrated by the syllabus in Table 1, where NL is the number of lectures allotted to the specific topics listed in all caps. Bold entries represent new topics specific to biological systems. Italicized entries are theoretical topics often considered optional in a traditional course but which are viewed as important for a biologically oriented course.

The introduction of state-space models and associated analysis tools is essential for the treatment of biological systems due to their complexity (e.g., high order, multivariable, highly nonlinear), which often precludes simple Laplace domain treatment. A few lectures on matrix algebra and linear state-space systems are necessary to review core material and ensure that students with deficient backgrounds understand the basic concepts. When combined with the linear systems analysis lecture, this material allows the calculation of eigenvalues to determine stability and matrix rank for the analysis of controllability and observability. The nonlinear systems theory lecture includes the traditional topic of Jacobian linearization as well as introductory coverage of phase plane analysis, multiplicity, and bifurcations. Biological systems are inherently nonlinear, given the existence of saturation phenomena, stable oscillations, etc. As such, a student must have a working knowledge of nonlinear systems to be able to identify such behavior and analyze system response in the presence of nonlinear phenomena. Without question, this topic could comprise a course unto itself. Some basic tools (e.g., phase planes, limit cycles, bifurcation) are easy enough to teach in a class or two, however. These provide students with an ability to identify nonlinear system characteristics, even if they cannot design a linearizing-state feedback controller to address the underlying nonlinearity. Feedback is a concept that is introduced naturally in the context of biological system examples. The representation of biological control systems using various elements of the traditional block diagram is particularly effective. This approach, however, should be used carefully to avoid concealing the complexity of the underlying biological processes.

Throughout the topic sequence in Table 1, a number of examples serve to highlight the breadth of opportunities for application of the theoretical concepts presented in the course. Table 2 provides a list of potential case studies. For each

<table>
<thead>
<tr>
<th>TABLE 1</th>
<th>Proposed Syllabus for a Biologically Oriented Dynamics and Control Course</th>
</tr>
</thead>
<tbody>
<tr>
<td>NL</td>
<td>Topics</td>
</tr>
<tr>
<td>-----</td>
<td>---------------------------------------------------------------</td>
</tr>
</tbody>
</table>
| 4  | DYNAMIC MODELING  
Principles of fundamental modeling; chemical and biological process examples; introduction to empirical modeling |
| 7  | LINEAR AND NONLINEAR SYSTEMS ANALYSIS  
Matrix algebra and linear state-space systems; linear systems theory; introduction to nonlinear systems theory; dynamic simulation; chemical and biological process examples; introduction to the Laplace transform |
| 7  | FEEDBACK SYSTEMS  
Basic principles of feedback; physiological control systems; homeostasis as a setpoint-free feedback system; feedback in biochemical reaction networks; closed-loop response analysis; servo vs. load behavior; feedback control of chemical process systems; closed-loop drug delivery |
| 8  | FEEDBACK CONTROL SYNTHESIS  
Basic principles of model-based controller design; PID controller design and tuning; advanced single-variable control techniques; multivariable control techniques; model predictive control; chemical and biological process examples |
| 4  | ADVANCED TOPICS  
Large-scale systems and plantwide control; parameter estimation and experimental design; state estimation; introduction to systems biology |

TABLE 2

Possible Case Studies for the Process Dynamics and Control Course

<table>
<thead>
<tr>
<th>Chemical Processes</th>
<th>Biotechnological Systems</th>
<th>Biomedical Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuous and/or fed-batch polymerization reactor; distillation column; continuous pulp digester; paper machine; simple plantwide example (e.g., reactor and separator); semiconductor process (e.g., lithography); photovoltaic film processing; fuel cell</td>
<td>Continuous and/or fed-batch fermentor; yeast energy metabolism; cell stress response (e.g., heat shock); eukaryotic cell cycle; bacterial chemotaxis</td>
<td>Baroreceptor vagal reflex (blood pressure control system); insulin-dependent diabetic patient (glucose-insulin metabolism/ control); circadian rhythm gene regulatory network; anesthesia control; drug delivery for HIV treatment; drug delivery for cancer treatment</td>
</tr>
</tbody>
</table>
A major conclusion of the MIT-organized education workshops was that multiscale phenomena should be incorporated throughout the undergraduate chemical engineering curriculum. A useful connection between the traditional chemical and biological examples listed in Table 2 is the wide range of time and length scales at which these systems can be analyzed. Polymerization reactor models can be developed using input-output representations, detailed descriptions of the individual polymer particles and their interactions, or a variety of scales in between. Analogous models can be developed for microbial fermentors where lumped descriptions of cellular processes are provided by unsegregated models and detailed descriptions of the individual cells are provided by cell population models. While the introduction of biological systems content is not necessarily required to illustrate these concepts, we feel that an integrated program of chemical and biological examples will reinforce key concepts and demonstrate that these diverse examples are conceptually similar.

UMASS CHE 446: INCORPORATING BIOTECHNOLOGY

The process dynamics and control course at the University of Massachusetts (<http://www.ecs.umass.edu/che/che446>) has traditionally focused on Laplace transform methods and chemical process applications. This course usually represents the only extensive exposure to dynamic modeling and feedback control in the undergraduate curriculum. Biological systems were chosen as an appropriate vehicle for introducing the key elements of biological transformations, multiscale phenomena, and systems-level analysis identified in the MIT-sponsored education workshops. Rather than completely change the existing course content, a more conservative approach based on the integration of biological systems and the requisite analysis techniques was pursued.

The current syllabus for the UMass course (ChE 446) is shown in Table 3, where new topics introduced in the past two years are italicized. The first few weeks are focused on fundamental modeling because undergraduate students typically have little experience formulating dynamic balance equations. Two biological examples—a continuous yeast fermentor model and a structured yeast cell model—are introduced and revisited throughout the semester. Both time domain and Laplace domain analysis techniques receive extensive coverage. A major focus is the formulation and stability analysis of linear state-space models. Engineered and natural-feedback systems are introduced in parallel to highlight their common features and unique properties. While most of the material on single-loop controller synthesis is traditional, an introduction to time domain controller design and analysis techniques is provided to parallel the Laplace domain methods. The final few weeks are focused on multivariable control systems with an emphasis on linear model predictive control.

To accommodate the new material on biological systems and time domain techniques, material previously covered in the course had to be de-emphasized or virtually eliminated. Topics that received reduced coverage included transfer function models, Laplace domain analysis and design techniques, advanced single-loop control strategies, and traditional chemical process examples. Frequency domain techniques received very limited coverage. While these topics are admittedly important, a broader view of dynamic systems and feedback

<table>
<thead>
<tr>
<th>NL</th>
<th>Topics</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>FUNDAMENTAL MODELING</td>
</tr>
<tr>
<td></td>
<td>Basic principles; chemical process examples (nonisothermal chemical reactor; binary flash unit; binary distillation column); biochemical system examples (continuous fermentor model; metabolically structured yeast cell model)</td>
</tr>
<tr>
<td>7</td>
<td>DYNAMIC SYSTEM ANALYSIS</td>
</tr>
<tr>
<td></td>
<td>Linear algebra (solution of matrix equations, state-space models; eigenvalues and eigenvectors); time domain analysis (basic stability concepts, linearization of nonlinear models, linear stability analysis, continuous fermentor example); Laplace transforms; transfer function models; empirical models; parameter estimation</td>
</tr>
<tr>
<td>6</td>
<td>FEEDBACK SYSTEMS</td>
</tr>
<tr>
<td></td>
<td>Process control systems; biological feedback systems (engineered vs. natural feedback systems, yeast sulfate assimilation pathway, baroreceptor vagal reflex); closed-loop transfer functions; closed-loop stability</td>
</tr>
<tr>
<td>7</td>
<td>FEEDBACK CONTROL SYNTHESIS</td>
</tr>
<tr>
<td></td>
<td>PID-controller tuning; internal model control; time domain controller design (state feedback, pole placement, model matching, continuous fermentor example); feedbackforward control; cascade control</td>
</tr>
<tr>
<td>5</td>
<td>MULTIVARIABLE CONTROL</td>
</tr>
<tr>
<td></td>
<td>Control loop interactions; decentralized control; discrete-time models (discretization of continuous-time models, convolution models, prediction models); model predictive control (controller design and tuning, constraint handling, real-time optimization, continuous fermentor example)</td>
</tr>
</tbody>
</table>
control was deemed to be more important given current trends in the chemical engineering profession. In fall 2003, each student was asked to evaluate the biological systems content using a score ranging from “5” if they strongly agreed the objective was achieved to “1” if they strongly disagreed the course objective was achieved. Results obtained from the 21 respondents are summarized in Table 4. The average scores are similar to those obtained for the other course objectives, thereby indicating that the biological content was successfully integrated into the course.

PITT CHE 0500: INTRODUCING BIOMEDICINE

The biology component in the Systems Engineering I: Dynamics Modeling course (ChE 0500, <http://sage.che.pitt.edu/~che0500>) at Pittsburgh focuses on the analysis of, and controller synthesis for, biomedical systems at the whole-organism level. By integrating the research activities in modeling and control of diabetic and cancer case studies within the undergraduate class, students are exposed to a novel application area. This format has resulted in a steady flow of undergraduates interested in undergraduate research, and an increased interest in graduate study. Students at Pitt were posed the same questions as those at UMass; responses can be found in Table 4. While confidence in dynamic balance construction is not as high as that shown in the UMass course, the other questions return similar quantitative responses indicating that the biomedical topics were well received.

ChE 0500 is approached from a model-based perspective; approximately half of the course is focused on modeling systems using both fundamental and empirical approaches, in both continuous and sampled-data (i.e., discrete) domains. From the fundamental modeling perspective, the students are taught to distinguish pharmacokinetics (the time profile of a drug) from pharmacodynamics (the disease dynamics, effect of the drug on the disease, and toxicity) in much the same way valve dynamics and process output response are captured by separate blocks in a block diagram. The remainder of the course focuses on the model-based synthesis and analysis of classical and advanced control systems, as in Table 1.

As a case study, consider the insulin-dependent diabetic patient depicted in Figure 1. Fundamental model construction introduces students to the key variables of the diabetic-patient problem and demonstrates the utility of skills developed elsewhere in the curriculum (e.g., dynamic mass balance with reaction, transport resistance) in the modeling of biomedical problems. Students then work with this model, or suitable lower-order approximations, throughout the semester on in-class problems, homework, etc.

The case study method[14] is commonly employed in teaching to facilitate in-depth treatment of problems in limited

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**TABLE 4**

<table>
<thead>
<tr>
<th>Question</th>
<th>Score UMass</th>
<th>Score Pitt</th>
</tr>
</thead>
<tbody>
<tr>
<td>I can construct a dynamic model of a biological system.</td>
<td>3.83</td>
<td>3.23</td>
</tr>
<tr>
<td>I can perform dynamic system analysis and controller design in the time domain.</td>
<td>3.78</td>
<td>3.71</td>
</tr>
<tr>
<td>I can apply dynamic system analysis techniques to evaluate properties such as stability.</td>
<td>3.89</td>
<td>3.76</td>
</tr>
<tr>
<td>I can describe the relevance of feedback control theory to biological systems.</td>
<td>3.83</td>
<td>3.77</td>
</tr>
</tbody>
</table>

---

*Figure 1. Open-loop schematic of the diabetic patient. Small solid blocks represent the fundamental model, with manipulated input insulin delivery rate, meal disturbance, exercise disturbance, and glucose concentration measurement.*
classroom time. An added benefit would be to use a unifying application, thereby allowing students to focus their attention on a single problem. The diabetic patient is one such problem, and case studies from the literature have been mapped onto the course outline (Table 1). The map in Table 5 provides a guide to focused literature reading that allows biomedically motivated problems to be quickly brought into the classroom. Case study-specific tables of this form are most useful to faculty who are not dynamics and control experts, but who are responsible for teaching the course, because the dynamics and control class is a challenging course for nonexperts to teach. A collection of these paper-topic maps, for traditional and biological case studies, would provide those teaching the dynamics and control course with a variety of examples tailored to each section of the course.

**TABLE 5**

Integration of Sample Case Study (insulin-dependent diabetic patient) with Course Outline Topics

<table>
<thead>
<tr>
<th>DATA-DRIVEN MODELING</th>
<th>Sorensen FOTD, Bolie two-state linear, Bergman “minimal” model</th>
</tr>
</thead>
<tbody>
<tr>
<td>FIRST PRINCIPLES MODELING</td>
<td>Physiologically based pharmacokinetic/pharmacodynamic</td>
</tr>
<tr>
<td>LINEAR SYSTEMS ANALYSIS</td>
<td>Bolie two-state linear ODEs</td>
</tr>
<tr>
<td>LINEAR SYSTEMS ANALYSIS w/ LINEARIZATION</td>
<td>Linearize and analyze Bergman “minimal”</td>
</tr>
<tr>
<td>DYNAMIC SIMULATION</td>
<td>All models, including AIDA as a different performance classification</td>
</tr>
<tr>
<td>FEEDBACK SYSTEMS</td>
<td>Glucose-insulin interactions; nonlinear feedback response; healthy pancreas response</td>
</tr>
<tr>
<td>CLOSED-LOOP ANALYSIS</td>
<td>Sorensen healthy patient</td>
</tr>
<tr>
<td>PID CONTROL</td>
<td>Controller design from FOTD, low-order ODEs, and linearized systems and/or effects of nonlinearity</td>
</tr>
<tr>
<td>ADVANCED CONTROL</td>
<td>Feedforward for meal disturbances and exercise, with simple or complex case studies</td>
</tr>
<tr>
<td>MULTIVARIABLE CONTROL</td>
<td>MISO (glucose and insulin inputs; G, I, and exercise inputs) or MIMO (glucose and insulin control) for a variety of systems</td>
</tr>
<tr>
<td>MODEL PREDICTIVE CONTROL</td>
<td>Linear MPC in analytical or data-driven forms; MPC with a linearized model; nonlinear MPC if desired</td>
</tr>
</tbody>
</table>

**TABLE 6**

Syllabus for UCSB Course: ChE 154 – Engineering Approaches to Systems Biology

<table>
<thead>
<tr>
<th>NL</th>
<th>Topics</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>CELLULAR REGULATION</td>
</tr>
<tr>
<td></td>
<td>Central dogma; genome sequences; genome expression; genomic circuits; protein, metabolic, signaling networks; high throughput biological data; biological databases</td>
</tr>
<tr>
<td>6</td>
<td>MATH MODELING AND SYSTEMS ANALYSIS TOOLS</td>
</tr>
<tr>
<td></td>
<td>Modeling strategies; boolean models; nonlinear ODE models; discrete stochastic models; systems biology modeling packages; network analysis—robustness, identifiability; design of experiment issues</td>
</tr>
<tr>
<td>6</td>
<td>BIOSYSTEMS CASE STUDIES</td>
</tr>
<tr>
<td></td>
<td>Bacterial chemotaxis; lambda phage virus; circadian rhythm gene network; signal transduction in apoptosis; synthetic biological circuits</td>
</tr>
<tr>
<td>2</td>
<td>COURSE PROJECTS</td>
</tr>
<tr>
<td></td>
<td>Midterm progress reports; final presentations</td>
</tr>
</tbody>
</table>
The course focuses on the emerging problems in systems biology and computational biology. There is a substantial level of effort being invested in these areas in both academia and industry, and the demand for training of students has increased in proportion. These advances have been facilitated by developments in both computational modeling and high throughput biology—enabling a systematic approach to analyzing complexity in biophysical networks that was previously untenable. These studies provide increasingly detailed insights into the underlying networks, circuits, and pathways responsible for the basic functionality and robustness of biological systems. They also create new and exciting opportunities for the development of quantitative and predictive modeling and simulation tools. Model development involves translating identified biological processes into coupled dynamical equations that are amenable to numerical simulation and analysis. These equations describe the interactions between various constituents and the environment, and involve multiple feedback loops responsible for system regulation and noise attenuation and amplification.

The discipline of “systems biology” has emerged in response to these challenges, and combines approaches and methods from systems engineering, computational biology, statistics, genomics, molecular biology, biophysics, and other fields. The recurring themes include: (i) integrative viewpoints toward unraveling complex dynamical systems, and (ii) tight iterations between experiments, modeling, and hypothesis generation. In response, there have been a number of courses introduced in a variety of departments across the country that address elements of systems biology and computational biology. These have been targeted at both undergraduate and graduate audiences, and in some cases involve continuing education participants from industry. The balance of topics in the syllabus in Table 6 is approximately one-third on basic cellular regulation, one-third on applications of systems engineering tools to biological problems, and one-third on detailed case studies to illustrate current methodologies and future challenges. Although the UCSB curriculum is based on quarters, the same general template could be extended to a semester-long course without significant modification.

Assignments for this course consist of short homework problems, primarily at the beginning of the course, and a major course project. The project entails a midterm progress report, a final presentation, and a written report. The case study offers a mechanism to tailor the course to a diverse student population—seniors work in teams with a reduced scope, while graduate students work as individuals on a more detailed project.

OPEN ISSUES

Laplace Domain Methods

Traditional process control courses emphasize Laplace transform methods for analyzing and designing feedback systems. While traditional analysis may be facilitated by Laplace domain representations, the applicability of these methods to the complex systems commonly encountered in biological problems is severely limited. Biological systems are inherently nonlinear with phenomena ranging from protein interactions in gene regulatory networks to adaptation in systemic reflexes. Furthermore, modeling of biological systems at resolutions below the macroscopic scale often leads to high-state dimension. As is evident from Table 1, Laplace domain methods have been de-emphasized and frequency domain techniques have been effectively removed from the proposed curriculum. While we do not dispute their potential value, transform-based methods introduce conceptual difficulties that cause many students to lose their physical insights and view the material as applied mathematics. On the other hand, the syllabus in Table 1 is sufficiently flexible that limited coverage of frequency domain methods at the expense of other topics is possible.

Time Domain Methods

Complex dynamic system models are most effectively formulated and analyzed in the time domain using conservation equations. Consequently, the syllabus in Table 1 focuses on linear and nonlinear state-space models. Connections with the corresponding Laplace domain concepts can be introduced as appropriate (e.g., stability via eigenvalues vs. poles). On the other hand, the Laplace transform is a particularly useful tool for single-input, single-output (SISO) systems with time delay and/or zero dynamics. We acknowledge that analytical treatment of zeros in the time domain is more involved than the corresponding Laplace methods. Time domain analysis of transportation and measurement delays is most conveniently performed using a discretized framework based on state augmentation. Because this approach can lead to potentially large state dimensions, evaluating student understanding of this material can be challenging. A possible solution is to use a combination of relatively simple exam questions and more detailed homework problems. While control system design issues can be addressed using continuous state-space models, we believe that a discrete-time framework is preferred for introducing data-driven model identification and sampled-data systems. Recent results have shown that a properly tuned SISO model predictive controller cannot be outperformed by a conventional proportional-integral-derivative (PID) controller. Because we expect this fact to be reflected in industrial practice, the syllabus in Table 1 offers increased exposure to controller synthesis techniques based on discrete-time representations such as step response models. While a comprehensive treatment is beyond the scope of this course, model predictive control (MPC) should be foremost among the topics covered due to its industrial importance. As outlined in the UMass course syllabus (see Table 3), the introduction of MPC necessitates limited discussion of real-time optimization and draws on the discrete-time modeling tools discussed above.
Multivariable Control

While most traditional courses treat multivariable systems as a straightforward extension of SISO systems, a more comprehensive approach that addresses the unique challenges of multivariable controller design is warranted. A formal introduction to decentralized control would support the systems viewpoint of multivariable processes—a set of optimal SISO feedback loops generally does not result in overall system optimality. Another advantage of introducing MPC is that multivariable system complexity is handled in a transparent and systematic manner. Students can gain appreciation for the effects of constraints and optimization-based methods for constraint compensation.

Robustness

A critical topic in the analysis of both process control systems and biological regulation is robustness. While the remarkable levels of robust performance attained in nature are enviable from an engineering perspective, this issue is not widely appreciated in biology. The critical importance of robustness in understanding disease states, as well as evolution and development, motivates its incorporation in the system dynamics and control curriculum. While a detailed theoretical treatment is beyond the scope of a typical undergraduate course, key concepts of robustness can be emphasized using simple tools such as sensitivity analysis—effectively capturing the gains from uncertain system elements to the controlled output or performance measure. Students would be well positioned to evaluate parametric sensitivities using state-space models in the proposed curriculum. Robustness analysis could also be used to study closed-loop strategies such as redundancy, feedback, filtering, and modular protocols commonly used in nature.

Nonlinear Analysis and Control

Most biological systems are not adequately described by linear dynamic models since nonlinear effects such as saturation phenomena are ubiquitous. Consequently, linear and linearization-based analysis techniques are rarely sufficient. Nonlinear analysis techniques, such as phase plane analysis and bifurcation theory (see Table 3), can be introduced explicitly, thereby exposing students to theoretical concepts and analysis tools with wider applicability than Laplace domain methods. Nonlinear phenomena are also common in industrial plants, and linear control methodologies often require specialized tools to handle strong nonlinearities. Linear controllers exhibit poor performance for some nonlinear processes (e.g., high purity distillation columns) and completely fail for particularly difficult processes (e.g., those displaying input multiplicity). Given increased exposure to linear MPC in the revised curriculum, a brief introduction to nonlinear MPC is entirely feasible.

Teaching Control for Nonexpert Faculty

Our experience indicates that the process dynamics and control class is not a popular choice as a teaching assignment among nonexperts in the field. This lack of interest is due to a variety of issues, including the mathematical complexity of the material and the significant focus on feedback controller synthesis. An additional concern is that the material is challenging to students, who have had limited exposure to dynamical systems prior to this course. The syllabus in Table 1 represents a significant departure from the traditional controller-synthesis-dominated course to a more balanced presentation of system dynamics and feedback.

A notable benefit of the proposed syllabus is the degree of potential customization. While our focus has been on the introduction of biological systems content, the treatment of other application areas such as advanced materials can be accomplished in a similar manner. This flexibility provides an excellent opportunity for instructors to integrate their research interests into the course. In fact, the three courses described here were heavily influenced by the work performed in our research groups. Possible benefits of such integration include: (i) increasing the diversity of application examples by encouraging nonexperts to teach the course; and (ii) introducing students to cutting-edge research that influences their perception of the field and may affect their future career directions.

SUMMARY

Biological processes have assumed an increasingly important role in chemical engineering research and practice. Modifications of the existing chemical engineering curriculum are necessary to provide undergraduate students the needed exposure to this emerging field. We believe that the capstone process dynamics and control course provides an excellent opportunity to integrate biological systems content and draw parallels with chemical process applications that have been the traditional focus of this course. This paper provides a summary of work on this problem at our respective institutions.

