**EDITORIAL AND BUSINESS ADDRESS:**
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# Chemical Engineering Education

**Volume 37 Number 3 Summer 2003**



*CHEMICAL ENGINEERING EDUCATION (ISSN 0009-2479) is published quarterly by the Chemical Engineering Division, American Society for Engineering Education, and is edited at the University of Florida. Correspondence regarding editorial matter, circulation, and changes of address should be sent to CEE, Chemical Engineering Department, University of Florida, Gainesville, FL 32611-6005.*  *Defective copies replaced if notified within 120 days of publication. Write for information on subscription costs and for back copy costs and availability. POSTMASTER: Send address changes to Chemical Engineering Education, Chemical Engineering Department., University of Florida, Gainesville, FL 32611-6005. Periodicals Postage Paid at Gainesville, Florida and additional post offices.*

# University of California Berkeley

*The Campanile overlooking San Francisco Bay.*

Arup K. Chakraborty, P.B. Plouffe, Stacey Shulman
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The academic year 2003-2004 marks the 56th anniversary of the Department of Chemical Engineering at the University of California, Berkeley. Developed as an academic discipline in the United States near the turn of the century, chemical engineering moved toward engineering science in the late 1940s and 1950s. During those years, Berkeley's young department rose to prominence. It took the lead in developing new areas of research such as electrochemical engineering, molecular thermodynamics, semiconductor processing, and biochemical engineering. The department has consistently ranked among the top three research and teaching programs in the country. It continues to be at the forefront in developing programs in emerging areas of chemical, materials, and biological technology.

The success of the department has been facilitated by being part of a world-famous university with leading departments in all fields of engineering, the natural sciences, social sciences, and the humanities. Strong synergies with research programs at the Lawrence Berkeley National Laboratory have also added to the richness of the intellectual culture of the department.

The Chemical Engineering Department at Berkeley is part of the College of Chemistry, which also houses the nation's top-ranked chemistry department. Nineteen members of the faculty work together congenially with 115 graduate students, 333 undergraduates, and 31 postdoctoral fellows in the pursuit of excellence in teaching and scholarship.

The current faculty has received many awards and honors recognizing their accomplishments in teaching and research. These awards include four members of the National Academy of Engineering, one member of the National Academy of Science, two Allan P. Colburn Awards (AIChE), two Professional Progress Awards (AIChE), three Food, Pharmaceutical and Bioengineering Awards (AIChE), the Award in Heterogeneous and Homogeneous Catalysis (ACS), the Marvin Johnson Award in Biochemical Technology (ACS), The Colloid and Surfaces Chemistry Award (ACS), the EV Murphree Award (ACS), two Emmett Awards in Heterogeneous Catalysis (North American Catalysis Society), two Amgen Awards in Biochemical Engineering (Engineering Foundation), one Dillon Medal (APS), one AVS Award in Plasma Physics, three Camille Dreyfus Teacher Scholar Awards, and numerous Presidential Young Investigator, National Young Investigator, and CAREER Awards (NSF).

Research groups in the department are housed primarily in

Gilman Hall, a National Historic Chemical Landmark where plutonium was discovered, and Tan Kah Kee Hall (dedicated in 1997). These buildings provide state-of-the-art facilities and infrastructure for research.

## HISTORY OF THE DEPARTMENT

The appointment of the first Professor of Chemical Engineering in July of 1946 marked the administrative decision that ultimately led to the present chemical engineering program at Berkeley. As the university began to more fully recognize the importance of chemical engineering—especially through its contributions to the war effort in the development of the atomic bomb and in the petroleum and chemical industries—the need for a full-fledged program became appar-

### TABLE 1
**Chronology of Events in Chemical Engineering at Berkeley**

1912 ► **G.N. Lewis** institutes a chemical technology major.

1942 ► An interdepartmental graduate group offers the MS degree in chemical engineering.

1945 ► Provost **Monroe Deutsch** authorizes establishment of a Chemical Engineering program in the College of Chemistry.