The proposed curriculum allows biological content and time domain concepts to be introduced in a synergistic manner without adversely affecting the coverage of traditional material. As outlined in the proposed syllabus, this requires a decrease in time spent on traditional topics such as PID controller synthesis, Laplace transform techniques, and frequency response analysis. Advances in feedback controller tuning (e.g., autotuning and model-based methods) combined with the availability of simulation/analysis tools (e.g., MATLAB, LabVIEW) bring into question the need for extensive treatment of pencil-and-paper analytical techniques that are rarely employed, even at the graduate level. While focused time on these topics has been reduced in the name of incorporating biology, it should also be noted that the analysis tools introduced in the dynamics and control class are applicable to problems beyond biological systems. Hence, students are no less prepared for “traditional” industrial positions, and they are certainly more equipped for positions in pharmaceuticals and systems biology.
A key hurdle that must be overcome is the lack of instructional materials to support the new process dynamics and control curriculum. For the courses outlined above, the authors are using new textbooks (System Modeling in Cell Biology, MIT Press) or have developed supplementary materials to complement existing textbooks. Researchers in process dynamics and control can contribute in a variety of ways. The extension of extended case studies such as Table 5 for various applications would ease the burden on nonexperts teaching the course. Software tools such as the Process Control Modules[22] and Java-based Control Modules[22] are well suited for introducing traditional concepts and applications. New software tools are needed to expose chemical engineering undergraduates to biological complexity and to allow the application of theoretical concepts to representative biological systems. Ongoing efforts, such as those organized by MIT and the CACHE Corporation, are focused on the development of biologically focused systems courses. A task force headed by the second author of this paper is currently working on course revisions as well as software module development as a means to integrate biological content throughout the chemical engineering curriculum. More details on this effort will be made available at <http://www.cache.org>.

ACKNOWLEDGMENTS
Support for RSP was provided by the National Science Foundation CAREER program (CTS #0134129).

REFERENCES


This column provides examples of cases in which students have gained knowledge, insight, and experience in the practice of chemical engineering while in an industrial setting. Summer internships and co-op assignments typify such experiences; however, reports of more unusual cases are also welcome. Description of the analytical tools used and the skills developed during the project should be emphasized. These examples should stimulate innovative approaches to bring real-world tools and experiences back to campus for integration into the curriculum. Please submit manuscripts to Professor W.J. Koros, Chemical Engineering Department, Georgia Institute of Technology, Atlanta, GA, 30332-0100.

THE ROLE OF INDUSTRIAL TRAINING IN CHEMICAL ENGINEERING EDUCATION

MAMDOUH T. GHANNAM
United Arab Emirates University • Al-Ain, United Arab Emirates

Industrial training plays an important role in preparing engineering students to be future professional chemical engineers. The training offers a golden opportunity to acquire numerous technical and nontechnical skills that can not be obtained in a classroom environment. Some of the benefits of industrial training are:

1. Observing daily work activities firsthand in a real setting.
2. Gaining the ability to apply technical and theoretical knowledge to industrial problems.
3. Direct exposure to nontechnical skills such as oral and written communications.
4. Understanding the diversity of the chemical engineering industries.
5. Applying computer software programs to real industrial situations.
6. Teamwork experiences.
7. Time management and deadline objectives.
8. Getting familiar with the industrial environment to set and achieve future career goals.
10. Boosting the student’s self-esteem and confidence by gaining today’s industrial skills.

UNDERGRADUATE INDUSTRIAL PROGRAMS

There is no classroom course that could simulate or replace the industrial experience gained from working with several operators in a real industrial environment. Numerous universities allow their students to gain industrial experience through a variety of programs.

Cooperative Education Program

One such program is the cooperative education program. Co-op education is based on rotation between schooling and full-time work periods. It connects undergraduate students directly with industry to gain strong fundamentals and invaluable insight into the chemical engineering profession, acquire technical knowledge, earn academic credits, and receive wages. Some universities offer co-op programs on an optional basis while others are mandatory. Among the colleges of engineering offering an optional program are the University of South Alabama, the University of Minnesota, and the University of Pittsburgh. Mandatory programs can be...
found in universities such as Drexel, Ryerson, Toledo, and Cincinnati. Cooperative education programs have been well established in these universities for a long time. For example, cooperative education was founded at the University of Cincinnati in 1906 and at Drexel University in 1919. Most cooperative education programs offer financial benefits to students. The financial reward for students is usually based on location and type of task. Students’ wages from their co-op jobs can even help finance their educations. At the University of Cincinnati, average salaries for co-op jobs are almost twice the tuition fees. Therefore, students do not have the burden of having a part-time job, giving them more time to devote to academics and other activities. At the University of Pittsburgh’s Department of Chemical and Petroleum Engineering, approximately 40-50% of the students take advantage of the available co-op program. According to a study completed by the co-op office in Cincinnati, 96% of graduating students acknowledged that the college program including co-op experience provided a better education than the traditional program without co-op.

Most engineering schools that offer cooperative education have certain requirements for a student to participate in the program. For example, at the University of Minnesota, the undergraduate student needs to be in good standing, have completed all program course requirements including fall semester of the third year, have completed at least five out of seven elective courses, and maintain a minimum GPA of 2.8. The co-op student will work full time for one year continuously in the industry. After successfully completing their co-op programs, students earn two credit hours per semester, which count toward technical elective courses.

**Industrial Training Program**

Around 10 years ago, the College of Engineering at the United Arab Emirates University (UAEU) recognized the importance of industrial training and its crucial role in preparing students for professional engineering. In 1995, a very committed program was established by the Unit of Industrial Training and Graduation Projects at the college. This program is mandatory—i.e., part of the engineering education curriculum—for all engineering students in the disciplines of chemical, civil, electrical, mechanical, and petroleum engineering. Students can be granted 15 credit hours after successful completion of their industrial training. The following discussion focuses only on the chemical engineering industrial training program (ITP). The industrial training program at UAEU is selected in this article as an example to address its benefits and highlight areas that can be improved.

**PROGRAM LOGISTIC OF ITP**

To ensure that students have enough theoretical background to comprehend industrial training tasks, the program requires students have a minimum GPA of 2.5 and to have completed 114 credit hours. Any student with a lower GPA will be required to complete 126 credit hours (the total credit-hour requirement to earn a B.S. degree in engineering is 168). Each eligible student should prepare and submit a file to the industrial training unit that contains academic records, a one-page resume, and a completed application form.

The industrial training unit works with each candidate to find a training position with the available participating industrial partners. Students will be required to interview with

![Figure 1. Participating industries.](image)
potential companies to be placed. If a student is not accepted by one company, he/she will have an opportunity with another company since the number of industrial partners exceeds the number of training candidates. The industrial training unit ensures that each candidate will receive placement in a relevant industry within the country or abroad.

At the beginning of the training period, each student will receive a training-program schedule outlining the whole 16-week period. This schedule includes a weekly job description with tasks, academic advisor visits, and deadlines for reports and presentations. The schedule is established by the industrial supervisor in agreement with the student’s academic advisor. The student is also advised of the evaluation process used to determine his or her grade. Student evaluation during this program is based on weekly progress reports submitted to the academic advisor (15% of total score), academic advisor visits to the industrial site (15%), industrial supervisor’s evaluation report (20%), and final report and oral presentation (50%). The presentation and final report are assessed by an examination committee consisting of a college representative, a departmental faculty member, and two or three professional engineers.

Upon successful completion of the ITP, student participants are eligible to register into the final academic year in chemical engineering. Failed participants must repeat the ITP program at another industrial site. With this in mind, most students are committed very seriously to the ITP.

From the above ITP description, it is notable that the objectives are similar to cooperative education in allowing students to gain industrial experience and learn the basics and fundamentals of the industry. The ITP, however, strictly considers students as trainees without financial compensation, not as employees with wages as in co-op programs.

**COMPANIES INVOLVED IN THE INDUSTRIAL TRAINING PROGRAM**

The number of participating companies in the ITP for the whole college increased tremendously from around 10 companies during the initial year of 1995-1996 to approximately 140 companies in the academic year of 2004-2005. This increase in participating companies, both locally and internationally, reflects industrial appreciation of the important role of the ITP. The total number of chemical engineering students who participated in the program from 1999-2005 is 198. The number of academic advisors involved in these activities changed from one semester to another based on the number of students. For example, the number of faculty members involved in the first semester of 2004-2005 was four, and in the second semester of 2005-2006 it was seven. For the chemical engineering discipline, the specialties of the involved industries vary widely, as can be seen in Figure 1.

The reported percentage represents the number of students completing the program for each industry during the period of 1999-2005. In addition, Figure 2 displays the various regions within the United Arab Emirates, with exception of France and Qatar, in which students of the UAEU carried out their training. These percentages also cover the period of 1999-2005.

The following is a brief description of the ITP for a chemical engineering student who completed his training program at the oil service company Dowell Schlumberger, in Abu Dhabi.

![Figure 2. Industrial locations by region.](image-url)
Based on a study performed by the Industrial Training Unit . . .
86% of the students who completed the ITP gained strong technical skills.

IMPACTS AND POTENTIAL IMPROVEMENT OF ITP

Impact

By becoming a part of the ITP, students gain practical experience, technical knowledge, confidence, time management skills, teamwork capability, and a better understanding of what they’ve learned in class. Based on a study performed by the Industrial Training Unit at UAEU in the first semester of the 2003-2004 school year, 86% of students who completed the ITP gained strong technical skills. A total of 69 students having completed their industrial training in 42 industrial sites participated in this study. This training mechanism enables students to define their career goals and provides an opportunity to find a permanent employment position.

Additionally, this program is an excellent recruiting tool for participating companies. Employers will have the chance to train, evaluate, and select candidates for future job opportunities. A study was done by the industrial training unit at UAEU to survey participating industrial employers from the first semester of 2003-2004 to the first semester of 2005-2006. This study investigated the responses of the industrial employers on the trainees’ performance with regard to the ABET2000 criteria (a to k criteria). A total of 75 industrial employers were involved in this study. The study showed that most of the employers’ evaluations exceeded the 70% limit (the acceptable limit established by the UAEU training office) for all the criteria of a to k with a few exceptions. These exceptions occurred during the second semester of 2003-2004 and first semester of 2005-2006. The employers’ evaluation was slightly less than the 70% limit for criteria c and j (the ability to design a system, component, or process, and knowledge of current engineering trends).

Improvement of ITP

If the faculty members are not significantly involved in industrial-site supervision, project choice, follow-up, and academic evaluation of student performance during the training period, the chances of an undergraduate student achieving industrial experience are not very good. As an academic advisor participating for the last seven years in the ITP, I feel improvements can be made to the current program. Implementing these ideas will enhance the overall performance and outcomes of the ITP. Suggested improvements are:

(a) Site Selection

To ensure the success of the training program for students, an academic advisor should be involved from the very beginning. The advisor needs to work closely with each student in selecting the appropriate training site since there can be several choices. Doing so guarantees matching the student with an industrial site that meets the program objectives, and avoids having students select an industry based on convenience rather than relevancy.

(b) Industrial Field Visits

The department should encourage and enforce a one-day field visit once a semester for all students, especially freshmen, to provide early exposure to different daily industrial activities. Doing so allows students to start forming an opinion as to what type of industry they want to pursue.

(c) Industrial Short Residence

Due to the short period of the ITP (i.e., four months) in comparison with that usually spent by a trainee at other schools such as Pittsburgh, Drexel, Cincinnati, and Minnesota participating departments should develop a yearly industrial event in which sophomore and junior students spend two to four weeks during the summer at a local industry in the residence city. Of course, each student should achieve certain limited objectives during this period and be required to provide a written report and oral presentation detailing his/her activities and experiences gained. To make this idea...
even more practical, one industrial site can be selected for each student. This requires the student to spend each summer break in different departments of an industrial site.

(d) Nontechnical Skills Course

To improve the nontechnical skills of undergraduate students in general and the ITP in particular, the college of engineering should develop a special course equivalent to two credit hours. The course would focus on enhancement of nontechnical skills such as communication, effective presentation, technical writing, accessing information, judgment, software applications in industry, job interviews, resume building, and explaining technical information to nontechnical customers.\cite{4,12}

This course would be offered to all students during the second academic year, thus allowing enough time before the ITP stage. In this way, students will be well prepared for the ITP. They will be able to maximize the benefits and achieve all the expected objectives of the ITP.

(e) Graduation Project Proposal

One requirement for the successful completion of the ITP is the submission of a graduation project proposal within the final report. This proposal should reflect a valuable idea that attracted the trainee’s attention during the training period. The proposal may then be selected as a graduation project by a faculty member within the chemical engineering department. Based on my own experience over the period of 1998-2005, I noticed problems associated with the graduation project proposals such as unclear or incomplete proposals and the lack of technical description and industrial data. It seemed students completed their proposals just to meet the requirement criteria, or did not complete them at all.

The requirement to submit a graduation project proposal itself is a great idea. For greater benefit, however, it needs more involvement and commitment from each side. The following are some suggestions to strengthen the process of the graduation project proposal:

1. All graduation projects should be based on students’ industrial proposals.
2. Clear, limited, and well-defined criteria for graduation projects should be established by the department at the beginning of each academic year.
3. Each group of three students will be assigned an academic advisor relevant to their industrial training site.
4. Forming a solid project proposal should be one of the main duties of trainees in coordination with the industrial supervisor and the academic advisor.
5. Both the industrial supervisor and academic advisor should be involved with students to achieve this task by the end of the training period.
6. The proposal should cover the details of problem definition, industrial importance, negative impacts, alternative solutions, suggested solution and reasoning, and positive impacts.
7. A significant grade should be assigned to the project proposal.
8. The academic advisor should involve the industrial supervisor throughout the graduation project stages.
9. The industrial supervisor will be entitled to attend the final project exam and to receive a copy of the final report with all results and recommendations.

(f) Academic/Industrial Interaction

One of the main benefits of the suggested mechanism of the ITP and graduation project proposal is the strong link and interaction made possible between the industrial supervisor and the academic advisor. This relationship can help both parties advance their mutual interests, including:

1. Faculty member can make a strong connection with different industries leading to research and technical cooperation.
2. Industrial supervisor will have better access to the university environment for assistance such as technical recommendations, hiring new graduates, acquiring samples and data analysis, and participating in scientific activities sponsored by the university.
3. Research cooperation between the two parties resulting in scientific publication reflects well on the image of the industrial partner.

Due to the large number of activities requiring faculty involvement, these modifications will be better suited for departments with a small number of students. A larger number of students would require too much faculty time investment, negatively affecting research.

SUMMARY

It is clear that industrial experience in any program format can be beneficial to students. Some programs may have more benefits than others, but each provides valuable skills and training for our future engineers. It is important that we continue to study and evaluate these programs to make improvements and adopt new ideas. What may work in one university may not work in another. By sharing the fundamentals of the programs, however, engineering colleges may find useful information to improve their current programs. After all, the main objective of any engineering education program is to produce the best possible engineers and to develop, enhance, and advance our society.
REFERENCES

11. <http://www.eng.uc.edu/welcome/coop/>
Validating 
THE EQUILIBRIUM STAGE MODEL 
for an Azeotropic System in a Laboratorial Distillation Column

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D uring their fourth year of undergraduate studies, chemical engineering students at the Instituto Superior de Engenharia de Coimbra (ISEC), Portugal, take a full laboratory course in unit operations and process control. The topics covered include evaporation, distillation, absorption in packed columns, solid-liquid extraction, drying, and the control of variables often found in industrial units (e.g., pressure, flow, level, and temperature) employing laboratory units or bench-scale kits. The course’s basic aim is the practical demonstration of theoretical concepts taught in courses on process separation, chemical thermodynamics, and process dynamics at laboratory scale. It also provides students with experience in operating and controlling complex units. Regarding the work on distillation, the students are asked to validate the steady-state behavior of a laboratory unit used for separating an azeotropic mixture of aniline and water. The interest in this binary system arose from an intensive research program carried out in the chemical engineering department of ISEC in collaboration with a Portuguese company that produces aniline—with the aim of optimizing the aniline production section. In addition, this work also aims to validate knowledge relating to the distillation of heterogeneous azeotropic mixtures, of which the aniline-water system is a simple and easily handled example.

The conceptual basis used to describe the phenomena involved in a distillation column is the equilibrium stage model, which assumes thermodynamic equilibrium between the species and perfect mixing in each phase and tray. But it is quite common for equilibrium not to be achieved in vapor-liquid-liquid dispersions arising from heterogeneous azeotropic mixtures. This is because of the occurrence of kinetically controlled phenomena, such as mass transfer, coalescence, and nucleation in liquid phases. Regardless of

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the mismatch of theoretical assumptions and real behavior, the equilibrium stage model is still used to represent the operation of distillation columns phenomenologically, and several research groups have presented data for three-phase distillation experiments to validate it.⁶ Thus, this work aims simultaneously to enable students to gain experience in operating and analyzing a distillation procedure, to use vapor-liquid equilibrium (VLE) prediction methods, and to contribute to the research community’s efforts to validate the equilibrium stage model for the aniline-water system.

Three four-hour sessions are required to complete the work. The first is devoted to a review of the basic theory behind mixture thermodynamics and methods for predicting activity coefficients for VLE, analysis of the column layout, and understanding its operation and control. Between the first and second sessions, the students develop an Excel workbook to obtain the VLE prediction for the aniline-water system at atmospheric pressure. Each group of three or four students is asked to use a different prediction method for the activity coefficients among UNIFAC, UNIQUAC, two-constant Margules, and van Laar,⁷ then to compare the results with experimental data published in the literature for the aniline-water system at atmospheric pressure.⁸

During the second session, the students carry out the experimental work with the distillation column, running it until steady-state conditions are reached. Next, they use Aspen Plus v. 11.1 to compute the unit steady state with an equilibrium stage-model-based module. Finally, in the third session, the results are presented, compared with those given by simulation, and discussed.

EXPERIMENTAL EQUIPMENT AND SAMPLING

Aniline, even in low concentrations, is a fairly toxic aromatic hydrocarbon. Its handling therefore requires students take some safety precautions, that is, to wear protective clothing, gloves, and eye/face protection to avoid skin contact. Furthermore, the work is carried out in a well-ventilated area to reduce the toxicity risk.

The schematic diagram of the column where experiments are performed is shown in Figure 1. The unit is formed by three column sections, each with 10 bubble-cap trays, a total condenser, and a kettle-type reboiler (reference Labodest 250 from Fischer). The column body is made of glass with an internal diameter of about 0.05 m.

The feed stream enters in tray 11, and the reboiler, which is the last tray of the column, operates simultaneously as a heat exchanger and equilibrium tray, since it contains an electrical-resistance element with maximum heating capacity of 3 kW.

The schematic representation of trays is shown in Figure 2. The net area for vapor flow (6) is 10% of the total area of the tray. Two cavities for liquid inlet (1) and outlet (2), with slightly different heights, separated by a wall (3), form the bubble caps. The liquid falls from the upper tray into the reflux zone (4) through the downcomer, circulates around the wall to the opposite position, and is discharged to the lower tray through the tube (5). This design increases the contact time between the vapor and liquid phases.

A solenoid valve controls the reflux flow to the column.

Figure 1. Schematic diagram of laboratory unit used for experiments.
(Figure 1). When the valve is open, a glass stem is pulled magnetically from the seat and the liquid from the condenser is collected in the distillate receiver. When the valve is closed, the stem is pushed back, the seat is closed, and, when it is partially filled, the liquid overflows through a side tube and returns to the column (Figure 3). The reflux ratio value is set by employing two time preselectors on the control device, thus establishing the valve dead band. For the aniline-water binary system, however, the control of the distillation column based on the reflux ratio causes severe problems due to the formation of two immiscible liquid phases in the condenser—the organic being denser than the aqueous at the temperature at which it leaves the condenser. The difference in density means that, when the valve opens after being closed for a while, a small volume of liquid retained in the valve seat (below the side tube level) is poured into the distillate receiver. This produces significant changes in the distillate composition since it is rich in the heavier phase (the organic phase). Table 1 indicates the density values for the aqueous and organic phases formed at different temperatures for the aniline-water system.

To overcome this drawback, instead of reflux ratio adjustment, an on-off control scheme based on the boiling point limit in the upper tray of the column is employed, with the head temperature measured through a resistance thermometer (Figure 1). Whenever it exceeds the value selected at the control unit (98.7 °C—the azeotropic temperature), the distillate flow rate is automatically interrupted, and the condensate starts to flow back to the column. Consequently, the temperature of the upper tray starts to fall, and when it reaches the preselected value the distillate starts to be collected again. This control scheme leads to small changes in the position of the solenoid valve, which is open most of the time.

The feed stream is preheated to 99.3 °C before entering the column in liquid state at atmospheric pressure. The feed stream is sampled for the quantitative determination of aniline concentration in the mixture.

When the steady state is reached, the students collect the distillate and bottom products in graduated receivers for a period of 90 minutes. At the end, the distillate is transferred to a separatory funnel, and after the separation of the two phases, the volume of each layer is measured in graduated cylinders.

The aniline concentrations in the aqueous phase of distillate, in the bottom product, and in the feed sample are quantitatively determined by spectrophotometry, after appropriate dilution. The absorbance of the solutions is measured at 279.5 nm in a UV-Vis spectrophotometer unit after setting the calibration line. The quantitative analysis of water concentration in the organic phase of the distillate is determined by titration with Karl Fisher reagent.

For the range of flows used in the experiments, the column manufacturer indicates that the Murphree efficiency is 92%. The experimental confirmation of this value is not performed exactly because of the column configuration, which does not allow the extraction of liquid samples in consecutive trays.

MODEL VALIDATION

Aspen Plus v. 11.1 is used to validate the equilibrium stage model; the steady-state flows, compositions, and temperatures of the upper tray and bottom stream result-
ing from the model solution are compared with laboratory data. The Radfrac module is chosen to describe the column unit since it is based on the rigorous solution of the equilibrium stage model for multistage vapor-liquid fractionation, steady-state operations. The model consists of a set of nonlinear algebraic equations, comprising the material balance (M) and thermodynamic equilibrium relation (E) for each component and tray, and the summation of mole fractions (S) and enthalpy balance (H) for each tray, generally called MESH equations.

This system can be augmented with the trays’ hydraulic relations and pressure-drop profiles across the column when the unit geometry is known. The broader generality of the Newton-Raphson algorithm led this to be chosen to solve Radfrac module in rating mode. The Newton-Raphson algorithm implemented is based on the classic Naphtal and Sandholm algorithm. First, the number of equations and variables resulting from unit modeling is reduced through the condensation of mole fractions, liquid, and vapor flows into new variables representing component molar flows. Next, the complete set of variables is ordered, and the resulting algebraic equation system solved iteratively by employing a Newton-type algorithm. The convergence is checked after each iteration by comparing the sum of squares of all variables, conveniently weighted by scale factors, with a tolerance defined as a function of the number of degrees of freedom the system involves and inlet flows.

An azeotropic convergence algorithm is chosen to handle the current binary system that forms a minimum-boiling azeotrope in the region of low aniline concentrations. The operating conditions, including the molar flow of distillate stream, the heat consumed in reboiler, the stages at which streams enter/leave the unit, the pressure-drop profile across the column, additional information regarding the condenser operation, and the characterization of the second liquid phase—formed essentially by aniline—are introduced into Aspen Plus. Molar flows are set equal to the experimental steady-state values, and the pressure drop is disregarded due to the small flows involved in the operation. The characteristics of the feed stream, including its temperature, pressure, and molar composition, are also entered into Aspen Plus. It is considered that there is no sub-cooling in the condenser and the Murphree stage efficiency is set to 92%. The Appendix at the end of this paper presents the Aspen Plus Input Summary file for a successfully converged model.

RESULTS

The first step in analyzing the results is to compare the VLE data calculated by the Aspen Properties module with the prediction obtained by students. Next, both must be validated with experimental data. The diagram in Figure 4 shows the agreement between the VLE data predicted using the UNIFAC method and the experimental data published in the literature. The system presents a heterogeneous azeotrope at 98.7 °C and 0.044 of aniline mole fraction, where three phases are in equilibrium: a vapor phase and two liquid phases [an organic phase with 30.3% (mole/mole) water, and an aqueous phase with 98.6% water].

This happens because the vapor-liquid envelope overlaps the liquid-liquid envelope, as illustrated in Figure 4. This task allows students to understand that for heterogeneous azeotropes the vapor formed during boiling has the same composition as the overall liquid, but the three phases in equilibrium have distinct compositions, contrary to what

![Figure 4. Comparison of experimental data from literature vs. VLE data determined through UNIFAC for aniline-water system.](image-url)
happens for homogeneous azeotropes, where the liquid and vapor formed have the same composition.

The VLE prediction methods using UNIQUAC, two-constant Margules, and van Laar activity-coefficient models require binary parameters for the aniline-water system, which students estimate by employing the following procedure and theoretical basis.

For a binary system containing two liquid phases and one vapor phase in equilibrium, the fugacities of each compound in each of the phases are equal. That is:

\[ \frac{y_{\text{org}}^{\text{P}} x_{\text{org}}^{\text{P}}}{y_{\text{as}}^{\text{P}} x_{\text{as}}^{\text{P}}} = \frac{y_{\text{org}}^{\text{s}} x_{\text{org}}^{\text{s}}}{P} \]

and

\[ \frac{y_{\text{ws}}^{\text{P}} x_{\text{ws}}^{\text{P}}}{y_{\text{ws}}^{\text{s}} x_{\text{ws}}^{\text{s}}} = \frac{y_{\text{ws}}^{\text{a}} x_{\text{ws}}^{\text{a}}}{P} \]

where the vapor phase behaves like an ideal gas mixture. The expressions \( y_{\text{org}}^{\text{P}} \) and \( y_{\text{as}}^{\text{P}} \) represent the activity coefficients of component \( i \) in the organic and aqueous phases, respectively; \( x_{\text{org}}^{\text{P}} \) and \( x_{\text{as}}^{\text{P}} \) are the molar fractions of component \( i \) in the organic phase and aqueous phases, respectively; \( P_{i} \) is the vapor pressure of the pure component \( i \) at temperature \( T \); \( P \) is the pressure; and \( y_{i} \) is the mole fraction of component \( i \) in the vapor phase. The subscript \( s \) stands for saturated liquid phases.

According to the phase rule, a binary system with three phases in equilibrium has just one degree of freedom, which means that by fixing the pressure (atmospheric pressure) the system becomes determined. Setting the activity coefficient model, the functional forms of \( y_{a} \) and \( y_{w} \) can be explicitly written, and the preceding equations lead to

\[ \gamma_{\text{org}}^{\text{a}} \left( A_{\text{a},w}, A_{\text{a},w}, x_{\text{org}}^{\text{a}} \right) x_{\text{org}}^{\text{a}} = \gamma_{\text{as}}^{\text{a}} \left( A_{\text{a},w}, A_{\text{a},w}, x_{\text{as}}^{\text{a}} \right) x_{\text{as}}^{\text{a}} \]

and

\[ \gamma_{\text{ws}}^{\text{w}} \left( A_{\text{a},w}, A_{\text{a},w}, x_{\text{ws}}^{\text{w}} \right) x_{\text{ws}}^{\text{w}} = \gamma_{\text{ws}}^{\text{w}} \left( A_{\text{a},w}, A_{\text{a},w}, x_{\text{ws}}^{\text{w}} \right) x_{\text{ws}}^{\text{w}} \]

where \( A_{a,w} \) and \( A_{w,a} \) are the binary interaction parameters of the model chosen for the aniline-water system. When the liquid-liquid equilibrium data is available, the fractions \( x_{\text{ws}}^{\text{org}}, x_{\text{ws}}^{\text{org}}, x_{\text{ws}}^{\text{org}}, x_{\text{ws}}^{\text{org}} \) can be used to evaluate the two parameters \( A_{a,w} \) and \( A_{w,a} \). Solubility data of aniline in water and of water in aniline for a temperature range of 20 °C to 100 °C can be found in the reference [8, Appendix G], thus allowing students to estimate mutual solubility values at the azeotrope temperature (98.7 °C). The parameters obtained are used to calculate activity coefficients for subsequent vapor-liquid equilibrium calculations in the regions of \( 0 < x_{\text{ws}} < x_{\text{ws}}^{\text{org}} \), and \( x_{\text{ws}}^{\text{org}} < x_{\text{ws}} < 1 \).

Table 2 lists the parameters obtained by the students for the UNIQUAC, two-constant Margules, and van Laar activity coefficient models.

The results of the Radfrac module are compared with experimental results in Table 3, showing the agreement
Using the Profiles form, it is possible to view the results from Radfrac as compositions, temperatures, and flow rates for each column tray. Figure 5 shows the profiles of aniline composition in both liquid and vapor phases across the column. As expected, the aniline concentration in both liquid and vapor streams increases from the bottom to the top of the column, with the aniline mole fraction in the vapor always being greater than that in the liquid since the feed stream is located to the right of the azeotropic point of the VLE diagram (see Figure 4). The composition profiles provide strong evidence that the number of trays is over-projected for the experimental conditions tested. Indeed, in some of the stages the enrichment of vapor phase in aniline is quite small, thus leading to the conclusion that the column can successfully separate a higher flow of feed stream (with a similar composition) with the same efficiency, provided the heat supplied to the reboiler increases and flooding does not occur.

Figure 6 shows that the liquid and vapor flows across the column are approximately constant in the enrichment and stripping zones. Since stage 11 (12 in Figure 6) is the feed stage and the state of the stream is saturated liquid, the liquid flow rate in the stripping zone is increased by an amount equal to the feed flow rate. These conditions enable the McCabe-Thiele graphical construction[13] to be used to estimate the number of theoretical trays required to perform the separation. Typical values achieved by students are about 14 trays plus the condenser and the reboiler.
CONCLUSIONS

Operating a laboratory distillation column is a good experiment for demonstrating the application of some concepts of unit operations, vapor-liquid equilibrium prediction, and process simulation. The experiment described in this paper embraces a wide range of topics including process control, chemical analysis, and numerical methods for handling rigorous distillation models. It also enables students to gain experience in operating and controlling a distillation unit. Moreover, the results provide the research community with sufficient evidence to support the validation of the equilibrium stage model for the heterogeneous azeotropic system formed by aniline and water. The results show that the column is too large for the experimental conditions tested, and additional knowledge regarding its behavior can be acquired if the inlet flow is increased and digital temperature meters are installed in each tray to validate the temperature profile. But the experiment might be successfully applied to other azeotropic systems, such as a benzene-monomonitrobenze-water mixture.

REFERENCES


APPENDIX

AspenPlus Input Summary file


DYNAPLUS
DPLUS RESULTS=ON
TITLE 'Coluna do Isec'
IN-UNITS SI
DEF-STREAMS CONVEN ALL
SIM-OPTIONS
IN-UNITS ENG
SIM-OPTIONS NPHASE=3 ATM-PRES=1. <atm>
PARADIGM=EO
ACCOUNT-INFO USER-NAME= "BELMIRO DUARTE"
PROP-SOURCES PURE / AQUEOUS / SOLIDS / INORGANIC / & NOASPENCID
PROP-SOURCES PURE / AQUEOUS / SOLIDS / INORGANIC
COMPONENTS
WATER H2O / ANILINE C6H7N-1
FLOWSHEET
BLOCK Cl IN=FEED OUT=DESTIL RESID
PROPERTIES UNIFAC
PROPERTIES NRITL / UNIQUAC
PROP-DATA NRITL
BPVAL WATER ANILINE 2.238300000 362.5433000 .3000000000 0.0 & 0.0 0.0 0.0 & 372.1500000 441.1500000
BPVAL ANILINE WATER -.8969000000 509.3646000 .3000000000 & 0.0 0.0 & 372.1500000 441.1500000
PROP-DATA UNIQUAC
BPVAL WATER ANILINE .6554000000 -168.0642000 0.0 0.0 372.1500000 441.1500000
BPVAL ANILINE WATER -.4676000000 -172.2809000 0.0 0.0 & 372.1500000 441.1500000
STREAM FEED
SUBSTREAM MIXED TEMP=99.3 <C> PRES=1 <atm> MASS-FLOW=2.427 <kg/hr> MAXIT=100 MASS-FRAC WATER 0.977 / ANILINE 0.023
BLOCK Cl RADFRAC
PARAM NSTAGE=32 ALGORITHM=STANDARD EFF=MURPHREE & INIT-OPTION=STANDARD MAXOL=100 TOLOL=0.0001
JMETH=INIT & LL-METH=GIIBBS NPHASE=2 DAMPING=NONE COL-CONFIG CONDENSER=TOTAL REBOILER=KETTLE FEEDS FEED 12 ON-STAGE PRODUCTS RESID 32 L / DESTIL 1 L P-SPEC 1 L <atm> / 2 L <atm>
COL-SPECS QN=335, MOLE-D=17.72 <mol/hr> 14 SC-REFLUX OPTION=0 STAGE-EFF 1 0.92 / 2 0.92 / 3 0.92 / 4 0.92 / 5 & 0.92 / 6 0.92 / 7 0.92 / 8 0.92 / 9 0.92 / 10 &
EO-CONV-OPTI
SENSITIVITY S-1
DEFINE Z1 BLOCK-VAR BLOCK=C1 VARIABLE=RR
SENTENCE=RESULTS
DEFINE Z2 BLOCK-VAR BLOCK=C1 VARIABLE=VRATE &
SENTENCE=PROFILE ID1=2
TABULATE 1 "Z1"
TABULATE 2 "Z2"
VARY BLOCK-VAR BLOCK=C1 VARIABLE=QN
SENTENCE=COL-SPECS
RANGE LOWER="250" UPPER="350" INCR="10"
SENSITIVITY S-2
DEFINE Z1 BLOCK-VAR BLOCK=C1 VARIABLE=RR
SENTENCE=RESULTS
DEFINE Z2 BLOCK-VAR BLOCK=C1 VARIABLE=VRATE &
SENTENCE=PROFILE ID1=2
TABULATE 1 "Z1"
TABULATE 2 "Z2"
VARY MASS-FLOW STREAM=FEED SUBSTREAM=MIXED
COMPONENT=ANILINE
RANGE LOWER="5.0E-6" UPPER="4.0E-5" INCR="2.5E-6"
CONV-OPTIONS
PARAM TEAR-METHOD=NEWTON SPEC-LOOP=INSIDE
STREAM-REPOR MOLEFLOW MASSFLOW
PROPERTY-REP NCES NOPARAM-PLUS

8.999E-006 / 26 8.990E-006 / 27 9E-006 / 28 9E-006 / &
29 9E-006 / 30 9E-006 / 31 9E-006
BLOCK-OPTION FREE-WATER=NO
A TIRE GASIFICATION
SENIOR DESIGN PROJECT
That Integrates Laboratory Experiments
and Computer Simulation

BRIAN WEISS AND MARCO J. CASTALDI
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The Accreditation Board for Engineering and Technology (ABET) requires that students in accredited engineering programs complete certain requisites to graduate. One constituent is engineering design, “the process of devising a system, component, or process to meet desired needs,” specifically Criterion 4—Professional Component, which is particularly focused on a major design project incorporating appropriate engineering standards and multiple realistic constraints. To fulfill the program, the Department of Earth and Environmental Engineering at Columbia University allows undergraduate seniors the opportunity to work independently under the supervision of a faculty advisor. The faculty advisor’s purpose is to guide the student’s activities and ensure progress.

The student typically decides on a topic area, such as waste to energy, in consultation with a faculty member. Once the overall project area is identified, a rigorous task plan and schedule are given to the student to begin the design effort. Clearly, this plan must be consistent with any guidelines outlined by the department (e.g., midsemester report, final presentation). In this case, Figure 1 (next page) details the efforts to be undertaken by the student and that are aligned with the department’s requirements of a fall and spring term presentation (not shown) and the final report.

One recent student’s project involved the conversion of waste tires by thermal treatment to either energy generation or chemical synthesis. The field of study was selected based on the expertise of the mentoring professor and capabilities of the laboratory. Weekly meetings between the student and professor were arranged and a schedule of activities was drafted to facilitate progress toward the design. The first semester (fall) concentrated on researching the topic, creating a design, and justifying the initial feasibility of the design with eco-

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Brian Weiss received his B.S. from the School of Engineering and Applied Sciences at Columbia University in spring 2005. The work with tire gasification culminated his education in the Department of Earth and Environmental Engineering. Currently, he looks forward to pursuing similar projects in efficient chemical conversion as a chemical engineering graduate student at the University of California, Berkeley.
**Plan for Fall Semester**

0) **Motivation** (*September 22*)
   a. Market demand
   b. Environmental/Economic/Global impacts/benefits
   c. Type of waste

1) **Previous work** (*October 15*)
   a. Patent office (*Next Week*) ([www.USPTO.gov](http://www.USPTO.gov))
   b. Textbooks
   c. General literature (journals)
   d. Company info

2) **Identify most promising processes** (*November 15*)
   a. Product yields
   b. Feedstock accessed
   c. Prototype built
   d. Economics
   e. Energy balance

3) **Understand** (*December 10*)
   a. Flow diagram
   b. Chemistry and reactions
   c. Thermodynamics
   d. Pitfalls
   e. Lab work

4) **Improve** (*Ongoing*)
   a. Imagination
   b. Lab work

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**Plan for Spring semester (Due dates in bold):**

0) **Review of tire pyrolysis and combustion characteristics.** (*Jan 14*)
   a. Literature search

1) **Materials list for Prototype** (*Jan 21*)

2) **Lab Work** (*Feb 25*)
   a. Combustion – TGA, micro GC (*Jan 28*)
   i. Test Plan (*Jan 14*)
   ii. Kinetics
   iii. volatile fraction; CO₂/CO; optimum atmosphere
   b. Gasification – Same apparatus (*Feb 25*)
   i. Test Plan (*Jan 28*)
   ii. w/ H₂O (g + 1); CO₂, CO, air
   iii. GC/MS product analysis
   iv. Effect of Temperature; optimum atmosphere;

3) **Computer simulation** (*Apr 8*)
   a. Aspen Plus
   b. Use TGA data
   c. Team with Kimberly?

4) **Prototype build** (*Apr 29*)
   a. Wire and Cellophane
   b. Smoke experiments

5) **Final Report** (*May 2*)

---

**Notes to plan:**

The prototype build might run overtime depending on the complexity of the project. The priorities will be physically observing the design, i.e. the lab work and the prototype build. The main benefit of a computer simulation could be a comparison with the models from last semester so it need not be the focus.

---

**Figure 1.**
The student and professor drafted a schedule of activities at the beginning of each semester. The schedule followed the guidelines given by the academic department.

---

Economic and thermodynamic calculations. The second semester (spring) focused on executing laboratory work necessary to provide data for input to a theoretical modeling of an overall system. Typically an industry-accepted modeling package is used to conduct simulation and analysis of an overall process. The package used during this project was Aspen Plus v. 12.1 by Aspen Technology, Inc.

Other design projects in which students combined experimental work and computer simulation have demonstrated positive results. In such projects, students can gain a profound understanding of industry in a more stimulating setting than a lecture class. In one project, students were instructed to use theory and experimentation to execute a boric acid dehydration process. The result won recognition from education competitions and Borax Europe, Ltd., an industry leader. In another case, students were prompted to design, fabricate, and test single-component, mechanical products. In both projects, an emphasis was made to complete the curriculum within one or two semesters. In the latter, computer aided design was necessary for compressing the work into the desired time frame. The success of each example project lay in the ability to organize a broad scope of activities into
manageable blocks.

The first step of the present design project was for the student and professor to propose a schedule of activities ensuring the student gained exposure to all aspects of the design experience. Shown in Figure 1, this type of work plan allows the student to understand the usefulness of preliminary calculations in guiding subsequent work. All segments of the plan were executed. The prototype build was attempted but not completed, however, because unanticipated opportunities to present the work arose and demanded more effort be devoted to refining what was already accomplished. The remaining sections of this paper are taken from work done by the student during the two-semester design project.

This paper is an example of how to integrate environmental issues such as pollution prevention, reuse, and recovery into the design experience. While this particular project did not use life-cycle assessment methods and tools, it could be a very worthwhile effort to employ them to explore the outcomes for waste tire and other waste-to-energy processes.

BACKGROUND WORK

The project began with a literature survey of academic papers, government programs, and business efforts. Currently in the United States, 290 million waste tires are generated annually. Additionally, nearly 300 million tires (~6 million tons) reside in environmentally unsound stockpiles. Accordingly, government impetus has created a market for waste tires that currently awards tipping fees to users between $50-100 per ton. Discarded tires have applications as a co-combustion fuel and ground rubber fills in construction materials. Only 9% of the tires currently generated in the United States go to landfills. Current applications for tires are both economically practical and regulated by national standards, but initial research showed opportunities for improvement. Most tires are used as supplementary feed in processes for which they were not explicitly designed. Since many advantages can be realized from a method specifically adapted to the feed, the purpose of the project became to design a system specific to scrap tires.

Since tires possess several distinct qualities as a fuel, thermal processing may offer a broad range of opportunities to improve existing practices. In the United States, three facilities have been established to convert exclusively scrap tires to electricity: Exeter Energy in Connecticut, Modesto Energy in California, and the Ford Heights facility in Illinois. Each facility was built in the early 1990s with a capacity to handle 8-10 million scrap tires per year on conventional equipment to produce 25-30 MW of electricity. Only one remains in business, however, indicating that their profitability is, in the current environment, only marginal. It is anticipated that, with rising energy and landfill prices, an innovative approach may enable a more successful business.

PRELIMINARY DESIGN AND ECONOMICS

Before drafting a reactor design, the economics and thermodynamics of the process were investigated using information found in the literature. These steps were intended to provide a “first-cut” analysis and set the boundaries of feasibility and profitability. A process was proposed with unit operations including: a standard thermal reactor; an electricity-producing system with boiler, turbine, and generator; a gas clean-up system consisting of an electrostatic precipitator, a scrubber and a stack; and auxiliary capital (pipes, pumps, etc.). Costing estimates were obtained from a chemical engineering textbook; size, efficiency, and inflation were incorporated into the model. Tires consist of a mixture of rubber polymer (C5H8)n and carbon black with added fillers such as light oils, fibers, trace metals (zinc), and a steel wire belt. A chemical and elemental analysis of tires was taken from a published source and showed a combustion enthalpy of 35 kJ/g.

The economic model was created for a process scaled to 10 million tires per year (164 thousand tons). The results showed that 16.7% of the tire’s enthalpy of combustion could be converted to an output of 28.6 MW of electricity. The revenue generated by the system included tipping fees from the tires ($100 per ton) and electricity sales ($0.05 per kWh). At an interest rate of 5%, the revenue after a 40% tax totaled to $21.5 million per year. The net present value was $201.5 million, which annualized to $8.4 million per year. The profits were $13.1 million per year indicating an internal rate of return of 19%. These results include all relevant parts such as working capital, debt servicing, permitting, and citing. The experiences of the other facilities combusting tires support the estimate.

Although the process proves profitable, the return is lower than most investors would prefer for new technology, indicating that a technological breakthrough is necessary to secure the business. Several reactors for converting waste-to-energy were researched including fixed beds, moving beds, fluidized beds, and rotary kilns. A fixed-bed type reactor was selected for its cost effectiveness, ease of use, and appropriateness to the feed. Additionally, it was proposed that the end product would be syngas (primarily CO and H2), which was thought to enable more controllable conditions. Syngas can be created by reforming the tires with CO2 and H2O. Because these reactions are endothermic, a heat source is required. Thus it was proposed that the combustion of tires with air could provide that heat to drive the reactions. Using sewage sludge as the water source could minimize costs, extending the scope of the design to a truly novel integrated waste converter. The ideas behind the design evolved by employing the principles of process intensification to existing technologies. Process intensification basically is the reduction of process volumes by combining and consolidating multiple unit operations into one physical unit.
DESIGNING THE REACTOR

The reactor was sketched in StudioTools (Alias). Anticipated flow patterns are shown in Figure 2. Scrap tires and stoichiometric air are fed separately into the combustor through an annular pipe. Tires fall and combus through a ceramic plate similar to a grate-type combustion system. The wall of the combustor has two layers: an outer impermeable steel barrier and an inner screen within which primary air emerges. This concept was adapted from the gas turbine industry to maintain moderate metal temperatures of the combustor. The purpose of the double wall is to maintain a unidirectional flow pattern that minimizes the amount of hot gases impinging on the wall. Secondary air actively cools the struts supporting the ceramic plate and assists the combustion. The combustion product leaves the combustor from below and enters the gasifier. The material to be gasified falls from the top in a counter-current flow to the hot gases. Heat transfers to the gasifier across the dividing wall of the combustor and via the enthalpy contained in the combustion product stream. The syngas produced is extracted through a pipe from the bottom. Baffles ensure the flow patterns run along the planned routes.

Figure 2. A rendering of the proposed reactor. Tires and air flow in an annular pipe and combus on a ceramic plate in the center. The combustion product exits the inner chamber from below and mixes with additional water, sludge, and tires. The syngas is extracted from a pipe in the side or on top and the ash falls to the bottom. Baffles ensure the flow patterns run along the planned routes.