1946 ► Initial faculty members are appointed to teach chemical engineering: **Philip Schutz** (deceased, 1947); **LeRoy Bromley** (retired, 1972); **Charles Wilke** (chair 1953-63; retired, 1987).
► Undergraduate instruction begins.

1947 ► **Theodore Vermeulen** (chair 1947-53; deceased, 1984), **Donald Hanson** (chair 1963-66; retired 1989), **Charles Tobias** (chair 1966-71; retired, 1991; deceased, 1996), join the faculty.
► PhD program is approved.

1948 ► BS degree program in Chemical Engineering is approved.
► **F. Campbell Williams** joins the faculty (left for Petrobas and University of Brazil, 1952).

1949 ► The Chemistry Department is renamed the Department of Chemistry and Chemical Engineering.
► BS program is accredited by the AIChE.

1952 ► A Division of Chemical Engineering is created within the Department of Chemistry and Chemical Engineering.
► **Kenneth Gordon** joins the faculty (left for University of Michigan, 1954).

1953 ► **Eugene Petersen** (retired, 1991) joins the faculty.

1954 ► **Andreas Acrivos** joins the faculty (left for Stanford, 1963).

1955 ► **John Prausnitz** joins the faculty.

1956 ► **Donald Olander** joins the faculty (left for UCB Nuclear Engineering Department, 1961).

1957 ► Chemical Engineering is established as a separate department.

1958 ► **David Lyon** (retired, 1982) joins the faculty.

1961 ► **Alan Foss** (retired, 1994) and **Michel Boudart** (left for Stanford, 1965; appointed Adjunct Professor, 1994-97) join the faculty. **Simon Goren** (chair, 1994-97; retired, 2001) and **Richard Wallace** (resigned, 1965) join the faculty.

1963 ► **Edward Grens** (retired, 1987), **C. Judson King** (chair, 1972-81), **John Newman, Richard Ayen** (left for Stauffer Chemical Co., 1968), join the faculty.

1964 ► **Robert Merrill** joins the faculty (left for Cornell, 1977).

1965 ► **Michael Williams** (retired, 1989) joins the faculty.

1966 ► **Robert Pigford** joins the faculty (returned to University of Delaware, 1975).
► Room 307 Gilman Hall is designated a registered National Historic Landmark by the U.S. Department of the Interior as the location for the discovery of plutonium.

1967 ► **Scott Lynn** (retired, 1994) and **Alexis Bell** (chair, 1981-91) join the faculty.

1969 ► **Mitchell Shen** joins the faculty (deceased, 1979).

1970 ► **Lee Donaghey** (left for Chevron, 1977) and **Thomas Sherwood** (deceased, 1976) join the faculty.

1975 ► **Clayton Radke** joins the faculty.

1977 ► **Dennis Hess** (left for Lehigh University, 1991) joins the faculty.

1978 ► **Elton Cairns** and **Harvey Blanch** (Chair, 1997-2001) join the faculty.

1979 ► **David Soane** (Soong)( left for Soane Technologies 1994; appointed Adjunct Professor, 1994) and **Edward Reiff** (left for DuPont, 1982) join the faculty.

1981 ► **Morton Denn** (Chair, 1991-94; left for CCNY, 1999) joins the faculty.

1982 ► **Jeffrey Reimer and James Michaels** (left for Mobil, 1989) join the faculty.

1986 ► **Douglas Clark, David Graves,** and **Doros Theodorou** (left for University of Patras, 1994) join the faculty.

1988 ► **Arup Chakraborty** (Chair, 2001-) joins the faculty.

1991 ► **Susan Muller** joins the faculty.
► Room 307 Gilman Hall is designated a Nuclear Historic Landmark by the American Nuclear Society as the site of the first chemical identification of plutonium on February 23-24, 1941).

1992 ► **Jay Keasling** joins the faculty.

1993 ► **Enrique Iglesia and Roya Maboudian** join the faculty.
► Construction of Tan Hall begins.