MATERIAL AND ENERGY BALANCES

Material and energy balances were performed for both the combustor and the gasifier. For a reactor that consumes 10 million tires per year (164 thousand tons), combusting 30% in stoichiometric air and gasifying the remainder with 87,600 m³ of water per year, the results of the calculations showed the syngas to consist of 18.9% H₂, 16.6% CO, 6.0% H₂O, 8.4% CO₂, and 49.9% N₂. The total energy output is 37 MW of sensible heat and 103 MW of chemical energy. The temperatures of the combustor wall and gasifier are 1,040 °C, and 614 °C, respectively. A flame temperature for the combustion of the tires was calculated to be 1,469 °C. Based on a material residence time of one hour, a combustor size of 27 m³ was calculated with a 2.8 m base diameter.

The gasifier was sized to allow a moderate flow rate of the syngas produced, while enabling most of the large ash particles to settle. This led to a unit of 77 m³ that is 5.0 m diameter and 3.8 m in height.

The success of the process will be determined by the ability to control the material and heat flow. Because combustion temperatures can run higher than the limitations of most metals, the wall must be kept cool, which will be accomplished by air flow augmented by the fresh tire/sludge mixture entering the gasifier. The double wall will create a unidirectional air-flow pattern and minimize the impingement of hot combustion gases onto the wall. Both the temperature...
and the syngas quality will be regulated by the composition of the feeds: adding more tires produces more energy and higher temperature whereas more water yields more hydrogen in the product stream.

LABORATORY WORK

While most, and probably all, parameters could be obtained from the literature, one of the advantages of having individual design projects is the ability for students to get hands-on experience working in a laboratory. This enables them to generate pertinent data needed for their design. It also forces students to think of the experimental outcomes before doing the work, thus preparing them to develop practical test methods for efficiently generating data. To enable realistic engineering, basic thermodynamic and kinetic parameters of tires were required. Some of these parameters were obtained from equipment readily available in the faculty advisor’s combustion laboratory. An oxygen bomb calorimeter (Parr) yielded the heat of combustion of tires. The bomb calorimeter adiabatically combusted the tire sample at constant pressure. The temperature rise of a water bath correlated to the enthalpy of combustion of the tires. The enthalpy of combustion of tire was determined to range from -33.37 to -36.33 kJ/g which was consistent with established data. Kinetic information was obtained from thermogravimetric analysis (TGA). A Netzsch TG 409 PC instrument was used to record the mass loss of a sample as the temperature was increased at a constant rate. Constant flow rates (100 mL/min) of air (20% O₂; 80% N₂) and inert purge gas (20% CO₂; 80% N₂) flowed over the sample. The air enabled evaluation of combustion parameters while the inert atmosphere was selected to resemble the gasification zone. A plot of the fractional weight loss, α, versus temperature, T, showed that the sample mass decreased as temperature increased. A derivative plot of α showed reaction rates as peaks. At a constant temperature ramp, the reaction rate can be described by dα/dT, which follows an Arrhenius rate law.

\[ \frac{d\alpha}{dT} = A\beta e^{\frac{E_a}{RT}} (1 - \alpha)^n \]  

(1)

where A, Eₐ, and n are the Arrhenius frequency, activation energy, and reaction order, respectively; R is the universal gas constant, and \( \beta \) is the heating rate.

A representative TGA analysis is shown in Figure 2 in which the student had to convert that raw data to usable data for input into a model for design simulations. Combustion of tires in air revealed five peaks in the derivative plot implying an equal number of reactions, which have been proposed to correspond to light oils, natural rubber, synthetic rubber, and tars. Under inert atmospheres only the first three peaks were observed, implying that the tar only combusts in the presence of oxygen. At higher heating rates the peaks overlap but maintain recognizable reactions.

Because Eq. (1) cannot be solved explicitly, quantitative parameters were derived from a method from the literature. Plotting 1/T versus 
\[-\log\left[1 - (1 - \alpha)\right]/T^2 (1 - n) \text{ for } n \neq 1 \]  

(2a)

\[-\log\left[-\log(1 - \alpha)\right]/T^2 \text{ for } n = 1 \]  

(2b)

reveals a linear plot for the appropriately chosen reaction order. The Arrhenius rate parameters can be related to the slope, m, and the intercept, b, by

\[ E_a = 2.3 R m \]  

(3a)

\[ A = 10^{6.695} / R (1 - 2 R T / E_a) \]  

(3b)

By this method, rate parameters for air and 20% CO₂/N₂ atmospheres could be obtained as shown in Table 1.

| TABLE 1 |
| Parameters Derived from TGA Experiments |

The “Weight” column refers to the amount of mass change that can be accounted for by the reaction. Under air, there was a 5% residual, whereas under an inert atmosphere there was a 38% residual.

<table>
<thead>
<tr>
<th>Reaction under Air</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight</td>
<td>15%</td>
<td>13%</td>
<td>23%</td>
<td>20%</td>
<td>24%</td>
</tr>
<tr>
<td>Eₐ (kJ/mol)</td>
<td>120</td>
<td>180</td>
<td>187</td>
<td>325</td>
<td>258</td>
</tr>
<tr>
<td>A (Hz)</td>
<td>5.5 x 10⁶</td>
<td>1.3 x 10¹⁰</td>
<td>2.3 x 10¹¹</td>
<td>4.0 x 10¹⁰</td>
<td>2.7 x 10¹⁰</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reaction under 20% CO₂</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight</td>
<td>18%</td>
<td>12%</td>
<td>32%</td>
</tr>
<tr>
<td>Eₐ (kJ/mol)</td>
<td>95</td>
<td>203</td>
<td>176</td>
</tr>
<tr>
<td>A (Hz)</td>
<td>1.4 x 10⁶</td>
<td>2.5 x 10¹⁴</td>
<td>3.0 x 10¹⁰</td>
</tr>
</tbody>
</table>

Summer 2006
The outflow of the TGA was connected to an Agilent 3000 micro-GC gas chromatograph (GC). Figures 3 and 4 show a typical species analysis of the product gases by the GC, and allowed the student to conduct a material balance ensuring the integrity of the data generated. Combustion under air revealed that CO2 was the main constituent of the exhaust. Pyrolysis of tires under CO2 indicated that the amount of CO2 in the product gas increased slightly during the reaction and no CO was detected. The GC proved useful for determining the product species and can be used in future work to identify important constituents.

SIMULATION

Following the laboratory work, the student then reduced the data and calculated the parameters needed to input into a simulation. There were two sets of simulations done, one was thermodynamic and the other used kinetics obtained from the laboratory experiments to more accurately simulate the combined combustor-gasifier reactor. This allowed the student to better understand the type of information thermodynamics can provide versus an actual operating system where the kinetics play an important role. Results are shown in Table 2.

Thermodynamic Simulation

The thermodynamic data obtained from literature and the student’s experiments (bomb calorimeter) were input into Aspen. Tires were defined as a mixture of the rubber monomer (C5H8), graphite, iron, and zinc so that the final assay equaled the literature value. Figure 5 shows the process flow diagram of the equilibrium simulation. The combustor and gasifier were represented as two Gibbs reactors connected by material and heat streams. The ideal “separators” surrounding the gasifier selectively remove solids from the streams. A calorimeter module was programmed to combust the syngas with stoichiometric amounts of oxygen only, to enable the student to conduct an energy balance and compare that with initial calculations. The model output of 170 MW total power from 18,700 kg per hour (5.2 kg per second) indicates an energy input for tires of -33 MJ/kg kinetic simulations. The kinetic simulations first attempted to model the TGA experiments to ensure the results were consistent. The simulated TGA was a semi-batch reactor with a charge of the tire sample and a constant flow rate. Due to the kinetic parameters’ sensitivity to the phase of the reactants, the tires were modeled as a mixture of coal and graphite—both present in the Aspen database. The Aspen-defined coal had many similar properties to tires. The mixture was modified so that the final analysis of the material would have an enthalpy of -33 MJ/kg.

<table>
<thead>
<tr>
<th>Reactant Flow Rates</th>
<th>Product Flow Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tires (total)</td>
<td>H2</td>
</tr>
<tr>
<td>Combusted</td>
<td>CO</td>
</tr>
<tr>
<td>Gasified</td>
<td>CO2</td>
</tr>
<tr>
<td>Water</td>
<td>H2O</td>
</tr>
<tr>
<td>Air</td>
<td>N2</td>
</tr>
<tr>
<td>ton/hr</td>
<td>Nm³/hr x 10³</td>
</tr>
<tr>
<td>18.7</td>
<td>25.8</td>
</tr>
<tr>
<td>5.6</td>
<td>11.6</td>
</tr>
<tr>
<td>13.1</td>
<td>11.5</td>
</tr>
<tr>
<td>18.0</td>
<td>11.2</td>
</tr>
<tr>
<td>97,490 Nm³/hr</td>
<td>47.2</td>
</tr>
</tbody>
</table>

Temperature (°C) | Energy (MW)
----------------|-------------
Combustor        | Chemical    | 130 (eq) |
Gasifier         | Sensible    | 40        |
and a total chemical assay of the literature. For the combustion reactions, the tire was separated into six components based on the reactions determined by TGA in Table 1. The gasification simulation used four components. The simulation results of Figure 6 show that the simulation closely approximates the measured data. The correspondence suggests that the kinetic model can be developed further to simulate the combustion-gasification reactor. Although the ultimate plan was to simulate the design of the integrated gasifier and combustor, time did not permit this step. The exercise of conducting a thermodynamic simulation of the entire design and programming the kinetics to simulate the TGA experiments provided the student with sufficient experience to complete the project had time permitted. Upon completion of this task, the student was keenly aware of the many ways to arrive at designing a new technology or modifying an existing technology. Moreover, the student was now well prepared to understand the importance of experimental data generation and how to attack such a process in the future.

OUTCOMES

The undergraduate design project taught the student how to address engineering challenges. The literature research aided in the design of the combined combustion-gasification system, which was devised solely by the student. The professor’s role was to provide insights into the merits and limitations of such a device. Using a more experienced knowledge base, the professor was able to recommend calculations and experiments that would prove the design.

The independence of the student allowed greater opportunities for learning about the business environment surrounding waste manage-
ment, industrial thermal processes, reactor designs, and the engineering process. Performing the laboratory experiments helped the student comprehend the operation of standard analytical tools. Further, the student began to understand how to devise a test plan and allocate adequate time to attain a sufficient amount of data. The Aspen simulations were instructive in demonstrating the next level of design execution and evaluation. Finally, to expose the student to the experience of communicating the work, poster or lecture opportunities were pursued with presentations at two academic departments in Columbia University and Barnard College, at a university-wide undergraduate research symposium, and at an American Chemical Society meeting.

The individual responsibility for the project encouraged a greater commitment from the student and allowed a wider platform for innovation. The development and successful implementation of the project, however, may have benefited from a larger undergraduate or graduate team. Nonetheless, the student was able to maintain the directives assigned in the predetermined schedule and provide a report at the end of each term. The time frame of the project allowed ample time to understand basic aspects of designing a reactor and carry out the preliminary steps. The student was able to identify future directions for the project in the final report. It is anticipated that the student will be better prepared for future work as a professional engineer and that the project described herein may be continued under other circumstances.

IMPLEMENTATION

A suggested implementation strategy is briefly presented for those who wish to augment a traditional chemical or environmental engineering capstone experience with a similar effort. Provided the scope of the project is contained and a schedule is put forth at the beginning of the semester, a project such as this becomes very manageable. As evidenced in Figure 1, all elements of engineering design are covered. An important aspect of this type of project is to have the course span two semesters to give students time to assimilate material, develop and design processes, and possibly build devices or conduct limited experiments.

So as not to risk skipping or eliminating any of the critical areas of the design process, the real task, for the student and faculty advisor, is not to spend extensive time on any one area. All components should be developed to the extent that the student can see a clear path to the outcome of each task. Most engineering departments maintain a software license to the common programs used in industry and typically have some level of laboratory capabilities. This leaves only the task plan and timing to be formulated and strictly followed. For reference, the hours spent by the student and faculty advisor on this project were no more than a typical design course and the cost of everything except for the software license was under $200. Typically, software licenses are heavily discounted for educational institutions.

REFERENCES

4. EPA in Management of Scrap Tires (2005)
Demonstration and Assessment of
A SIMPLE VISCOSITY EXPERIMENT FOR HIGH SCHOOL SCIENCE CLASSES

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The objective of this demonstration and assessment was to develop an instructional model to inform and enthuse students about chemical engineering. Figure 1 shows the number of B.S. degrees granted nationally in chemical engineering. Rhinehart observed a 13-year-cycle period for the production of B.S. degrees in chemical engineering at Oklahoma State University, dating back to the 1930s. It is not clear at this time if the 13-year-cycle period for chemical engineering degrees awarded will hold, but it is clear that the peak has dropped from approximately 7,500 degrees awarded to approximately 6,500 degrees awarded, representing a 13% decline. Rhinehart attributes the cycling to B.S. chemical engineering supply/demand being out of phase but does not discuss the magnitude of the peaks. Halford, however, suggests the decline is due to a rising attraction of potential chemical engineers to the environmental engineering and bioengineering fields. The cause of the decline in chemical engineering enrollment has not been determined conclusively, but regardless of the cause—the effect is that when enrollment is low, administrators may question the benefit of maintaining an expensive chemical engineering program.

B.S. chemical engineers are indirectly supplied by the nation’s high schools. Therefore, one potential approach to positively impact enrollment in chemical engineering undergraduate programs is to conduct outreach programs for high schools. Ross and Bayles describe a method for incorporating high school outreach into chemical engineering courses. Their goal is to provide role models for high school students by assigning chemical engineering students enrolled in their courses to participate in an outreach project. In contrast, this work describes an outreach program administered and conducted by professors for the purpose of informing high school students about chemical engineering and attracting them to the profession.

Figure 1. Annual national B.S. chemical engineering degrees awarded.

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Academic Year

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Paul Jones recently retired as director of product supply for the Snacks and Beverages Division at the Procter & Gamble Corporation in Cincinnati.

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†: Procter & Gamble Corporation, Cincinnati, OH
The overall objectives of this demonstration were twofold. First, the authors wanted to develop a presentation giving an overview of the field of engineering with emphasis on chemical engineering. Second, the authors wanted to conduct a simple experiment with the high school students so that they have an opportunity to learn a chemical engineering concept and be exposed to principles and problems that practicing chemical engineers will expect to encounter.

**PRESENTATION DESCRIPTION**

The demonstration was conducted at Martin Luther King, Jr., High School in Dekalb County, Georgia, in November of 2004. A junior/senior-level physics course (a chemistry course may also be appropriate) was chosen for an introductory presentation followed by hands-on viscosity experimentation. Twenty-six students participated in the demonstration during a class period of 90 minutes.

General engineering, chemical engineering, and the concept of viscosity were discussed first. In the general discussion of engineering, the major engineering disciplines were described in basic terms (e.g., civil engineering was described as the branch of engineering responsible for designing municipal structures such as bridges and roads).

After a general discussion on engineering, the presentation was focused on chemical engineering. The facilitator discussed the kinds of jobs that chemical engineers are responsible for and the types of engineering fundamentals that chemical engineers study. The job areas described included petrochemicals, intermediate chemicals, food processing, cleaning products, plastics, and pharmaceuticals. When describing what chemical engineers study, several core examples were included. The list of what chemical engineers study included accounting for material flows (material and energy balances), how fluids move (fluid mechanics), how heat is transferred, and how materials react to create new things (reaction engineering). The students were informed that the viscosity experiment for the day was related to fluid mechanics. During the discussion on heat transfer, the example of an egg cooling was introduced. As expected, the students had a good idea about how long it would take for an egg to cool under different conditions (free vs. forced convection, in air vs. in cool water) but overall were surprised that it is something that chemical engineers expect to predict theoretically and/or empirically. During the discussion of reaction engineering, the example of how an antacid helps indigestion was introduced. The students were aware of acid/base reactions from their chemistry class, but again didn’t realize that chemical engineers are involved in producing the antacids (bases) that are administered to neutralize excess stomach acid.

The presentation ended with a discussion on viscosity. Viscosity was described as a fundamental physical property in the study of how fluids move or how “thick” and “slippery” a fluid is. Several examples including paste, pancake syrup, water, and motor oil were discussed. Viscosity was not mathematically defined during the presentation, and a discussion on Newtonian vs. non-Newtonian fluids was not included because the facilitators thought that it was beyond the scope of what was appropriate for a high school science class.

**APPARATUS AND THEORY**

The viscometer used for the demonstration has been described previously. The viscometer is a tank-tube viscometer as illustrated in Figure 2. It consists of a tank and a vertical drain tube attached at the bottom of the tank. In addition, a balance, a thermometer, a stopwatch, and a bottle of water at room temperature are required for the experiment. The viscosity of a fluid is inferred from the drain rate of the fluid through the drain tube of the viscometer tank. The drain rate is dependent on the viscosity of the fluid and follows the behavior described in Eqs. (1) through (4). The detailed derivations of these equations have been described previously.

\[
\ln \left( \frac{H+L}{h+L} \right) = \frac{g R_0^4 \rho}{8 \mu R^2 L} \left( t \right) \tag{1}
\]

\[
h = H - \frac{m}{\pi R^2 \rho} \tag{2}
\]

\[-\ln \left( 1 - \frac{m}{(H+L)\pi R^2 \rho} \right) \left( \frac{g R_0^4 \rho}{8 \mu R^2 L} \right) \left( t \right) \tag{3}
\]

\[m^* = -\ln \left( 1 - \frac{m}{(H+L)\pi R^2 \rho} \right) \tag{4}
\]

where

- \(H\): initial height of the fluid in the tank (9.3 cm, illustrated in Figure 3)
- \(h\): height of the fluid in the tank
- \(L\): length of the drain tube (56.4 cm)
- \(g\): acceleration due to gravity
- \(R_0\): equivalent radius of the tank
- \(\rho\): density of the fluid
- \(\mu\): viscosity of the fluid
- \(t\): drain duration
- \(R\): radius of the drain tube (0.0509 cm)
- \(m\): accumulated amount of a fluid drained from tank
- \(m^*\): left-side value of the viscosity equation, as shown in Eq. (3)

During the experiment a tank with a rectangular cross section, illustrated in Figure 3, was used instead of a tank with a radial cross section. This modification was made because the tank with the rectangular cross section is easier to fabricate. Thus, the equivalent radius \(R_0\) was computed with the
following equation
\[ R_o = \left( \frac{DW}{\pi} \right)^{1/2} \]  \hspace{1cm} (5)

where

- \( W \): width of the rectangle (25.4 cm)
- \( D \): depth of the rectangle (3.81 cm)

The experimental procedure for determining the viscosity of water using the tank-tube viscometer is as follows:

- Fill the reservoir with water.
- Set up the balance with automatic data acquisition so that the data from the balance are input directly into Microsoft Excel in real time. Use a sampling rate of 1/s.
- Remove the end cap on the drain tube and allow the water to collect on the balance.
- After \( \sim 90 \) s, stop the data acquisition.
- Plot \( m^* \) [left-hand side value of the viscosity equation as shown in Eq. (3)] vs. \( t \) (time) and obtain the slope of the line.
- Extract \( \mu \) from the expression of the slope as illustrated in Eq. (6).

\[ \mu = \left( \frac{gR^4p}{8 \pi L} \right) \frac{1}{\text{slope}} \] \hspace{1cm} (6)

- Measure the temperature of the water used in the experiment.
- Compare the experimental \( \mu \) to the literature value.
- Calculate the measurement error based on a percent difference.

In addition to the experimental procedure outlined, brief explanations on linear regression, Microsoft Excel features, and standard deviation (\( \sigma \)) were provided to the class. Units were not discussed and, due to time limitations, only one experimental run was performed.

**RESULTS AND DISCUSSION**

The viscosity experiment was demonstrated using water at room temperature. The experiment was successful with a measurement error of \( \sim 3\% \) which is the typical result obtained in a simple viscosity experimental setting with the tube-tank viscometer in the absence of a temperature regulating circulator.

**Facilitator’s Perception**

Overall, the students were enthusiastic and attentive, suggesting that the activity was structured appropriately to maintain the interest of a high school student. The students were also willing to interact with and participate in the presentation and the hands-on viscosity experimentation. The experiment could be improved by structuring it for more student participation. Ideally, there should be one station per four students so that the students can perform the experiment themselves. Excluding the computer and the balance, the fabrication cost is \$100 so the concept is economically feasible. Also, if time permits, it would be illustrative to measure the viscosity of more than one fluid. For example, in addition to measuring the viscosity of water, one could measure the viscosity of an alcohol and its aqueous solutions or water with the viscosity modified by adding a second component such as sugar.

**Student Survey**

Students were asked to rate the following five questions on a scale of one to 10 before and after the demonstration, where
one is “no knowledge” and 10 is “very knowledgeable”:
1. How much do you know about engineering?
2. How much do you know about chemical engineering?
3. How much do you know about viscosity?
4. How interested are you in engineering?
5. How interested are you in chemical engineering?

The students were also asked to comment on what they liked most about the presentation/experiment and what could have been improved.

Survey Results

Table 1 shows the results from the survey given to the students. The results summarize the students’ knowledge and interest before and after the presentation followed by the hands-on viscosity experimentation. The table also shows the difference between the two values and the statistical significance of the results. Using a paired-sample t test, it was concluded that the students gained by at least 36% in the knowledge of and interest in general engineering, chemical engineering, and the viscosity topic. In the future, however, a short test may be more informative than the student self-assessment for determining how much the students learned during the demonstration. Overall, the survey shows that the students are more interested in general engineering, but their interest in chemical engineering increased between 95% and 230%.

Survey Comments

Approximately half of the students indicated that the most interesting part of the demonstration was the experiment. The other half indicated that they enjoyed learning about different types of engineering and/or learning about chemical engineering. Most students didn’t comment on potential improvements, but of those who did, the majority indicated that more audience (i.e., student) participation was preferred.

SUMMARY AND OUTLOOK

An experiment/presentation appropriate for high school students was developed and demonstrated. Based on the survey results, the students gained by at least 36% in the knowledge of and interest in engineering, chemical engineering, and fluid viscosity. Furthermore, interest in chemical engineering increased between 95% and 230%.

Based on the survey results and the facilitator’s perception, for any high school experimental demonstration, a significant portion of the time allotted should be devoted to talking to the students about engineering and chemical engineering. In the future, the facilitators would like to contact high schools and offer to send them simple tank-tube viscometer kits so that a viscosity experiment can be incorporated into their existing curriculum. Also, the facilitators would like to develop a program so that undergraduates can participate in the viscosity experiment at local high schools as one of the department’s outreach efforts.4

ACKNOWLEDGMENTS

The authors would like to thank the Procter & Gamble Corporation for funding this work under a curriculum grant.