1997 ► Gilman Hall designated as an ACS National Historic Chemical Landmark.
► Dedication of Tan Kah Kee Hall (April 12, 1997).

1999 ► **David Schaffer** joins the faculty.

2000 ► **Alexander Katz** joins the faculty.

2004 ► **Rachel Segalman** will join the faculty.

***. . . the [Berkeley] chemical engineering faculty has contributed to the emergence of a number of different areas that are now considered quintessential chemical engineering.***

***Professor John Prausnitz and students in the unit operations laboratory.***

ent. Initially, considerable controversy developed as to whether the program should be in the College of Engineering or the College of Chemistry. For a while, this led to the amusing situation where Berkeley had two chemical engineering departments—one housed in the College of Engineering and the other in the College of Chemistry. The stronger program in the College of Chemistry ultimately prevailed.

Philip Schutz, a professor of chemical engineering at Columbia University, was selected to head the fledging chemical engineering program. To assist him, Dean Wendell Latimer appointed Charles Wilke (PhD, University of Wisconsin) and LeRoy Bromley (MS, Illinois Institute of Technology). Sadly, shortly after the first class enrolled in September 1946, Philip Schutz passed away. Theodore Vermeulen (PhD, UCLA) joined the program in February 1947 and became its head. Don Hanson (PhD, University of Wisconsin) and Charles Tobias (a Hungarian émigré, PhD, Budapest) joined the faculty in the fall of 1947, and they were followed by F. Campbell Williams in 1948.

This initial faculty group remained in place without further additions until 1952 when Ken Jordan from MIT joined the faculty. During this period, a PhD program was formally approved (1948) and the BS program was fully accredited (1949). Charles Wilke succeeded Theodore Vermeulen as Chairman in 1953, and between 1953 and 1955, he recruited three more remarkable intellects: Eugene Petersen from Penn State (1953), Andreas Acrivos from Minnesota (1954), and John Prausnitz from Princeton (1955).

With these pioneers establishing standards of excellence that have consistently marked the department, new areas of research were established in the period between 1953 and 1985. The sub-field of electrochemical engineering (under the leadership of Charles Tobias) is a notable example. During those same years, John Prausnitz developed a systematic approach for obtaining activity coefficients and equations of state for substances central to the petrochemical industry. The major award in this field, now called molecular thermodynamics, is named after Dr. Prausnitz, who continues to be active in teaching, research, and administration.