REFERENCES


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PLANT DESIGN PROJECT: 
Biodiesel Production Using Acid-Catalyzed Transesterification of Yellow Grease

RAFAEL HERNANDEZ, TRENT JEFFREYS*, ANIRUDHA MARWAHA, AND MATHEW THOMAS
Mississippi State University • Mississippi State, MS 39762

Over the last 10 years, the chemical industry, federal and state agencies, and the chemistry and chemical engineering profession have been increasingly investing intellectual, technical, and financial resources on the research, development, and application of chemicals and fuels generated from renewable raw materials and sustainable processes. The main goal of the involved parties is to develop energy-efficient and cost-effective processes that prevent pollution and decrease our dependency on foreign oil. The number of papers describing sustainable processes and renewable fuels that have appeared in the publications and conferences of the American Chemical Society (ACS) and American Institute of Chemical Engineers (AIChE) have increased significantly over the last five years. The 2005 57th AIChE Institute Lecture was titled “Energy Supply Challenges and Opportunities.” The ACS dedicated one issue of Environmental Science and Technology, the society’s main publication on environmental research, to sustainable processes.\textsuperscript{[1]} Presently, that journal includes a section on sustainable technologies in every issue. Additionally, numerous papers were presented at the 2005 Annual AIChE Meeting (Cincinnati) on biorefineries, sustainable technologies, and renewable fuels.

*Albermarle Corporation in Orangeburg, SC

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Trent Jeffreys has a B.S. (2004) in chemical engineering from Mississippi State University. Currently, he works for Albermarle Corporation in Orangeburg, SC as a process technology engineer. He has worked on projects for cost reductions, automation and control system development, and sample campaigns for new products in the Fine Chemicals Division.

Matt Thomas received his B.S. in chemical engineering from Mississippi State University in 2004. He is currently seeking his master’s degree in chemical engineering at Mississippi State University, studying the remediation of nitroaromatic contaminated groundwater. After receiving his master’s, he plans on continuing his education at Mississippi State University by working toward a Ph.D. in chemical engineering and focusing on producing oils from glycerol for biodiesel production.

Anirudha Marwaha has his bachelor’s degree in chemical engineering (2003) from Mississippi State University. He is currently pursuing a M.S. degree in chemical engineering at Mississippi State. Since 2001, he has been working for the E-Tech Lab in the chemical engineering department. His thesis work is on the solidification and stabilization of high-level radioactive waste.

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The main contributing factor to the chemical engineering and chemistry professions’ focus on efforts to promote the development of sustainable technologies and the production of renewable alternative fuels such as ethanol, biodiesel, and hydrogen has been the commitment of resources by the U.S. Environmental Protection Agency (USEPA), the U.S. Department of Agriculture (USDA), the National Science Foundation (NSF), and the U.S. Department of Energy (USDOE). One way to develop creative new production processes for renewable chemicals is to educate future chemists and chemical engineers on the design, advantages, disadvantages, and economics of current production techniques.

The last core course in the chemical engineering curriculum at most universities in the United States is capstone design. In this course, students have the opportunity to practice, for the last time in an academic environment, the design and economic evaluation of industrial chemical plants. To our knowledge, most chemical engineering capstone design projects focus on the use of petroleum-based raw materials for producing specialty and commodity chemicals. To broaden the students’ perspective on the potential contributions of chemical engineering to areas such as new energy sources, global warming, and environmental sustainability, they should be introduced to the conversion of plants, natural oils, microorganisms, and other types of biomass into alternative energy sources and value-added products. The capstone course represents an excellent opportunity to assign projects in which students synthesize and analyze renewable-chemicals production facilities. The objective of this paper is to describe a project entitled “Design of a Biodiesel Production Facility Using Acid-Catalyzed Transesterification of Yellow Grease,” assigned to the capstone design course at Mississippi State University (MSU). Research on biodiesel is conducted by the class instructor’s research group. Thus, the design problem

Biodiesel is an alternative renewable fuel derived from vegetable oils or animal fats, which conforms to ASTM D6751 specifications for use in diesel engines.[2] Biodiesel utilization has increased significantly over the last 10 years, mainly due to environmental benefits and government efforts to reduce dependence on foreign oil. The use of biodiesel reduces emissions of CO₂, CO, SO₂, and particulates from operating diesel engines. Under a newly established sustainable energy policy by the U.S. Department of the Interior, over 20 national parks operate boats, trucks, heating systems, electricity generators, and other fuel related systems on 100 percent biodiesel and/or biodiesel/petroleum diesel blends. Blends of 20 percent biodiesel with petroleum diesel require no engine modifications. Furthermore, biodiesel/petroleum diesel blends have demonstrated lubricity enhancements over the newly required low sulfur petroleum diesel. Numerous school districts, transit authorities, public utility companies, and recycling companies have also successfully used biodiesel. Recently, the U.S. military has begun to procure biodiesel for use in on-base vehicles. These numerous experiences with the use of biodiesel have clearly shown the environmental and high performance characteristics of this alternative fuel.

In spite of the fact that Mississippi ranks 4th and 16th nationally in yellow grease generation and soybean production (main biodiesel feedstocks), there are no biodiesel production facilities in the state. The Swalm Engineering Design Group at MSU was asked by the Alternative Energy Company to perform a preliminary design of a 2,240 lb/hr biodiesel production facility using acid-catalyzed transesterification of yellow grease, and to evaluate the process economics. In order to perform sensitivity analysis of process variables, the company requires a simulation of the whole process using ChemCad. The company has acquired land adjacent to a fertilizer manufacturing company in Yazoo City, Miss., at the cost of $1,000,000 as the plant site. The design is to be based on a project life of 20 years. The major equipment, however, is to be depreciated in accordance with applicable IRS regulations. In your final design report, you are requested to provide estimations of the annual return on investment as well as the rate of discounted cash flow taking into account the most recent laws and regulations on corporate taxes. Design basis and specifications, available utilities, and other information will be provided in further communications.

Figure 1. Project description.
Some of the comments in the students’ course evaluations were . . . , “What I like most about this course was the fact that the project was broken into separate portions over the whole semester,” and “I loved the layout of the class . . . .”

also represented an excellent opportunity to integrate research and education. As part of the course, invited speakers and the course instructor presented seminars on ethics, job interview preparation, entrepreneurship, and the social and environmental implications of reducing our dependency on petroleum. A workshop on ChemCad (chemical process simulation software) was offered to students and faculty by the software creators.

PROJECT DESCRIPTION

The statement of the problem submitted to the students on the first day of class is presented in Figure 1. The class was divided into five groups and each group had four members selected by the instructor. The same project was assigned to all groups. The open-ended nature of the problem statement led to five different design configurations.

The design project was divided into three progress reports (memorandums) and one final report. Several activities and rules were established to maximize participation of all students:

(A) Progress reports and the final report were accompanied by an oral defense. The student in charge of presenting the oral defense was selected at the time of the presentation. Each member of a design group was questioned extensively during each progress report presentation.

(B) Written peer evaluations were required after each progress and final report. The evaluation forms were similar to those suggested by Fogler.⁷

C) A panel of industry and academic members judged and selected the best final presentation. The presence of industry representatives was additional encouragement for all the students to prepare for the presentation. The instructor selected the best report. The group or groups with the best presentation and final report received plaques and cash awards.

PROGRESS REPORTS

Division of the design project into progress reports had two objectives. The first objective was to evaluate an inductive approach to the teaching of plant design. This approach consists of the presentation of a general problem or concept, followed by closer focus on details and the solution of component small problems. This method is applied by the chemical industry and during academic and industrial research and development activities and it is an approach suggested by chemical engineering educators.⁴,⁵

The second objective was to facilitate the organization of the project and enhance students’ time-management skills. Some of the comments in the students’ course evaluations were related to the second objective. For example, “What I like most about this course was the fact that the project was broken into separate portions over the whole semester,” and “I loved the layout of the class—progress reports and the final presentation.” The tasks conducted for each progress report were as follows:

- **Progress Report 1**: Literature survey, calculation of gross profits, block diagram preparation, overall mass balance calculations, and input of yellow grease components into the ChemCad database.
- **Progress Report 2**: Preparation of process-flow diagram and simulation of the transesterification reactor and methanol recovery system.
- **Progress Report 3**: Simulation of all the biodiesel purification steps: neutralization, solids removal, glycerol recovery, and biodiesel and glycerol purification.

PROJECT SOLUTION

Yellow grease is the fat generated during animal rendering activities. It is mainly composed of oleic, palmitic, and stearic fatty acids attached to glycerol,⁶ and contains a relatively high percentage of free fatty acids (15%). Zhang (2000) used triolein (triacylglycerol) as a test compound to represent yellow grease during a Hysys simulation of a biodiesel production facility.⁷ The acid-catalyzed transesterification of this compound using methanol as the alcohol results in methyl oleate and glycerol. Zhang (2000) assumed that biodiesel could be represented by methyl oleate.⁷ To generate a mixture of transesterification products with similar biodiesel chemical and physical properties, the students were encouraged to use several triacylglycerols and oleic acid (free fatty acid) as representative of yellow grease for the ChemCad simulation of the biodiesel production facility. Figure 2 presents the reactions of acid-catalyzed transesterification of the selected triacylglycerols and oleic acid. The acid-

\[
\begin{align*}
C_{19}H_{34}O_{6} + 3CH_{3}OH &\xrightarrow{H_2SO_4} 3C_{19}H_{38}O_2 + C_{19}H_8O_3 \\
\text{Oleic acid} &\quad \text{Methyl Oleate} \\
C_{19}H_{34}O_{6} + 3CH_{3}OH &\xrightarrow{H_2SO_4} 3C_{19}H_{38}O_2 + C_{19}H_8O_3 \\
\text{Tripalmitin} &\quad \text{Methyl Palmitate} \\
C_{19}H_{34}O_{6} + 3CH_{3}OH &\xrightarrow{H_2SO_4} 3C_{19}H_{38}O_2 + C_{19}H_8O_3 \\
\text{Tristearin} &\quad \text{Methyl Stearate} \\
C_{19}H_{34}O_{6} + 3CH_{3}OH &\xrightarrow{H_2SO_4} 3C_{19}H_{38}O_2 + C_{19}H_8O_3 \\
\text{Triolein} &\quad \text{Methyl Oleate}
\end{align*}
\]

Figure 2. Acid-catalyzed transesterification reaction for producing fatty acid methyl esters (FAME).
catalyzed transesterification of the proposed components of yellow grease results in a mixture of methyl esters of oleic, palmitic, and stearic fatty acids. This mixture contains more than 90% of the methyl esters found in commercial biodiesel from yellow grease. Phase behavior of triglyceride- and alcohol-rich phases was ignored for simplicity. Students recognized that they were making this simplification.

The complete process flow diagram (PFD) and stream table are presented in Figure 3 (a and b) as well as in Table 1. Both were prepared using the ChemCad process simulation software licensed by Chemstation in Houston. Some of the physical and chemical properties of the yellow grease-assumed components were determined using the UNIFAC Group Contribution method in ChemCad. Other basic properties, such as boiling point and melting point, were input manually into the simulator.

The first main unit operation of the PFD is the transesterification reaction system (R200). To determine reactor volumes, it was assumed that the reactors were half full and the reactions followed first-order kinetics. Reactor volume meeting

| Table 1: Stream Properties Corresponding to the Process Flowsheet Presented in Figure 3 |
|---------------------------------|--------|--------|--------|--------|--------|--------|--------|--------|
| **Stream No.** | 2 | 7 | 8 | 9 | 10 | 11 | 12 | 14 |
| **Name** | **H₂SO₄** | **MeOH** | **YG** | **Rx Out** | **MeOH Rcy** | **Rx Feed** | **MeOH Bot** | **LLE Bot** |
| **Molar Flow, lbmol/h** | 3.93 | 7.85 | 3.35 | 178.07 | 162.57 | 178.07 | 15.5 | 32.32 |
| **Mass Flow, lb/h** | 385.12 | 251.52 | 2206.75 | 8200.12 | 5207.87 | 8200.09 | 2992.34 | 1057.53 |
| **Temperature, °C** | 25.12 | 25.16 | 25.19 | 80 | 64.41 | 59.02 | 140.35 | 139.57 |
| **Pressure, kPa** | 340 | 340 | 340 | 400 | 101 | 400 | 110 | 111 |
| **Vapor mole fraction** | 0 | 0 | 0 | 0 | 0.0032 | 0 | 0 | 0.7484 |
| **Average mol. weight** | 98.08 | 32.04 | 659.29 | 46.05 | 32.04 | 46.05 | 193.03 | 32.72 |
| **Actual dens. lb/ft³** | 114.42 | 49.28 | 55.17 | 49.07 | 15.53 | 5031 | 53.42 | 0.09 |
| **Std liq. ft³/hr** | 3.38 | 5.03 | 39.63 | 154.84 | 104.21 | 155.02 | 50.63 | 13.52 |
| **Flow rates in lbmol/h** | | | | | | | | |
| **Triolein** | 0 | 0 | 1.17 | 0.04 | 0 | 1.2 | 0.04 | 0 |
| **Tripalmitin** | 0 | 0 | 0.67 | 0.02 | 0 | 0.69 | 0.02 | 0 |
| **Tristearin** | 0 | 0 | 0.34 | 0.01 | 0 | 0.35 | 0.01 | 0 |
| **Oleic Acid** | 0 | 0 | 1.17 | 0 | 0 | 1.17 | 0 | 0 |
| **Sulfuric Acid** | 3.93 | 0 | 0 | 3.93 | 0 | 3.93 | 3.93 | 3.9 |
| **Methanol** | 0 | 7.85 | 0 | 162.64 | 162.49 | 170.34 | 0.16 | 0.15 |
| **Methyl Oleate** | 0 | 0 | 0 | 4.67 | 0 | 0 | 4.67 | 0 |
| **Methyl Palmitate** | 0 | 0 | 0 | 2.06 | 0 | 0.04 | 2.06 | 0 |
| **Methyl Stearate** | 0 | 0 | 0 | 1.28 | 0 | 0.26 | 1.28 | 0 |
| **Glycerol** | 0 | 0 | 0 | 2.18 | 0 | 0 | 2.18 | 2.18 |
| **Water** | 0 | 0 | 0 | 1.25 | 0.08 | 0.08 | 1.17 | 26.09 |
| **Calcium Oxide** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| **Calcium Sulfate** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
TABLE 1 CONTINUED

Stream Properties Corresponding to the Process Flowsheet Presented in Figure 3

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<td>NeutRxOut</td>
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<td>Calcium Oxide</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.9</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Calcium Sulfate</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.9</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.9</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

The conversion requirement (97% the initial triglycerides) was minimized by including two equal-size reactors in series. The first and second reactors achieve an overall 83% and 97% conversion, respectively. The volume of each reactor was 200 ft³ and the material of construction selected was 316 stainless steel. The reactions were performed at 80 °C and 400 kPa. The reactor influents were 3.35 lbmol/hr, 3.93 lbmol/hr, 170.42 lbmol/hr yellow grease, sulfuric acid, and methanol. The reactors were simulated in ChemCad using the equilibrium reactor. This reactor gives the user the capability to simulate multiple reactions.

The purpose of the methanol recovery system (T210) is to return excess, unreacted methanol to the reactor to save raw material costs. The major challenge in simulating the methanol recovery tower is to return as much methanol as possible to the reactor, thus minimizing water in the recycle stream. Conversion of triglycerides into biodiesel drops dramatically if the reactants contain between 0.5% and 5% water. The simulation was conducted using the ChemCad tower module. The column was operated using atmospheric pressure for the overhead stream and a bottom pump-out pressure of 110 kPa. The smallest number of theoretical stages that could be obtained while keeping the water-weight percent of the reactor feed below 0.10% was 13 with a feed stage of seven. This resulted in a water concentration 0.064% by weight in

Chemical Engineering Education
the feed to the reactor. The distillation column recycles 99.9% by weight of the methanol in the reactor effluent.

The remaining portion of the process after the methanol recovery system consists of separation and purification steps to obtain purified biodiesel, glycerol, and yellow grease recycle streams. The effluent of the surge tank (V-220) is pumped into the bottom stage of the liquid-liquid extractor (T-300). Water cascades down the column after being fed into the top stage. The wash water extracts the entrained glycerol while the biodiesel and unreacted yellow grease exit the top of the column. The ChemCad simulation of T-300 resulted in four theoretical stages for complete separation of biodiesel from glycerol. The students conducted a sensitivity analysis using ChemCad to determine the effect of reboiler operating temperature of the biodiesel distillation column and wash-water flow into the liquid-liquid extractor on cost and biodiesel purity, respectively. Figure 4 shows the effect of wash-water flow on biodiesel purity. It can be observed that water flows in excess of 500 lb/hr have a negligible effect on biodiesel purity. This type of analysis is essential to determine optimum plant operating conditions to meet biodiesel quality.

The crude glycerol stream from the bottom of the extractor flows to the reactor (R-500) for the neutralization of the sulfuric acid catalyst by the following reaction:

\[ \text{H}_2\text{SO}_4 + \text{CaO} \rightarrow \text{CaSO}_4 \text{ (gypsum)} + \text{H}_2\text{O} \]

Calcium oxide (CaO) was the base choice due to low cost, limited complications in regard to materials of construction, and low solubility of its salts formed by neutralization. A CSTR was selected to perform the transesterification reaction. The reactor was simulated in ChemCad using the stoichiometric reactor module and assuming 100% conversion of sulfuric acid. The reactor was maintained at 80 °C. Effective mixing of solids is easily maintained by physical agitation in a CSTR. Additionally, the CSTR should prevent any excess collection of calcium sulfate in the neutralization reactor. A centrifuge (CN-510) was used to separate the gypsum from the glycerol and water. A solids effluent moisture fraction of 10% was defined for the centrifuge. It was assumed that the gypsum recovered was sold to a cement company at $56/ton.¹

The liquid stream from the centrifuge flowed into the glycerol purification tower (T-600) to achieve a bottoms product of 99.5% by weight purity glycerol. Four theoretical stages were required to achieve the desired purity. To use high-pressure steam, the column must be operated at a reduced pressure so that the reboiler temperature is 250 °C. The final reflux ratio of 1.8 results in a reasonable reboiler duty while maintaining the desired purity of 99.5%.

The biodiesel purification column (T-400) must produce 99.6% by weight biodiesel by separating the methyl esters from the unreacted yellow grease. This column presented several challenges in simulating its operation due to the lack of experimental vapor-liquid equilibrium data for biodiesel.

¹ Communication with cement company.

Figure 4. Effect of wash-water flow into the liquid-liquid extractor on the biodiesel purity exiting the distillation tower.
and yellow grease. Operation of the column at atmospheric pressure required extremely high reboiler temperatures of up to 600 °C to achieve a sufficient biodiesel purity. Therefore, the column was simulated under severe vacuum with top and bottom operating pressures of 8 kPa and 20 kPa, respectively. The necessity of low vacuum for the separation of triglycerides from biodiesel also has been observed by other investigators. Under these conditions, the bottom product temperature was 330 °C. The vacuum necessary for this separation can be achieved using multistage steam injectors. Dowtherm G at 357 °C was selected as the heating medium for the reboiler.

Students prepared the final report following the format suggested by Peters, et al. Capital and operating costs were determined using the Cap Cost software included in the textbook by Turton, et al., Web sites, and communications with vendors. Several scenarios were evaluated to determine plant economics. For example, students evaluated return on investment (ROI), taking into consideration the biodiesel tax incentive ($1.00/gal) included in the current version of the Energy Bill. ROI also was determined after increasing the operating capacity of the plant. These scenarios helped students understand the economics of scale and the current situation of the biodiesel industry in the United States, which requires government incentives to be economically feasible.

The results of the estimation of capital and total product costs are presented in Tables 2 and 3. The information in these tables was essential to determine net present value and the ROI. The prices used for raw materials costs were: yellow grease, $0.1175/lb; methanol, $0.6/gal; sulfuric acid, $67/ton; and calcium sulfate, $56/ton. Except for the price of calcium sulfate, all the other prices were obtained from the September 2003 issue of the Chemical Market Reporter. The students assumed that the solid recovered during the neutralization step (calcium sulfate) was sold to a local cement company. They contacted a local cement company to obtain a calcium sulfate purchasing price. Utilities costs were the following: low-pressure steam, $2.50/1000 lb; high-pressure steam, $5.50/1000 lb; natural gas, $2.70/1000 SCF; electricity, $0.04/kWh; cooling water, $0.05/1000 gal; wastewater treatment, $56/1000 m³; and process water, $0.5/1000 gal.

Total income was calculated by adding biodiesel, glycerol, and calcium sulfate sales. The prices used for biodiesel, glycerol, and calcium sulfate were $2.40/gal (the price of petroleum diesel at the time was $1.40/gal and the $1.00/gal tax incentive was added), $0.72/lb, and $15/ton, respectively. The mass and volume rates are presented in Table 1. The total annual income was $7,083,700. Subtracting the total product costs shown in Table 3 results in annual gross earnings of $888,100. Assuming a 35% tax, the after-tax profit (ATP) was $577,200.

The after-tax cash flow (ATCF) is the sum of the ATP and depreciation. ATCF is calculated for every year of plant operation. The depreciation was calculated using straight-line depreciation with 9.5 years recovery period. Thus, depreciation and ATCF were given by:

\[
\text{d} = \frac{\text{original investment}}{9.5 \text{ years}} = \frac{\$2,291,642}{9.5 \text{ years}} = \$241,226 \quad \text{year}^{-1}
\]

\[
\text{ATCF} = \text{ATP} + \text{d}
\]

\[
\text{ATCF} = \$577,277 + 241,226 = \$818,503
\]

Only half of the depreciation was added in year 10 of operation and no depreciation was added in the final years of operation. ROI is a profitability measure defined as the ratio of profit to investment. Average profit over the 20 years of plant operation and fixed capital investment were used to calculate ROI for the biodiesel production facility. This value resulted in:

\[
\text{ROI} = \frac{\sum_{i=1}^{20} \text{ATP}_i}{\text{ATP}_{\text{ave}}} \times 100
\]

\[
\text{ROI} = \frac{\$577,277}{\$2,864,552} \times 100 = 20\%
\]

This value of ROI is considered acceptable for a new product entering into an established market. The payback period is the length of time necessary for the total

<table>
<thead>
<tr>
<th>TABLE 2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Estimation of Capital Investment for the Proposed Biodiesel Production Facility</strong></td>
</tr>
<tr>
<td>Cost components</td>
</tr>
<tr>
<td>Equipment (including service, installation, and instrumentation)</td>
</tr>
<tr>
<td>Distillation columns</td>
</tr>
<tr>
<td>Jacketed reactors</td>
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<tr>
<td>Liquid-liquid extractor</td>
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<tr>
<td>Heat exchangers</td>
</tr>
<tr>
<td>Tanks</td>
</tr>
<tr>
<td>Total equipment costs</td>
</tr>
<tr>
<td>Land (buildings and service facilities included)</td>
</tr>
<tr>
<td>Indirect costs (20% fixed-capital investment)</td>
</tr>
<tr>
<td>Fixed-capital investment</td>
</tr>
<tr>
<td>Working capital (15% of fixed-capital investment)</td>
</tr>
<tr>
<td>Total capital investment</td>
</tr>
</tbody>
</table>

1 Communication with cement company.
return to equal the capital investment. It was calculated using the following equation:

\[
\text{PBP} = \frac{\text{FCI}}{\sum_{t=1}^{20} \text{ATCF}}
\]

\[
\text{PBP} = \frac{$2,864,552}{\$13,837,187 / 20} = 4.14 \text{ years}
\]

To calculate ATCF, full depreciation was only added the first nine years of operation and only half of the depreciation was added for year 10. As mentioned above, no depreciation was added the final years of operation. The value of PBP obtained is also acceptable for a new product entering an established market.\(^9\) The students concluded that a biodiesel production facility is not economically feasible without government tax incentives. This result gave the students an understanding of the need for state and federal support for developing new industries associated with renewable energy.