In the 1970s, Dennis Hess headed up the first program in micro-

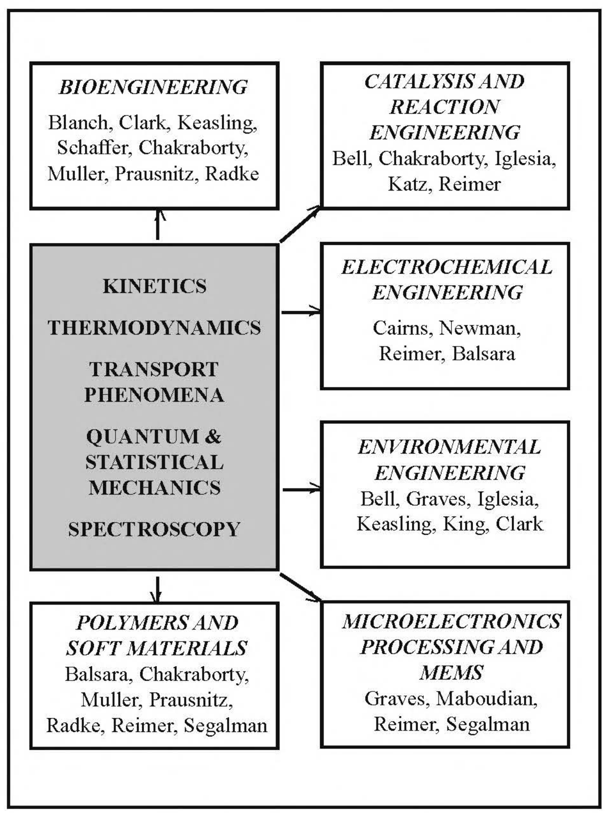



**Figure 1.** Research areas.

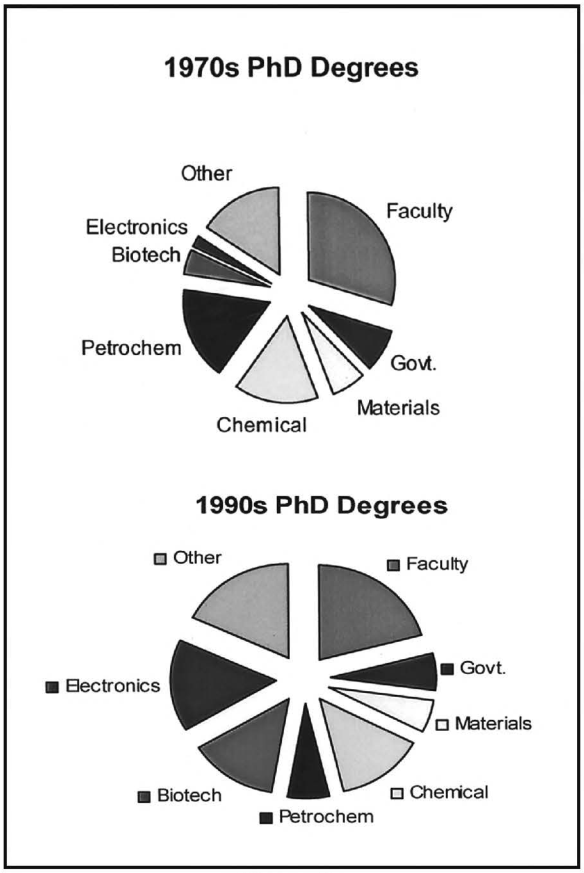
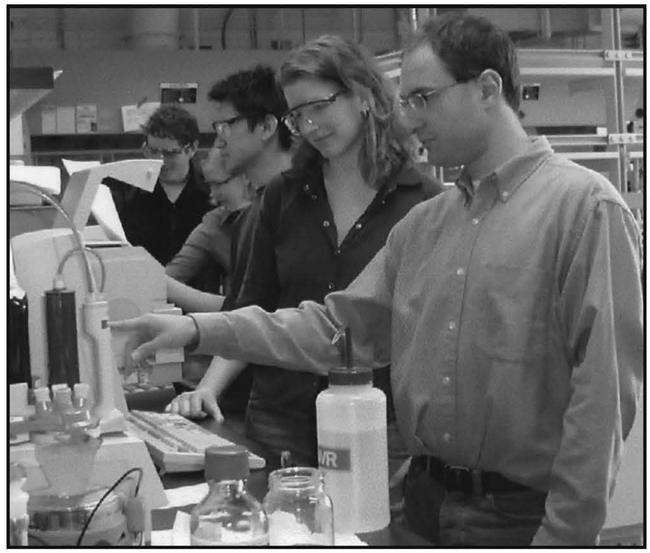



*Figure 2.*

**TABLE 2**
**Textbooks Published by Berkeley Faculty**

| | |
|---|---|
| Blanch & Clark | • *Biochemical Engineering* |
| Denn | • *Process Fluid Mechanics*<br>• *Process Modeling*<br>• *Introduction to Chemical Engineering Analysis* (with T.W.F. Russell)<br>• *Stability of Reaction and Transport Processes*<br>• *Optimization by Variational Methods* |
| King | • *Separation Processes*<br>• *Freeze Drying of Foods* |
| Hanson | • *Computation of Multistage Separation Processes* |
| Newman | • *Electrochemical Systems* |
| Petersen | • *Chemical Reaction Analysis* |
| Prausnitz | • *Molecular Thermodynamics of Fluid Phase Equilibria* (with Lichtenthaler and de Azevedo)<br>• *Properties of Gases and Liquids* (with B. Poling and R. Reid)<br>• *Regular and Related Solutions* (with J.H. Hildebrand and R.L. Scott) |
| Reimer | • *Chemical Engineering Design & Analysis* (with T.M. Duncan) |
| Sherwood, Pigford & Wilke | • *Mass Transfer* |