Some of the results presented above were taken from the class-best final report. Student course evaluations and senior exit interviews indicated that the application of research and teaching was an exciting and motivating experience for the class. Some of the students’ comments about the project included:

- “I liked the fact that the project was a real-life application.”
- “I became more competent with ChemCad.”
- “This class helped with my teamwork skills.”

Additionally the class benefited by:

- Access to the instructor’s extensive literature collection on biodiesel production technology.
- Excitement of working on the production of renewable fuel with clear environmental, health, and safety benefits.
- Discussing contemporary issues associated with the economic feasibility of a renewable fuel.
- Visualizing the importance of lifelong learning on the application of chemical engineering principles to contribute solutions to society’s dwindling energy resources.
- Determining the capital and operating cost drivers of the acid-catalyzed transesterification biodiesel production process.

### TABLE 3

| Estimation of Total Product Cost for the Proposed Biodiesel Production Facility |
|-----------------------------------|-----------------|
| **Cost Components**               | **Cost/Year**   |
| **Manufacturing Cost**            |                 |
| Raw Materials                     | $2,407,199      |
| Utilities                         | $367,178        |
| Labor (based on plant capacity kg/day\(^9\)) | $1,252,912 |
| Maintenance (7% of fixed capital investment minus land and indirect costs\(^9\)) | $90,415 |
| Operating (15% of maintenance costs) | $13,562 |
| Depreciation (straight line depreciation) | $241,226 |
| Local Taxes (1% of fixed capital investment\(^9\)) | $28,645 |
| Insurance (1% of fixed capital investment\(^9\)) | $28,645 |
| Overhead (56% of labor and maintenance\(^9\)) | $749,202 |
| **Total Manufacturing Cost**      | $5,178,984      |
| **General Expenses**              |                 |
| Administrative (20% of operating labor and maintenance\(^9\)) | $273,186 |
| Distribution and Marketing (7% of the total product costs\(^9\)) | $433,695 |
| Research and Development (5% of the total product costs\(^9\)) | $309,782 |
| **Total General Expenses**        | $1,016,663      |
| **Total Product Cost (Total Manufacturing + General Expenses)** | $6,195,647 |

**SUMMER 2006**
EXPERIMENTAL INVESTIGATION AND PROCESS DESIGN 

in a Senior Laboratory Experiment

KENNETH R. MUSKE
Villanova University • Villanova, PA 19085

A drying experiment for the senior unit operations laboratory course at Villanova University is described in this article. This experiment involves the determination of the drying rate of a solid material in a forced convection drying apparatus and the scale-up design of this process. The experimental drying rate data is used to determine the appropriate transport coefficients to mathematically describe the drying process. The students then use this mathematical model for the design of a large-scale dryer for a specified production rate of the material under study. Various solid materials such as sand, gravel, clay, sawdust, natural and synthetic fibers, and agricultural products have been used in this experiment. This variety of materials is intended to provide each student group with a different experience that can be compared and contrasted during student group oral presentations at the end of the semester.

The main goal of the laboratory exercise documented in this article is to provide the students with hands-on experience in the analysis and design of drying processes. Drying is an essential unit operation in the chemical process industries with applications ranging from forest products[1] and mineral processing[2] to food products[3] and pharmaceuticals[4]. Although this technology has been a key component of chemical engineering since its inception as an academic discipline, the science of drying continues to remain an active area of research and development.[5] Despite its widespread industrial importance, however, it is not emphasized in the heat and mass transfer courses due to time constraints. This laboratory experiment provides an opportunity for students to apply transport phenomena concepts presented in the classroom to the process of drying, while becoming familiar with this common unit operation.

A second goal of this experience is to provide students with an opportunity to apply the results of their experimental study to a process design. A similar approach to the unit operations laboratory course is advocated in Reference 6. The emphasis of this experiment is not simply to obtain data to determine transport coefficients. The students must also use their results in the scale-up design of the drying process. This addition of a design element to the laboratory provides a more practical objective for students and a more realistic application of their experimental investigation. This experience also provides additional learning objectives in the laboratory course, such as the development of engineering awareness, mathematical modeling, scale-up, and economic evaluation.[7]

There have been a number of chemical engineering laboratory drying experiments reported in the literature such as microwave drying of sand[8] and convection drying of a towel.[9] A bench-scale experimental drying apparatus[10] and the statistical treatment of drying data[11] have also been reported. The unique aspect to the experiment described in this article is both the incorporation of a design element and the study of a wide variety of materials with drastically different drying properties for each group.

Kenneth Muske is an associate professor of chemical engineering at Villanova University where he has taught since 1997. He received his B.S.ChE and M.S. from Northwestern (1980) and his Ph.D. from The University of Texas (1990), all in chemical engineering. Prior to teaching at Villanova, he was a technical staff member at Los Alamos National Laboratory and worked as a process control consultant for Setpoint, Inc. His research and teaching interests are in the areas of process modeling, control, and optimization.

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LABORATORY EQUIPMENT

The experiment is carried out using a batch cross-circulation cabinet dryer. A schematic of the dryer system is shown in Figure 1. Air is supplied at a rate of 0-440 ft³/min by a centrifugal blower with a gate-valve arrangement to adjust the air flow into the cabinet. The air is heated by two steam coil heaters located in the bottom half of the cabinet. The inlet air is passed through the heaters in the bottom half of the cabinet before being redirected to the drying section in the top half of the cabinet. A baffle arrangement (not shown in Figure 1) provides uniform air flow in the drying section. The volume of the drying section is 5.6 ft³ and the cross-sectional area for the air flow is 1.9 ft². The material to be dried is contained within a shallow tray or wire basket that is suspended in the air stream.

Dryer air temperature is controlled by a valve on the inlet steam line to the heaters with manual valves to isolate either heater. Steam is supplied from the high-pressure building main. Source pressure to the dryer is maintained at 30 psig by a regulator on the supply line. This reduction in the heater steam supply pressure is for both safety considerations and improved temperature control by increasing the normal operating range of the steam valve. The maximum dryer temperature is restricted to 200 °F for all experiments to prevent the possibility of thermal decomposition or ignition of the solid material.

Dryer process measurements include: the mass of the tray and material using a load cell (Transducer Techniques EBB-5 load cell [0-5 kg] and DPM-3 digital panel meter with analog output); the air temperature and relative humidity in the dryer using a humidity probe (Omega Engineering HX94C relative humidity/temperature probe); the surface temperature of the material in the tray and a second dryer air-temperature measurement using thermocouples (Analog Devices 2B52A type T thermocouple transmitters); and the inlet air flow rate inferred from the differential pressure across an orifice in the inlet air header to the blower (Setra Systems C239D differential pressure transmitter). The approximate cost of this instrumentation at the time of installation was $400. In addition to the electronic measurements, there is a thermometer inside the dryer cabinet, a wet/dry bulb thermometer to determine the conditions of the inlet air, and a water manometer connected to the orifice in the inlet air line. The data acquisition and control computer system displays the process measurements in real time and also records these values in a data file for later analysis by the students. A data sampling period in the range of 0.25 to 1 min is suggested to the student groups for data collection by the computer system.

LABORATORY EXERCISE

There are two three-hour laboratory sessions each week for the experiments in the senior laboratory course. These sessions are composed of two planning, experimental, and analysis sequences. The students only have access to the drying apparatus during the two experimental sessions. In the first planning session, the group is introduced to the material that they will be studying, the range of moisture content that they must consider, and the specifications on the final dried product. Because the students have essentially no practical experience with drying processes, they are expected to re-search the drying process and plan their experimental study during this session. Presentations on drying can be found in Perry’s chemical engineering handbook[12] and other process engineering handbooks such as Cooper, et al,[13] along with unit operation and mass transfer texts such as McCabe, Smith and Harriot,[14] Geankoplis,[15] and Treybal.[16]

The initial drying experiments are carried out during the first experimental session where the students determine the character of the drying curve for their material. An initial estimate for the tray loading is based on rules of thumb for the design of drying processes such as presented in Reference 13. The drying rate and moisture range for the constant rate period and the transition to the falling rate period are determined from the students’ initial experimental results during the first analysis session. An initial determination of the corresponding mass transfer coefficients is also carried out during this session.

In the second planning session, the group develops its experimental plan for the second experimental session. Depending on the drying behavior of their material and the results of their initial experimental session, during this session the student groups usually either concentrate on the falling rate period or consider the effect of different tray loadings. The incorporation of a second experimental session allows for the unstructured experimental approach adopted in this laboratory course. Benefits to the students of an unstructured approach include exposure to a more realistic experimental study, since
in reality the precise details of a procedure are rarely known in advance and the experimental plan often evolves as more information is discovered.

The final analysis session is used to analyze the data obtained from the second experimental session, and to design the scale-up drying process. Each student group is informed of the required production rate and initial moisture content of their source material after completion of the second experimental session. This practice is implemented in order to prevent the students from specifically targeting their experimental study to their scale-up process design requirements.

**EXPERIMENTAL ANALYSIS**

The process of drying can be described using an energy balance determined by the heat transfer rate between the hot gas and the moist solid, and a material balance determined by the mass transfer rate between the moist solid and the hot gas. The corresponding liquid component evaporation rate can be calculated using the relationships\(^{[14]}\)

\[
m = M_w h^A \frac{T_y - T_i}{\Delta H_f} = M_w A k_x (y_i - y_g) (1 - y)_{LM}
\]

where \(m\) is the evaporation rate of the liquid component from the moist solid, \(M_w\) is the molecular weight of the liquid component, \(A\) is the contact area between the moist solid and hot gas, \(h^A\) is the heat transfer coefficient, \(T_y\) is the bulk hot gas temperature, \(T_i\) is the solid-gas interface temperature, \(\Delta H_f\) is the latent heat of vaporization of the liquid component at the interface temperature, \(k_x\) is the mass transfer coefficient expressed on a mole fraction basis, \(y_g\) is the bulk liquid component mole fraction in the hot gas, \(y_i\) is the liquid component gas-phase mole fraction at the solid-gas interface, and \((1 - y)_{LM}\) is the log mean value of \((1 - y_i)\) and \((1 - y_g)\).

For reasons of convenience and safety, the liquid component is water and the gas is air for all of the experimental studies in this laboratory. Due to the time constraints in the laboratory sessions and the relatively slow evaporation rates for the materials under study, the dryer system is typically operated at near maximum air flow rate to maximize the evaporation rate. Under these conditions, constant air temperature and humidity can be safely assumed. Because the thermal changes to the system occur at a faster time scale than saturation changes, it is also appropriate to assume that the drying rate can be expressed in terms of the mass transfer relationship for drying process design calculations.\(^{[17]}\) This assumption is applied in both the experimental data analysis and scale-up design. It should be noted that a similar mass transfer expression to Eq. (1) in terms of partial pressure and humidity driving forces can also be employed. Although partial pressure has been the most popular, the student groups have tended to be rather evenly divided in their choice of driving force for their mass transfer coefficient.

The determination of the mass transfer coefficient depends on the behavior of the drying curve for the material under study. All of the materials considered in this experiment exhibit a constant-rate drying period and some exhibit a falling-rate drying period for the moisture range of interest. The constant-rate period is characterized by a constant rate of drying that is independent of the moisture content. During this period, a continuous film of water exists on the solid surface that is constantly replenished as the surface water evaporates. The falling-rate drying period occurs when the moisture content of the solid falls below some critical point. After this point, there is insufficient moisture present to maintain a continuous liquid film on the solid surface and the liquid mass transfer in the solid phase becomes limiting as opposed to interfacial mass transfer.\(^{[15]}\) The drying rate typically decreases as the moisture content in the solid decreases during this period.

Under typical experimental conditions during the constant-rate drying period, all of the parameters in Eq. (1) are relatively constant. The constant-drying-rate mass transfer coefficient can then be determined from the slope of the total tray mass vs. time, total material mass vs. time, or the free moisture mass vs. time drying curves as follows

\[
k_x = \frac{-a(1 - y)(1 - y_g)}{M_w A(y_i - y_g)}
\]

where \(a\) is the slope of the drying curve during the constant-rate drying period, \(y_g\) is the mole fraction of water in the inlet air determined from the humidity probe in the cabinet and checked with the wet/dry bulb thermometer, and \(y_i\) is the mole fraction of water at the solid-gas interface. The interface mole fraction is assumed to be the equilibrium saturation value at the interface temperature, which can be determined using steam tables or the Antoine equation. As discussed in Reference 15, it is possible to apply the dilute gas-phase mole fraction approximation \((1 - y)_i \approx 1\) in the analysis of the constant-rate-period mass transfer coefficient.

The determination of the mass transfer coefficient for the falling-rate period is more problematic due to the changing conditions of the material and the interface. Although many approaches exist to describe the falling-rate period,\(^{[14-15]}\) one of the simplest is to assume that the drying rate is proportional to the difference between the free moisture in the solid and the equilibrium free moisture,

\[
m = M_w A k_x (X - X^*) \quad \dot{X} = \frac{M_w A k_x}{m_s} (X - X^*)
\]

where \(k_x\) is the solid-phase mass transfer coefficient, \(X\) is the bulk solid free moisture, \(X^*\) is the equilibrium free moisture, \(m_s\) is the dry mass of the solid material, and the
other parameters are as defined previously. Eq. (3) can be integrated yielding

\[ t = \frac{m}{M_w A k_x} \ln(X - X^*) + b = a \ln(X - X^*) + b \]  

(4)

where \( a \) is the multiplicative constant and \( b \) is the constant of integration. The solid-phase mass transfer coefficient can be determined from the constant, \( a \), obtained by a logarithmic fit of the free moisture vs. time experimental data.

\[ k_x = \frac{m}{a M_w A} \]  

(5)

This fit is easily accomplished using Excel or any curve-fitting numerical package. The use of the free moisture vs. time curve, as opposed to the drying rate computed by central differencing the data as discussed in Reference 8, provides a more accurate estimate of the mass transfer coefficients for both the constant and falling rate periods because of the noise inherent in the load cell measurements.

**EXAMPLE EXPERIMENTAL RESULTS**

Figure 2 presents the total material mass (load cell reading minus the empty-tray mass) drying curve for a coarse sawdust material initially composed of a 2:1 volumetric mixture of sawdust (900 ml–156 g) and water (450 ml–450 g) with an average material thickness in the tray of 1 cm. Figure 3 presents the material interface temperature for this system determined by a thermocouple embedded in the surface of the sawdust. Linear regression on the material mass for the constant-rate drying time period between 5 and 80 minutes resulted in a slope of -3.89 g/min with a correlation coefficient of 0.992. Assuming an equilibrium interface temperature of 140 °F for the constant drying period, the resulting constant-rate drying period mass transfer coefficient is \( k_x = 11.2 \text{ gmol/m}^2\text{-min} \). Although not used in this calculation, the log mean value was \( (1 - y)_{LM} = 0.895 \), which is close to the dilute-gas phase mole fraction approximation. The specification on the final dried sawdust product was that it must be free flowing without any lumps. The student group concluded that the dried sawdust material met this criterion after
85 minutes at the end of the constant-rate drying period with a moisture content of 0.8 g H₂O/g dry solid.

Figure 4 presents the free-moisture drying curve for a clay absorbent material initially composed of a 3:1 mixture by mass of absorbent (474 g) and water (158 g). The average material thickness in the tray was 0.375 in. A logarithmic regression on the falling-rate data after 31 min resulted in a value of the multiplicative constant of -61.6 min with a correlation coefficient of 0.953. The corresponding solid-phase mass transfer coefficient is \( k_x = 0.427 \text{ gmol/ft}^2\text{-min} \). The specification on the dried absorbent product was that it must be dry enough to package. The student group concluded that the dried absorbent met this criterion after 60 minutes with a moisture content of 0.075 g H₂O/g dry solid. The justification of this decision was that the drying rate essentially goes to zero after this time resulting in little further drying being possible without a very long additional exposure.

**SCALE-UP PROCESS DESIGN**

The scale-up process design is based on manufacturing a specified production rate of some product from the wet solid material with a specified initial moisture content. The final moisture content of the material must be determined by the student group based on a subjective performance criterion as indicated in the initial laboratory handout. Examples of this criterion are that the solid must be dried to the point that it is free flowing or dry to the touch. This subjective criterion requires both experimental data and engineering judgment to determine the final moisture content. The intent is to demonstrate that product specifications are often not directly measured physical quantities.

Because the mass transfer coefficient is a function of the operating conditions of the dryer, the scale-up process operation must not deviate significantly from the experimental operating conditions if the experimental mass transfer coefficient is to be used in the design. This restriction does impose limitations on the scale-up design depending on the experimental conditions that were considered. Specifically, the material depth in the tray and the air velocity in the scale-up design must be representative of the experimental conditions used to determine the mass transfer coefficient. For example, the air velocity is determined by the air flow rate and cross-sectional flow area. To change the driving force for mass transfer by changing the air flow rate, the cross-sectional area must also be changed to maintain a similar air velocity. A benefit of the design aspect in this experiment is the exposure to this relationship between experimental investigation and scale-up design through hands-on experience. Such exposure is not available in the process design course because of the lack of an experimental component.

A further objective of the design aspect is the development of a physically realistic process design. Although most student groups have little difficulty in determining the required surface area and air rate for the scaled-up process, the actual physical design of the dryer can often be unrealistic. A common initial approach is to scale up the experimental apparatus to handle the required production rate. The result is a design with trays that are often too large and heavy to be physically managed. More realistic process designs evolve as the student groups are prompted to consider the size and weight of the material that must be handled. An example initial approach for the scale-up design of a wood-chip dryer with a production rate of 1 ton/day consisted of a batch cabinet dryer using a single 50-ft-long tray containing almost one-half ton of wet wood chips. The final design was also a batch cabinet dryer, but instead consisted of ten 5-ft-long trays stacked on top of each other where each tray initially contained approximately 120 lbs of wet wood chips. The consideration of the practical aspects of a process design is an additional benefit of this experience.

**PRESENTATION OF RESULTS**

The experimental and scale-up process design results for each student group are reported in a formal written
report and an oral presentation. The formal written report is due 10 days after the last analysis session for the experiment. The oral presentations are scheduled over a series of presentation days at the end of the semester. There are also short memo reports required after each laboratory session to document the planning, experimental, and/or analysis results and conclusions. The different materials and scale-up requirements incorporated into this experiment provide each group a slightly different experience that can be shared with the class during the presentation sessions.

Each student group is composed of three students and there are three experiments in the senior laboratory course. Therefore, each student in the group takes on the responsibility of group leader for one experiment in the sequence. Each group leader is responsible for the formal written report, oral presentation, and short memo reports on their experiment. The group leader responsibility also includes coordinating the activities of the other group members. When the class is not evenly divisible by three, there will either be one two-member or four-member student group. A two-member student group will not prepare a formal written report and oral presentation for one of the experiments although they will carry out this experiment and prepare the short memo reports. A four-member group will be given two objectives with a separate group leader for one of the experiments. Because of the length of the drying experiments, they have not been considered for two objectives in a four-member group.

STUDENT RESPONSE

There are no formal course evaluations for laboratory courses in the chemical engineering department at Villanova University. Student response data for the senior laboratory course is obtained from departmental surveys administered at the end of the semester. Qualitative assessment of the students’ experiences is also based on their comments during and after the experiment. This assessment indicates that the experience has been generally well received by the students. Student comments concerning the drying experiment reveal that the group spent more time on this experiment because of the design aspect, which required more use of the second planning and analysis sessions.

CONCLUSIONS

The laboratory experiment documented in this article has been developed and implemented over the past two years in the chemical engineering senior laboratory course at Villanova University. Based on the results of informal course surveys, the students have found the experience both challenging and worthwhile, in addition to providing an applied mass transfer and process design experience. The experiment has also provided valuable documentation of students’ ability to design, conduct, analyze, and interpret experiments for ABET\textsuperscript{[18]} Criterion 3b and their ability to perform as part of a team for ABET\textsuperscript{[18]} Criterion 3d.

ACKNOWLEDGMENTS

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REFERENCES

Many chemical engineering departments are wrestling with the following questions:

- When should computing be introduced to the chemical engineering student?
- How should computer programming in chemical engineering be taught, and how much formal programming instruction on languages such as C should be provided (vs. usage of computing tools such as MATLAB, Mathcad, spreadsheets, etc.)?
- Is a numerical methods course required and where is it in the course sequence? How many credit hours are needed? Which department teaches it?
- Should every chemical engineering course include some computing?

Since the mid-'80s two approaches have been taken toward introductory computing for engineers: “CS 101” and the engineering tools approach. The “CS 101” approach was catalyzed by the growth of computer science programs, which provided instruction in computer languages. Over the years the “CS 101” courses have migrated through several programming languages: Pascal, C, C++, and Java. In the engineering branch, software vehicles such as spreadsheets (first Lotus 123, then Quattro Pro, and now Excel), TK Solver, Mathcad, and MATLAB have gradually pushed out programming languages (primarily Fortran). Programming languages are becoming endangered species in these courses.

The “CS 101” branch would claim a number of reasons for existence:\(^{10}\):

- engineers should learn fundamental concepts of programming and computer science
- computing should be taught by computer scientists, not engineers
- engineering faculty are not interested in teaching computing languages to their students
- these courses provide a significant number of student credit hours (SCH) and budgetary resources

There are concrete benefits to an engineering education that incorporates the ability to write computer programs: Students learn what assumptions go into the program, i.e.,

- what the right answer should be
- what is the input, what is the output
- clear organization of thought, logic, and calculations is required
- that errors can exist in a program
- that programming is unforgiving for ambiguities and errors

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When it comes to assessing computing needs, faculty often confuse what is important for their students with what is important for themselves.

The “Engineering Tools Approach” branch believes:

- engineering students need a solid grounding in problem solving with modern computing tools
- engineering students need the knowledge and tools required in their professions
- engineering computing and problem solving are best taught by engineers
- there is no room in the curriculum for a separate three- or four-SCH course in programming

While the two branches are complementary and most engineering students could benefit from both courses, most chemical engineering program curricula are too congested to make room for both.