***Professor Alex Katz and students.***

electronics processing within a chemical engineering department. In that same decade, Charles Wilke and Harvey Blanch initiated a pioneering program in biochemical engineering. Under the leadership of Gene Petersen, Michel Boudart, and Alex Bell, an innovative program in catalysis and reaction engineering was established. When Mort Denn joined the faculty in 1981, he set up a world-class program in polymer processing on the Berkeley campus and at the Lawrence Berkeley National Laboratory. (The research programs that have evolved since 1985 are described in the "Graduate Program" section of this article.)

## THE UNDERGRADUATE PROGRAM

The BS degree in chemical engineering at UC Berkeley, accredited by ABET, is acknowledged as one of the most demanding majors on campus. The curriculum provides a strong background in mathematics and the basic sciences of physics, chemistry, and biology. The core principles of thermodynamics, reaction engineering, and transport phenomena are often illustrated by examples drawn from the petroleum, petrochemical, pharmaceutical, biomedical, and microelectronics industries. The program includes extensive laboratory experience, with mandatory laboratory courses in unit operations, transport phenomena, and control systems. In addition, elective courses in biochemical engineering, polymers, and microelectronics processing include large laboratory components. Under the supervision of a faculty member, the students work in teams to design a process in the capstone course.

In the final two years, students choose an option that allows them to more deeply study a sub-field of chemical engineering. In particular, option programs are available in biochemical engineering, materials science and engineering, chemical processing, and microelectronics. The options program, in place for 16 years now, constantly evolves to meet student and industry needs.

A special feature of the undergraduate program at Berkeley is the high premium placed on teaching students how to communicate technical information effectively, both orally and in writing. Each laboratory course and the design course include oral presentations and written reports. In addition, a required course in technical communication and ethics is taught by a lecturer in the department. Alumni and employers report back to us the great advantage and value of these experiences.

The undergraduate program in chemical engineering is constantly reviewed by the faculty. This has allowed it to continuously evolve, and perhaps it is the reason why we do not perceive an urgent need to make revolutionary changes to the curriculum. Constant fine tuning has allowed us to make necessary modifications to meet the needs of students who find employment in a wide range of corporate sectors.

The department values excellence in teaching and over the years several landmark textbooks have been written by the faculty (see Table 2). They include *Molecular Thermodynamics* and *Properties of Liquids and Gases* by Prausnitz, *Separation Processes* by King, *Process Fluid Mechanics* by Denn, *Biochemical Engineering* by Blanch and Clark, and *Introduction to Chemical Engineering* by Reimer. The faculty's excellence in teaching has been recognized by numerous campus awards, including four Distinguished Teaching Awards. Faculty from all departments on the Berkeley campus are eligible for this award, and only three distinguished teachers are chosen each year.

Our commitment to teaching has continued to inspire the next generation of teachers. Fifteen percent of the current fac-

### *The Emergence of High-Technology Industries*

Berkeley has developed research areas on the frontiers of chemical engineering. A Berkeley PhD, Andy Grove (1963), together with Gordon Moore (BS Chemistry, 1950) and Robert Noyce, founded the Intel Corporation. The growing importance of the semiconductor manufacturing industry led to Dennis Hess joining the department in 1977, and he initiated collaborations that were critical in the expanding role that chemical engineers have continued to play in many areas of electronic materials processing.

The proximity of Silicon Valley was a distinct advantage for the development of the program at Berkeley, and opportunities for undergraduate and graduate student employment increased. Today, nearly one-third of the students at all degree levels find employment in electronics materials processing. This area has been strengthened at Berkeley by the addition of David Graves (in 1986), with his interests in plasma processing and Roya Maboudian (in 1993), who studies surface processes occurring during electronic-materials processing (especially MEMS technologies). Jeff Reimer's research has complemented the research program in electronic materials. At the undergraduate level, Lee Donaghey first developed an elective course in electronic materials processing in 1970. Subsequently, Hess and then Graves expanded the course, which has become a key component of the options program in chemical engineering.