Many departments no longer require a course in a computer programming language such as Fortran, C, or C++. It has been suggested that teaching computer programming is analogous to teaching plane geometry. It is a way of thinking but you may not have to use it. On the other hand, without some programming ability, engineers are limited by the built-in capability of commercial software without any way to extend it. This has led a number of departments to switch from teaching C++ to using MATLAB as the programming tool. MATLAB is a structured programming language that incorporates many elements of Fortran, C, and C++. It allows for modularity, flow control, and input/output control and has the following programming features.

1. Loops: like DO and WHILE in Fortran, MATLAB has for and while
2. Conditional statements: like IF in Fortran, C, and C++; MATLAB has if for testing relational operations
3. Relational operations: like C and C++, MATLAB has the expected suite of <, >, <=, >=, ==, ~=. And like C and C++, the result of the operation is 1 or 0, and can be used outside of a conditional statement
4. Logical operations: like Fortran, C, and C++, relational operations can be strung together with AND(&), OR (|), and NOT (~)
5. Matching: like C, MATLAB has a switch/case syntax for matching string variables, integers, or logicals
6. I/O: not only can a user be prompted for input and then have results output to screen in formatted form (using fprintf, as in C), but MATLAB can read (load) and write (save) to files, in binary or ascii format
7. Modularity: like SUBROUTINE in Fortran or function in C and C++, MATLAB allows the user to create user-defined functions to be called by a main program; any number of inputs and outputs can be associated with a user-defined function
8. Error processing: using the try/catch syntax a user can attempt calculation(s) and then gracefully continue execution if an error occurs
9. Array math: like Fortran90, MATLAB transparently accommodates scalar and array math (i.e., implied FOR loops)

Reasons given by faculty for switching from C++ to MATLAB include ease of use and widespread availability due to an inexpensive student version. Because MATLAB is an interpreted rather than compiled language, the user can create (write), debug, and run code in the same environment. The built-in editor can pass code directly to the MATLAB application for execution. Also, MATLAB has a solid graphical interface for creating 2-D and 3-D plots; and plots can be created using appropriate MATLAB code from within a user’s program.

Based on informal surveys many chemical engineering departments now introduce programming and engineering problem solving in the freshman year. The view is that
these subjects are best taught by an engineering department in the context of an application. A typical introductory course has the following outline.

- problem-solving: engineering method, units, precision in calculations
- symbolic computing: algebra, calculus
- spreadsheet techniques: solutions to engineering problems, Visual Basic for Application (VBA) in Excel
- programming fundamentals: data types, program flow, modularity, object-oriented features
- elementary numerical methods: linear and nonlinear equation solving, linear regression
- software tools: Mathcad, MATLAB, Excel

When it comes to assessing computing needs, faculty often confuse what is important for their students with what is important for themselves. Faculty needs, more often than not, align with their research interests and activities, and these may be disconnected from the needs of their undergraduate students. Also, faculty may have an incorrect impression of the computing needs of professionals by either being out of date or out of touch. Discussions on computing needs do not always proceed on the basis of evidence from alumni and employer surveys. Finally, computing is not part of the daily professional existence of most faculty and is not expected to be. Their computing skills can be oxidized, and most of their computing is carried out by their students.

In the area of computing software, there is a noticeable disconnect between industry and academia. The appendix summarizes a survey of computing practices of recent graduates in chemical engineering, most of whom now work in industry. Typically chemical engineering departments teach the use of MATLAB, Mathcad, Mathematica, or Maple but not the use of spreadsheets. Yet in industry, spreadsheet software (e.g., Excel) is the dominant computer package in use. Of course, this may reflect the nature of many calculations that need to be performed by chemical engineers in industry, rather than a need to de-emphasize the teaching of sound numerical approaches in universities. Some faculty resist teaching spreadsheets, for example, because it is difficult to analyze the logic in the code, but this appears to be changing with the availability of VBA. Another objection is that a spreadsheet approach can encourage the use of inaccurate or inefficient numerical calculations (no error control, etc.) For complex calculations, it may be better to program spreadsheets using VBA, where programming logic is more transparent.

The survey of industrial usage of computing in the appendix also indicates that less than 50% of recent graduates in chemical engineering actually perform programming on the job (although there is no clear definition of what constitutes "programming" in industry). The use of spreadsheets in chemical engineering practice appears to be increasing. The application of spreadsheets in university courses may be attractive because of student-driven usage. David Clough (U. Colorado) and Brice Carnahan (U. Michigan) have developed many examples of spreadsheet applications, as presented at the 2002 ASEE Chemical Engineering Summer School.

TEXTBOOKS AND AFFILIATED SOFTWARE

The fragmented nature of software tied to leading undergraduate textbooks makes integration through the curriculum difficult, e.g.,

(a) material and energy balances: Felder and Rousseau\textsuperscript{121} – EZ Solve; Himmelblau and Riggs\textsuperscript{30} – POLYMATH
(b) thermodynamics: Sandler\textsuperscript{41} – MathCAD; Kyle\textsuperscript{81} – POLYMATH; Elliott and Lira\textsuperscript{61} – various programs
(c) separations: Wankat\textsuperscript{71} – Aspen
(d) process control: Seborg, Edgar, Mellichamp\textsuperscript{80} – MATLAB; Bequette\textsuperscript{90} – MATLAB; Riggs\textsuperscript{100} – MATLAB/Excel
(e) chemical reaction engineering: Fogler\textsuperscript{111} – POLYMATH; Ekerdt and Rawlings\textsuperscript{121} – Octave/MATLAB
(f) product and process design: Seider, Seader, Lewin\textsuperscript{131} – Aspen, HYSYS, CHEMCAD, PROII

In addition to these courses, many departments are teaching a statistics course, which involves still one more software package such as JMP, SAS, or Minitab. Clearly, using a subset of these textbooks sequentially through the sophomore, junior, and senior years will require a student to learn up to five or more different software packages. Adding software packages from outside of chemical engineering can push the total number of packages beyond 10, which becomes problematic for the typical student. It would be desirable to keep the number of software packages below three or four if possible [note that Excel is only mentioned once in (a)-(f) above although it is used with many of the textbooks listed]. But usually textbooks are not chosen because of the bundled software. In addition, departments must address issues of software availability, licensing, cost, and providing software in computer labs vs. student-owned computers. A textbook that is closely coupled to a software package, a CD-ROM, or a Web site is clearly an attractive option.

TEACHING PROCESS SIMULATORS THROUGH THE CURRICULUM

Several departments have found that the difficulty of integration of computing tools mentioned above can be avoided by more extensive use of process simulators. It is quite common to expose students to a commercial simulator in a thermodynamics or separations course. At Virginia Tech, ChE undergraduates have been using Aspen Plus and Aspen Dynamics to solve problems in all subjects, starting in the sophomore year. It is fairly straightforward to convert a steady-state model in Aspen Plus into a dynamic model (with PID control schemes) in Aspen Dynamics. The applicability ...
of Aspen Plus to mass and energy balances, thermodynamics (physical and thermodynamic property analysis, estimation and regression), multicomponent separations, reactor design, and process flowsheet simulation is well known. In process control Aspen Dynamics enables students to evaluate controller tuning, process dynamics, startup and shutdown, etc. HYSYS has similar features, and has been used at Rowan University for analysis in freshman-senior years.

Recently, Version 2.0 of a CD-ROM, Using Process Simulators in Chemical Engineering: A Multimedia Guide for the Core Curriculum,[14] has become available. Modules and tutorials are provided for self-paced instruction in the use of the process simulators to solve open-ended problems in courses on material and energy balances, thermodynamics, heat transfer, reactor design, separations, and product and process design. A 110-page document has been prepared for instructors suggesting the best instruction sequence and providing exercises and solutions, for each of the core courses (first introduced at the 2002 ASEE Chemical Engineering Summer School).

NUMERICAL AND ANALYTICAL APPROACHES IN MODELING OF PHYSICAL BEHAVIOR

Historically many engineering courses have been taught from an analytical viewpoint, but a transition is starting to occur in which numerical experiments are being gradually added in fluid flow or heat transfer courses. Problems and experiments should not be so simplified that they are not realistically formulated. Students are normally exposed to idealized fluid flow cases in the curriculum, for which application of theoretical concepts results in a solution of a one-dimensional ordinary differential equation or an algebraic equation. Therefore it is very easy for them to come away with the notion that theory is useless for most real-life situations.

Students should be able to select either analytical or numerical techniques to solve a problem, hence they should learn the advantages and disadvantages of either approach. Use of more sophisticated numerical tools such as CFD (computational fluid dynamics) will reduce the need to make many simplifying assumptions because you do not need as many assumptions to solve the problem numerically. Chemical engineering students should understand that there are both numerical experiments and physical experiments. In some cases we can make observations from numerical experiments that you cannot see in physical data, but the converse is also true. This does not suggest that all derivations should be replaced by numerical simulation, neither should every experiment be replaced with a simulator. There should, however, be a balance of experimental fluid dynamics (EFD), analytical fluid dynamics (AFD), and CFD.

To prepare students for industrial practice, there should be a department-level re-examination of the role of detailed analytical solutions. Is the purpose of some of these exercises the preparation of undergraduates for graduate school or industry? Today practicing engineers are not expected to carry out complex derivations in project work. Once a fluid flow situation is analyzed theoretically or the governing principles are discussed, that same situation can be visualized using the computer. This visualization of the flow phenomena can significantly facilitate and enhance the learning process, especially for the visual learner. CFD software makes flow visualization easy. Students can simulate flow processes in a transient or steady-state mode. Flow patterns can be displayed via velocity contours, velocity vector plots, or graphs of velocity profiles. A key element in flow visualization exercises is exploring the effects of different parameters. Using CFD, students can quickly change the size of the pipe, viscosity of the fluid, size of the particles, velocity of the feed, etc., and see the resulting changes in the flow behavior. This type of parametric analysis also ties in nicely with a discussion of dimensionless groups and geometric and dynamic similarity.

While computing and visualization can increase understanding, educators do not want students to view such simulators as black boxes. In the fluid mechanics course, simulations can become a mathematical exercise with little intuition, unless the instructor has the students solve a simple problem by hand first. More work on the software tools is needed, and it is critical to match the software tool to the student’s knowledge base.

Two specific recent packages that have been developed for educational usage are FlowLab (a finite volume-based code) by Fluent, Inc., and FEMLAB (a finite element-based code) by Comsol, Inc. Based on a survey by Professor Jennifer Curtis at the University of Florida, about 20 departments of chemical engineering in the United States expose their undergraduate students to CFD software. FlowLab allows students to solve fluid dynamics problems without requiring a long training period. Using carefully constructed examples, FlowLab allows students to get started immediately without having to spend the large time commitment to learn geometry and mesh-creation skills required by traditional CFD software. Current exercises that have been developed include sudden expansion in a pipe, flow and heat transfer in a pipe, flow around a cylinder, and flow over a heated plate, among others. In addition, professors can create their own examples or customize the predefined ones.

FEMLAB provides ready-to-use application modes, where the user can build his or her own model by defining the relevant physical quantities rather than the equations directly. The software also allows for equation-based modeling, which gives the user the freedom to create equations. FEMLAB’s programming language is an extension of the MATLAB language; this feature gives much flexibility to the user. FEMLAB’s graphical interface includes functions for automatic mesh generation of a user-defined geometry. Recently a k-ε turbulence model has been added to its menu of options.
Seider, et al., present the design of configured consumer products, which usually involves 2-D or 3-D simulations. In Chapter 19 (Product Design), momentum and species balances in a 2-D plasma CVD reactor are employed to produce thin Si films using CFD packages such as FEMLAB. This illustrates where it is very effective for students to use CFD packages to optimize designs—even without understanding all of the physical and chemical interactions in the transport-reaction processes.

Even with these recent advances in educational CFD software, this computing technology has been slow to penetrate undergraduate transport and reactor engineering courses. A 2002 CACHE survey of all chemical engineering departments in the United States on barriers to implementing CFD identified a lack of knowledge concerning available CFD resources, a lack of professor training in CFD, the relative difficulty of use and the long learning curve associated with using CFD software in a given course, and cost of CFD software.

VIRTUAL LABORATORY EXPERIMENTS

Laboratory courses are evolving, and new directions are being examined at specific universities, combining elements of simulation and also distance learning. In the chemical process industries, the high cost of pilot-scale equipment and operating manpower has led to more reliance on computer-based simulations rather than traditional pilot-scale experiments. During a typical day, the plant engineer works from a control room, or at least behind a computer screen. An engineer rarely is in the field adjusting valve positions, flow rates, and temperatures, because that is normally done using the computer interfaces of distributed control systems.

The fourth-year unit operations laboratory at Texas Tech University is emulating industrial practice, by providing computer-generated simulations based upon mathematical models for laboratory equipment. The unit operations laboratory can familiarize students with safety concerns and operational issues regarding each piece of equipment. Major pieces of equipment include a double-pipe heat exchanger, an ammonia gas-absorber packed column, and a cooling tower. The Virtual Unit Operations laboratory (VUOL) complements the existing laboratory to give students a realistic experience with industrial operations. LabVIEW computer interfaces of the VUOL permit students to control the equipment in addition to physically turning valves and checking temperatures.

In the Texas Tech course each student operates two physical and two virtual experiments. Based on preliminary assessment data, students reported that this type of laboratory class contributed either a great deal or considerably in all areas of ABET criteria a-k. Virtual and physical experiments complement each other and enhance student learning. In addition, there appears to be no significant difference in the student perception to their learning in using virtual vs. actual unit operations experiments, in 18 out of 20 ABET-related skill areas. While students believe both types of experiments are valuable, a total virtual unit operations laboratory would apparently not be well-received by the students. With the physical portion of the lab, students get a feel for the equipment and how it operates. With the virtual portion, the students 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.

Web-access of laboratory experiments enables real chemical engineering laboratory equipment to be controlled and monitored interactively by computers that are connected to the Internet, i.e., under the command of users over the Web. This capability is now available in the labs at University of Tennessee-Chattanooga as well as other schools.

Today practicing engineers are not expected to carry out complex derivations in project work. Once a fluid flow situation is analyzed theoretically or the governing principles are discussed, that same situation can be visualized using the computer.
such as University of Texas-Austin, Columbia University, University of Toledo, and MIT. Such labs permit faculty and students from any university to run Web-connected experiments at any time of the day or night, any day of the week. The laboratory station computer operates the equipment (pumps, valves, heaters, relays, etc.), collects the data (pressure, temperature, position, speed, concentration, etc.) and sends it to the Web user. The University of Tennessee site is accessed through the Web address <http://chem.engr.utc.edu/>, and even includes audio and video of the operating equipment.

All established chemical engineering programs are facing increased financial pressure to keep existing laboratory experiments up to date and in satisfactory operating condition. Major operating costs of unit operations laboratories include maintenance and teaching assistant support. Using highly automated experiments for remote operations will allow a drastic reduction in TA time requirements for those particular experiments. In addition, by sharing the operation of the experiments among several universities, there can be a pro rata reduction in maintenance costs. There is also the opportunity to add experimental assignments to a lecture class using this technology. In a lecture class, it may be desirable to have students individually or in small groups carry out an experiment, much like a homework assignment; in contrast, a traditional experiment would require continuous supervision by teaching assistants (e.g., one week of TA time for an entire class). Therefore, using an Internet-based experiment can greatly reduce the time commitment by the TA. It is clear that traditional experiments should remain in the curriculum to give students “hands-on” exposure, but they can be augmented with Internet labs.

**PROCESS AND PRODUCT DESIGN**

Historically there has been a process design emphasis in the curriculum that is now transitioning to a dual product and process design emphasis. This means that a framework is needed to make process decisions to make structured products. This has added a performance layer, i.e., not just purity of the product. Given a structure, we can often predict at some level what the properties of the material are likely to be. The accuracy of the results and the methods used to treat them depend critically on the complexity of the structure as well as the availability of information on similar structures. For example, various quantitative structure property relationship (QSPR) models are available for the prediction of polymer properties. The inverse engineering design problem, however—designing structures given a set of desired properties—is far more difficult. The market may demand or need a new material with a specific set of properties, yet given the properties it is extremely difficult to know which monomers to put together to make a polymer and what molecular weight the polymer should have. Today the inverse design problem is attacked empirically by the synthetic chemist with his/her wealth of knowledge based on intuition and experience. A significant amount of work is already underway to develop the “Holy Grail” of materials design, namely, effective and powerful reverse-engineering software to solve the problem of going backwards from a set of desired properties to the realistic chemical structures and material morphologies that may have these properties. After this is completed, a subsequent step would involve how to manufacture the desired new product.

A chapter on Molecular Structure Design in Seider, et al., [13] contains simple optimization procedures using GAMS to determine polymer repeat units, refrigerants, and solvents that have desired properties using group-contribution methods. Eventually, these will be replaced (and augmented) by molecular models.

Another subject related to product design is the scheduling of batch processes, which can be done using simple simulation techniques, as in BATCH PLUS and SUPERPRO DESIGNER. Hence design of optimal processing can be viewed as “product design” for specialty chemicals. Clearly, spreadsheets and optimization packages can also be used for many of these computations. Finally, the use of large databases and software systems, such as ASPEN IPE, for equipment sizing and purchase and installation cost estimation, is becoming common throughout the chemical industries for product and process design.

**MOLECULAR MODELING**

A molecular-level understanding of chemical manufacturing processes would greatly aid the development of steady-state and dynamic models of these processes. Process modeling is extensively practiced by the chemical industry to optimize chemical processes. One needs, however, to be able to develop a model of the process and then predict not only thermochemical and thermophysical properties but also accurate rate constants as input data for the process simulation. Another critical set of data needed for the models is thermophysical properties. These properties include such simple quantities as boiling points and also more complex phenomena such as vapor/liquid equilibria phase diagrams, diffusion coefficients, liquid densities, and the prediction of critical points. A key role of computational chemistry is to provide input parameters of increasing accuracy and reliability to the process simulations.
Under the NSF grant, “World Wide Web-Based Modules for Introduction of Molecular Simulation into the Chemical Engineering Curriculum,” seven university experts in molecular simulations have developed Web-based modules to facilitate introduction of molecular simulation into the chemical engineering undergraduate curriculum. These teaching modules can be integrated directly into chemical engineering core undergraduate courses, supplying for the instructor and the student the appropriate linkage material between macroscopic concepts currently taught in these courses and molecular simulations designed to aid student understanding of the molecular underpinnings of the phenomena. Modules are centered around Java Applets that run the molecular simulations and provide an “experimental” simulation platform for students to explore concepts. In addition, modules contain instructor materials, fundamental tutorials, student problems, and assessment materials.

A consistent Web-based interface has been designed that organizes all of the material in each module and develops scripts using perl; this eases the job of putting the written material into this common format. The developer of a module must construct simple text files, perhaps with HTML markup that permits inclusion of figures and tables. Then he or she runs the files through the perl script, which adds HTML formatting and links to put the set of files into the common configuration. The files are uploaded to the module site for anyone to access. This site is perhaps best accessed through the Etomica site. Etomica is a Java-based support environment developed for the modules project, which has now been expanded for other applications (<http://www.ccr.buffalo.edu/etomica>, contact is Professor David Kofke).

Following is a list of phenomena and concepts for which modules are completed or planned:

- Chemical reaction equilibrium
- Osmosis
- Diffusion
- Molecular dynamics
- Normal modes of a solid
- Chemical reaction kinetics
- Dissipative particle dynamics
- Surface tension
- Crystal viewer
- Joule-Thomson expansion
- Self-assembly
- Chemical potential
- Multicomponent phase equilibrium
- Heat transfer
- Atomic billiards
- Viscosity

**CONCLUSIONS AND RECOMMENDATIONS**

One way to foster renewal of the curriculum is to identify departments where curriculum revision is being carried out and to evaluate best computing practices and current trends. There may not be one answer because of different constraints under which various universities operate, such as number of faculty in the department and whether computing courses are taught outside the department. Contributions to this article came from nearly 20 universities, so we are aware of local issues.

CACHE makes the following recommendations to enhance computing through the curriculum:

1. There is increasing pressure on the total number of hours in the curriculum, especially with the addition of life science courses. Departments should continue to re-examine whether a formal three- or four-credit-hour computer programming course is required for the chemical engineering degree (vs. teaching how to use software or write m-files in MATLAB, for example). The chemical engineering computing course also provides students with a valuable experience in quantitative problem solving.

2. The number of software tools that implement numerical methods used by students should be minimized; departmental agreement on software used in each course should be reached within the faculty. Faculty need to reach consensus on how student computing skills can grow systematically through evaluating each course in the curriculum.

3. Courses such as transport phenomena and thermodynamics offer new possibilities for introduction of computing physical and chemical behavior, such as with computational fluid dynamics or molecular modeling. Process design can add a product design emphasis by using such tools as well.

4. Internet-based and virtual laboratories offer a new means of strengthening the student simulation experience in order to reinforce theoretical concepts.

5. To prepare students to optimize process designs, it helps to expose students to process simulators for solution of a problem(s) in the core courses of the chemical engineering curriculum. Also, as software develops and product design is added at the senior level, instructors must select from among optimization packages (such as GAMS), batch process simulators (such as BATCH PLUS and SUPERPRO DESIGNER), and packages for estimating equipment sizes and installation costs (such as Aspen IPE). The use of comprehensive software packages and databases is common in industrial design and needs to be introduced in design courses and used for solution of design projects.

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REFERENCES


APPENDIX

2003 Computing Survey of Recent Graduates

In 1997 the CACHE Corporation carried out a survey of recent graduates in chemical engineering from three universities to determine how much group used (or did not use) computing in performing their jobs. Since that time, there have been considerable changes in the field of information technology. Four universities volunteered to participate for the 2003 survey: Carnegie Mellon University, Clarkson University, McMaster University, and the University of Texas. A Web-based form was used to tabulate the responses using database software.

The four universities used different approaches for contacting their recent graduates, defined as students who graduated during the previous five years (1998-2003). Printed mail, e-mail, and/or Web forms were used depending on the specific school. The response rate for the four universities was estimated to be between 20% and 30%, which actually is quite good given the complexity and length of the survey (which took less than one hour to complete). The results of the survey are available in PowerPoint form on the CACHE Web site, <www.che.utexas.edu/cache/survey>.

The questionnaire asked for the nature of the work carried out and the degree level of the respondents. No attempt was made to remove current graduate students from the sample even though they are technically not in the workplace. The overwhelming majority of engineers value computing skills as critical to industrial problem solving. About 75% of recent graduates in the survey characterize their work as “technical.” Compared to 1997, there was a gradual increase in the use of the computer as a general productivity tool. The personal computer is ubiquitous in all business and engineering work, including standard office tasks, with 70% of respondents using a computer actively at least half the day. For the range of using the computer 3/4 to all day, the percentages doubled from 19% to 44% between 1997 and 2003.

Of the respondents, 99% report they use spreadsheets on a daily basis. Faculty have observed that spreadsheets are used by most if not all undergraduates, often with minimal formal instruction in the department. Industry clearly values the use of spreadsheets for a variety of applications based on the percentage of respondents who use them: data analysis (88%), numerical analysis (47%), material balances (25%), economic studies (23%), and other tasks such as financial modeling or emission calculations (17%).

Similar to spreadsheets, database software (70%) has the same level of penetration in daily work usage. It is noteworthy that even with continued improvement of packages such as MATLAB and MathCAD, they are used much more heavily in academia than in industry (26%). Numerical methods libraries are only infrequently used (6%), which illustrates their general decline in popularity since the 1970s.

Less than half of the survey respondents use a process simulator in their work, probably because a growing percentage of students are working in nontraditional industries (outside the CPI). Even in the CPI, not all chemical engineers are actively using simulators in the performance of their jobs.

In 2003 there was more emphasis on and time devoted to training new engineers to use computing in their jobs (compared to 1997). There is a continued reliance by recent graduates on learning new computing skills on their own or with the help of colleagues. This supports the notion that universities should prepare their graduates to “learn how to learn.” The amount of formal training to use computing tools continues to be fairly small.

A majority of the respondents (78%) replied that undergraduates should be exposed to some form of programming. This is not surprising even though a minority of engineers write programs in the workplace. Most people agree that use of programming logic is an important skill, whether it is C++, VBA, or MATLAB m-files. Of the respondents, 38% indicate they write computer programs at work (compared to 20% in 1997), but it is not clear what actually constitutes programming in the workplace today (is running simulations considered to be programming?). Use of VBA along with spreadsheets is a dominant practice. The growth of usage of VBA to 34% of the respondents is an important development. C++ leads the rest of the programming options (24%).
ChE class and home problems

The object of this column is to enhance our readers’ collections of stimulating problems in chemical engineering education. Ideal problems, which may be “open-ended,” are those that motivate the student either by the novel illustration of a particular principle, or by the elucidation of a difficult concept in a more traditional setting. Practical relevance is encouraged. The text portion of a manuscript (excluding figures) should not normally exceed 10 double-spaced pages (about 2,500 words). Please send manuscripts to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136. Preliminary ideas may be discussed with Prof. Wilkes before submitting a manuscript.

Design of a Fuel Processor System for GENERATING HYDROGEN FOR AUTOMOTIVE APPLICATIONS

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Fuel cell power systems for automotive applications have received increased attention in recent years because of their potential for high fuel efficiency and lower emissions. While there have been significant advances in fuel cell technology, this technology has not seen widespread application in the automotive industry due to the lack of an efficient hydrogen distribution system. One option is to develop a system that utilizes a commonly available carbon-based hydrocarbon fuel such as gasoline or methane to generate the necessary hydrogen in situ on an “as needed” basis.

In this paper, the objective is to design a fuel processor system that utilizes methane to generate sufficient hydrogen of desired purity, generating 50 kW of power, or enough to drive a small car.

PROBLEM STATEMENT

A schematic of the fuel cell system under consideration is shown in Figure 1 (next page). Methane enters the fuel processing system and is converted to hydrogen. Hydrogen enters the fuel cell where it reacts with oxygen to generate electrical power, driving an electric motor.

The fuel processing system has a train of three packed-bed reactors: (1) the reformer, (2) the water-gas shift reactor, and (3) the preferential oxidation reactor.

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Based on the Figure 1 schematic diagram, students are required to complete the following tasks:

1. Write the mole balance equations for the reformer, water-gas shift reactor, and preferential oxidation reactor.

2. Calculate the volume necessary for 75% conversion in the steam reformer. Assume isothermal operation at 1000 K, with the reactor operating at 5 atm pressure. The flow rate of methane into the reactor is 9 mol/min at room temperature, and the ratio of steam to methane is 3:1.

3. Calculate the maximum conversion in the water-gas shift reactor that can be obtained at 450 K and 600 K, respectively, and the minimum volume required.

4. Calculate the volume of the water-gas shift reactor to obtain 90% conversion if:
   (a) 20% of the total volume of the reactor is at 600 K and the rest of the reactor is at 450 K.
   (b) 60% of the total volume of the reactor is at 600 K and the rest of the reactor is at 450 K.

5. The input to the preferential oxidation reactor consists of exhaust from the water-gas shift reactor and air. The amount of air fed should be adjusted such that the amount of oxygen in the air is 2.1 times the amount of CO in the exhaust of the water-gas shift reactor. If the preferential oxidation reactor is operating at a temperature of 473 K and a pressure of 2 atm, calculate the volume required to bring the concentration of CO below 100 ppm. Assume 90% conversion in the steam reformer operating at 1000 K and 5 atm and a conversion of 90% in the water-gas shift reactor operating at 500 K and 2 atm.

6. Calculate the flow rate of hydrogen exiting the preferential oxidation reactor. How does this flow rate change when the flow rate of methane entering the reformer is changed?

7. Energy Balance:
   - Calculate the heat of reaction from the heat of formation for all the reactions, and list out the exothermic and endothermic reactions.
   - Calculate the enthalpies of all the feed and product streams and use this information to complete an overall energy balance for the reactor system.

**Data**

**Steam reformer**  In this reactor, methane is converted to hydrogen and carbon monoxide. Part of the carbon monoxide reacts with water to produce carbon dioxide and hydrogen, and some methane is totally oxidized to carbon dioxide.

\[
\begin{align*}
\text{CH}_4 + \text{H}_2\text{O} &\rightleftharpoons 3\text{H}_2 + \text{CO} \quad (1) \\
\text{CO} + \text{H}_2\text{O} &\rightleftharpoons \text{CO}_2 + \text{H}_2 \quad (2) \\
\text{CH}_4 + 2\text{H}_2\text{O} &\rightleftharpoons 4\text{H}_2 + \text{CO}_2 \quad (3)
\end{align*}
\]

Xu and Froment\(^\text{[4]}\) developed intrinsic rate expressions for steam reforming of methane, accompanied by the water gas shift reaction on a Ni/MgAl\(_2\)O\(_3\) catalyst. The following reaction rate laws were derived:

\[
\begin{align*}
\frac{r_1}{P_{\text{H}_2}^{0.5}} &= \frac{P_{\text{CH}_4}P_{\text{H}_2\text{O}}^2 - P_{\text{H}_2}^2P_{\text{CO}}}{K_1} \\
\frac{r_2}{P_{\text{H}_2}^2} &= \frac{P_{\text{CO}}P_{\text{H}_2\text{O}}^2 - P_{\text{H}_2}^2P_{\text{CO}_2}}{K_2} \\
\frac{r_3}{P_{\text{H}_2}^{3.5}} &= \frac{P_{\text{CH}_4}P_{\text{H}_2\text{O}}^2 - P_{\text{H}_2}^2P_{\text{CO}_2}}{K_3}
\end{align*}
\]

where \(r_1\), \(r_2\), and \(r_3\) are the rates of formation of CO, CO\(_2\), and CO\(_2\) in the reactions represented by Eqs. (1), (2), and (3) respectively. The \(P_i\) are the partial pressures of the reactants. The values of the constants are given in Table 1.

The adsorption coefficients can be found using the following relations for the respective species

\[
K_i = A(K_i)e^{\frac{-\Delta H_i}{RT}}, \quad \text{where } i = \text{H}_2, \text{CO, CH}_4, \text{H}_2\text{O}
\]

The rate constants are given by a similar Arrhenius-type equation.

\[
A_j = A(k_j)e^{\frac{-E_j}{RT}}, \quad \text{where } j = 1, 2, 3
\]

The equilibrium constants for the three reactions are given by the following expression,

\[
K_j = e^{\frac{A_j + B_j}{T}}, \quad \text{where } j = 1, 2, 3
\]
Water-gas shift reactor • In this reactor, most of the remaining carbon monoxide is converted to hydrogen. The following exothermic reaction occurs:

\[ \text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2 \]  \hspace{2cm} (10)

Choi and Stenger\(^5\) proposed a kinetic model for the water-gas shift reaction on a Cu/ZnO/Al\(_2\)O\(_3\) catalyst operating between 400 K to 700 K. The following rate law was developed.

\[ r_4 = k_4 \frac{P_{\text{CO}} P_{\text{H}_2\text{O}}}{P_{\text{CO}_2} P_{\text{H}_2}} \left(1 - \frac{P_{\text{CO}_2} P_{\text{H}_2}}{P_{\text{CO}} P_{\text{H}_2\text{O}}} K_{\text{eq}} \right) \]  \hspace{2cm} (11)

where \(r_4\) is the rate of formation of \(\text{CO}_2\) in the reaction represented by Eq. (10). The equilibrium constant \(K_{\text{eq}}\) varies with temperature as follows:

\[ K_{\text{eq}} = \exp \frac{-4577.8}{T} \]  \hspace{2cm} (12)

The rate constant \(k_4\) follows an Arrhenius type equation as given below:

\[ k_4 = A' (k_4) \exp \left(-\frac{E_{k_4}}{RT} \right) \]  \hspace{2cm} (13)

Other constant values used are given in Table 1.

Preferential oxidation reactor • The stream exiting the water-gas shift reactor may still have significant amounts of carbon monoxide that can poison the Polymer Electrolyte Membrane (PEM) fuel cell electrocatalyst. For this reason, it is necessary to have a preferential oxidation reactor where the carbon monoxide from the water-gas shift reactor is reacted with air to form carbon dioxide. Some of the hydrogen reacts with the oxygen to produce water.

\[ \text{CO} + \frac{1}{2} \text{O}_2 \rightleftharpoons \text{CO}_2 \]  \hspace{2cm} (14)

\[ \text{H}_2 + \frac{1}{2} \text{O}_2 \rightleftharpoons \text{H}_2\text{O} \]  \hspace{2cm} (15)

The following kinetic model was taken from Kahlich, \textit{et al.}\(^6\)

\[ r_5 = k_5 P_{\text{CO}}^{0.42} \left( \frac{2P_{\text{O}_2}}{P_{\text{CO}}} \right) \]  \hspace{2cm} (16)

\[ r_6 = 1.5 k_6 P_{\text{O}_2}^{0.42} \left( \frac{2P_{\text{O}_2}}{P_{\text{CO}}} \right) \]  \hspace{2cm} (17)

where \(r_5\) represents the rate of formation of \(\text{CO}_2\) in the reaction represented by Eq. (16), and \(r_6\) represents the rate of formation of \(\text{H}_2\text{O}\) in the reaction represented by Eq. (17). The rate constant \(k_5\) follows an Arrhenius-type equation:

\[ k_5 = A' (k_5) \exp \left(-\frac{E_{k_5}}{RT} \right) \]  \hspace{2cm} (18)

SOLUTION

Each reactor is modeled as an isothermal plug-flow reactor. It is assumed that no axial mixing or axial heat transfer occurs. This implies that the reactors are operating at high

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A_1)</td>
<td>29.3014</td>
</tr>
<tr>
<td>(A_2)</td>
<td>25.225</td>
</tr>
<tr>
<td>(A' (k_1))</td>
<td>9.886x10^16 [mol atm^0.5/m^3 min]</td>
</tr>
<tr>
<td>(A' (k_2))</td>
<td>4.665x10^7 [mol atm^-1/m^3 min]</td>
</tr>
<tr>
<td>(A' (k_3))</td>
<td>2.386x10^6 [mol atm^0.5/lt min]</td>
</tr>
<tr>
<td>(A (K_{\text{H}_2}))</td>
<td>6.209x10^-8 [atm^-1]</td>
</tr>
<tr>
<td>(A (K_{\text{CO}}))</td>
<td>8.339x10^-6 [atm^-1]</td>
</tr>
<tr>
<td>(A (K_{\text{H}_2O}))</td>
<td>1.77x10^9</td>
</tr>
<tr>
<td>(B_1)</td>
<td>-26248.4 [K^-1]</td>
</tr>
<tr>
<td>(B_2)</td>
<td>4593.17 [K^-1]</td>
</tr>
<tr>
<td>(B_3)</td>
<td>-21825.28 [K^-1]</td>
</tr>
<tr>
<td>(E_{\text{f1}})</td>
<td>240.1 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(E_{\text{f2}})</td>
<td>67.13 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(E_{\text{f3}})</td>
<td>243.9 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(\Delta H_{\text{f1}}^O)</td>
<td>-82.90 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(\Delta H_{\text{f2}}^O)</td>
<td>-70.65 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(\Delta H_{\text{f3}}^O)</td>
<td>-488.68 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(\Delta H_{\text{f1}}^O)</td>
<td>-38.28 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(A' (k_4))</td>
<td>6.195x10^8 [mol atm^-0.5/lt min]</td>
</tr>
<tr>
<td>(A' (k_5))</td>
<td>2.333x10^6 [mol atm^-0.5/hr min]</td>
</tr>
<tr>
<td>(E_{\text{f4}})</td>
<td>47.53 [kJ/(mol K)]</td>
</tr>
<tr>
<td>(E_{\text{f5}})</td>
<td>71 [kJ/(mol K)]</td>
</tr>
</tbody>
</table>

Peclét numbers for both heat and mass transfer. A more detailed analysis incorporating these diffusive effects has been conducted by Bell and Edgar\(^7\). The automotive application puts a constraint on the total volume of the reactor train, since the entire system has to fit under the hood. The design equations are solved numerically in MATLAB. The process is also simulated in the process simulator CHEMCAD. The results are given below.

Mole Balance Equations

The general mole balance equation for a PFR is given by:

\[ \frac{dF_j}{dV} = r_j \]  \hspace{2cm} (19)

where \(j\) represents the species present in the reactor. It is necessary to determine the reaction rate for each species in the three reactors.
In the reformer, the reactions taking place are represented by Eq. (1)-(3). The reaction rates in terms of the species involved can be expressed in terms of the reaction rates represented by Eq. (4)-(6) as shown below.

\[ r_{\text{CH}_4} = -r_1 - r_3 \]  
\[ r_{\text{CO}} = r_1 - r_2 \]  
\[ r_{\text{CO}_2} = r_2 + r_3 \]  
\[ r_{\text{H}_2} = 3r_1 + r_2 + 4r_3 \]  

There is only one reaction occurring in the water-gas shift reaction as shown by Eq. (10). We can express the reaction rate of each Eq. (10) species in terms of the reaction rate of Eq. (11) as follows:

\[ r_{\text{CO}} = -r_4 \]  
\[ r_{\text{H}_2}\text{O} = -r_4 \]  
\[ r_{\text{CO}_2} = r_4 \]  
\[ r_{\text{H}_2} = r_4 \]  

In the preferential oxidation reactor, the reactions taking place are represented by Eq. (14)-(15). The reaction rates, in terms of the species, involved can be expressed in terms of the reaction rates represented by Eq. (16)-(17).

\[ r_{\text{O}_2} = -0.5r_5 - 0.5r_6 \]  
\[ r_{\text{CO}} = -r_5 \]  
\[ r_{\text{CO}_2} = r_5 \]  
\[ r_{\text{H}_2}\text{O} = r_6 \]  
\[ r_{\text{H}_2} = -r_6 \]  

**Volume of Steam Reformer**

Rate expressions for the different reactions are given in terms of partial pressures of reacting species. The given molar feed rate of the gases, \( F_r \), should be converted to partial pressures. Using the molar feed rates, we can calculate the mole fraction of the feed used to calculate the partial pressures as follows:

\[ X_j = \frac{F_j}{F_r} \]  
\[ P_j = X_jP_r \]

The partial pressure obtained is substituted into the rate expression to calculate the change in flow rate along the volume of the reactor.
The mole balance equations for the species in the steam reformer are given in the mole balance equation section. A volume for the reformer was estimated, and the mole balance equations were integrated numerically in MATLAB for this guessed volume using the initial conditions given in the problem statement. The methane concentration exiting the reformer was computed, and the methane conversion was calculated. The reactor volume was iteratively adjusted using a secant method until the computed conversion was 75% as specified in the problem statement. Students found a reformer volume of 6.38 liters resulted in the specified conversion. The concentration profiles, as a function of reactor volume, are shown in Figure 2(a).

This reactor configuration was also simulated in CHEM CAD. Shown in Figure 2(b), the reformer with a volume of 6.38 liters resulted in a conversion of 75%.

Volume of Isothermal Water-Gas Shift Reactor

The mole balance equations for the species in the water-gas shift reactor are given on pp. 241-242.

This reactor was simulated in CHEM CAD and MATLAB, producing identical results. The specific reaction rate constants were computed for the temperatures given in the problem statement first. Using the exit conditions of the reformer as the initial conditions of the water-gas shift reactor, the mole balance equations were integrated numerically for a variety of reactor volumes till the maximum conversion was attained. The conversion of carbon monoxide as a function of reactor volume at two different isothermal conditions (450 K and 600 K) is shown in Figure 3. If the reactor is operated isothermally at 450 K, the maximum conversion possible is 98.8%. The minimum volume required to obtain this conversion is about 250 liters. The maximum possible conversion at a temperature of 600 K is only 86.6%, and the minimum volume required is 9.4 liters.

Volume of Two-Temperature-Zone Water-Gas Shift Reactor

At low temperatures, the reaction is kinetically limited. At high temperatures, the reaction conversion is limited, i.e., the extent of reaction is limited by the thermodynamics. To minimize the volume, the reactor is operated at a high temperature (600 K), and to increase the conversion it is operated at a lower temperature (450 K). The reactor volume for 90% conversion under two different reactor temperature regimes is calculated in CHEM CAD, and verified with MATLAB. The results are shown in Table 2. It is observed that the reactor volume can be substantially reduced as compared to the isothermal operation if 20% of the reactor is operated at 600 K.

Volume of Preferential Oxidation Reactor

The last reactor in the series is the preferential oxidation reactor. Here, the concentration of CO is brought to less than 100 ppm. Along with the combustion of CO, some hydrogen is also burned. For the gases that have a 75% conversion in the reformer and a 90% conversion in the water-gas shift reactor, the amount of conversion in the preferential oxidation reactor (PROX) is approximately 98.7%. The volume obtained for this conversion is 0.335 liters.

Hydrogen Flow Rate

From calculations performed in the section on “Volume of Preferential Oxidation Reactor,” the flow rate of hydrogen exiting the preferential oxidation reactor is 28.08 moles/min. Using the reactor volumes given above, the reactor train was simulated for varying methane flow rates. A plot of hydrogen flow rate out of the fuel processor vs. methane flow rate into the reformer is shown in Figure 4. Note that the relation between the two flows is linear, and 3.12 moles of hydrogen are formed for every mole of methane entering the reformer.

Energy Balance

The standard heat of reaction can be obtained from the standard heat of formation of individual species involved in the reaction using Hess’s Law. The standard heat of formation can be obtained from the NIST Chemistry Web book.[8] For oxygen and hydrogen, the standard heat of formation (at 298
TABLE 3
Standard Heats of Formation

<table>
<thead>
<tr>
<th>Species</th>
<th>Standard Heat of Formation (kJ/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>-110.53</td>
</tr>
<tr>
<td>CO₂</td>
<td>-393.51</td>
</tr>
<tr>
<td>H₂O</td>
<td>-242</td>
</tr>
<tr>
<td>CH₄</td>
<td>-74.5</td>
</tr>
</tbody>
</table>

TABLE 4
Standard Heats of Reaction and Type of Reaction

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Standard Heat of Reaction (kJ/mol)</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄ + H₂O ⇌ 3H₂ + CO</td>
<td>205</td>
<td>endothermic</td>
</tr>
<tr>
<td>CO + H₂O ⇌ CO₂ + H₂</td>
<td>-41</td>
<td>exothermic</td>
</tr>
<tr>
<td>CH₄ + 2H₂O ⇌ 4H₂ + CO₂</td>
<td>164</td>
<td>endothermic</td>
</tr>
<tr>
<td>CO + (1/2)O₂ ⇌ CO₂</td>
<td>-283</td>
<td>exothermic</td>
</tr>
<tr>
<td>H₂ + (1/2)O₂ ⇌ H₂O</td>
<td>-242</td>
<td>exothermic</td>
</tr>
</tbody>
</table>

K) is zero. The heat of formation for other species is given in Table 3. Using heat of formation data, the standard heats of reaction were found. These results are given in Table 4.

There are two feed streams going into the reactor train and one product stream coming out. The enthalpies of these streams can be computed easily in CHEMCAD. The enthalpy of the stream containing steam and methane is -8.261 MJ/min, the air stream is -0.003 MJ/min, and the product stream is -6.042 MJ/min. Air is assumed to be 79% nitrogen and 21% oxygen. Enthalpies are calculated based on the same reference states as those used for the heat of reaction. The net heat to be supplied to the fuel processor is 2.22 MJ/min.

**DISCUSSION**

The purpose of this work was to demonstrate that standard reaction engineering principles could be utilized to design a fuel processor that uses methane to generate hydrogen and oxygen from the required purity for a PEM fuel cell used for automotive applications. The total volume required for the fuel processor to generate hydrogen of the required purity is small enough to fit under the hood of small cars. Furthermore, the energy balanced reactions involved indicate that there is a net depletion of energy, and so it is necessary to provide a small amount of heat to the reactors. This project gives the instructor the opportunity to discuss several reactor design issues such as:

- The importance of changing the temperature in the water-gas shift reactor to minimize the volume. This is a common approach when one looks at equilibrium limitations in exothermic reactions.
- The necessity of having the preferential oxidation reactor. While the reactor volume is small (the size of a soft drink can), it is necessary to have this reactor so that the concentration of carbon monoxide is reduced to a level acceptable for the PEM fuel cell.
- The importance of doing an overall energy balance on the process. This exercise demonstrates it is necessary to burn some of the methane feed or the hydrogen generated for the reactions to proceed at the specified conditions.
- For every mole of methane utilized, more than 3 moles of hydrogen are produced. This demonstrates that hydrogen is produced not only from methane, but also from water.
- The equivalence of results in MATLAB and CHEMCAD for reactor design calculations.

This problem was given as a reactor design problem in our department in summer 2005. All design teams were ultimately successful in producing an acceptable design report for this problem. A discussion with the students at the end of the semester indicated a great deal of enthusiasm in tackling this problem. Students appreciated that a practical design problem had been assigned instead of a problem from a textbook.

All the reactor design calculations were done assuming steady state. In an automotive application, however, the demand for hydrogen will fluctuate, so it is necessary to compute the dynamic response of the reactor train to sudden changes in methane flow rate and utilize this information to design a suitable control system. This requires the solution of a set of partial differential equations, and is beyond the scope of an undergraduate class in reaction kinetics.

**REFERENCES**