The second area to benefit from Berkeley's location was biochemical engineering. Charlie Wilke turned his research effort from diffusion and mass transfer to this new field in the 1960s. His early studies on the kinetics of microbial growth and gas-liquid mass transfer provided the engineering underpinnings for the revolution in molecular biology that was to come. The advent of recombinant DNA and cell fusion (hybridoma) technology in the mid-1970s led to tremendous opportunities for the production of new, high-value therapeutic proteins and specialty chemicals. The Bay Area soon became home to start-up companies such as Cetus, Chiron, and Genentech. The department's research in this area expanded with the addition of Harvey Blanch in 1978, Douglas Clark in 1986, Jay Keasling in 1992, and David Schaffer in 1999.

The biochemical engineering program is now one of the largest in the United States. Jay Keasling introduced environmental biotechnology to the undergraduate curriculum, highlighting the increasing role of biological routes to environmental remediation.

Environmental engineering has also become a leading career option for BS graduates. Jay Keasling has developed a major program in synthetic biology. David Schaffer has brought cutting-edge biomedical research to the department, developing vectors for gene delivery. Arup Chakraborty's work on how cells in the immune system communicate and Clay Radke's interest in contact lenses are two other examples of biomedical research in Berkeley's Chemical Engineering Department.

In recent years, many new technologies have emerged that require advance materials with specific functionality. Precise control of these properties requires a detailed knowledge of the molecular constitution and mesoscopic structure of the material. Berkeley's Chemical Engineering Department has been able to capitalize on the strengths of the Chemistry Department and develop collaborations that elucidate the relationship between materials structure and their function. Synthesis, quantum and statistical mechanical theory, and characterization are being employed by several groups to develop novel catalytic and polymeric materials (*e.g.,* Balsara, Bell, Chakraborty, Katz, Iglesia, Muller, Reimer, Segalman).

ulty at MIT and 18% of the faculty at Cal Tech received their PhDs from Berkeley's Department of Chemical Engineering.

## THE GRADUATE PROGRAM

Both the MS and PhD degrees in chemical engineering are granted, but a preponderance of graduate students pursue the PhD. The central focus of graduate education is research conducted under the supervision of a faculty advisor. The faculty-advisee relationship is truly collaborative and is one of the most enriching aspects of graduate (and, indeed, faculty) life at Berkeley. As noted earlier, the chemical engineering faculty has contributed to the emergence of a number of different areas that are now considered quintessential chemical engineering. Research areas represented in the department today can be broadly classified as shown in Figure 1.

**Professor David Schaffer and graduate student Karen Lai working on an I-cycler, a quantative PCR machine.**

A special feature of a chemical engineering education at Berkeley is that a deep knowledge of phenomenological concepts pertinent to transport phenomena, reaction kinetics, and thermodynamics is buttressed by a strong foundation in the underlying molecular phenomena. Thus, experimental methods such as scattering and spectroscopy, and the conceptual frameworks of statistical and quantum mechanics, are as much a part of the basic tools in the arsenal of a PhD chemical engineer as are continuum models, macroscopic reaction studies, and measurements of macroscopic mechanical properties of materials. As shown in Figure 2, graduate research at Berkeley can be viewed as bringing to bear the chemical engineer's rare ability to think across molecular, mesoscopic, and macroscopic scales to develop knowledge that can aid the development of new technologies and discover new phenomena in the related sciences.

Research in areas pertinent to biotechnology and microelectronics processing are facilitated by our geographical location. The San Francisco Bay area is a hotbed for biomedical research and companies focused on developing new biochemical and microelectronic products, and there are many collaborations between research groups in the department and these companies.

Another facilitator of research in biological engineering has been the establishment of an institute called QB3, a multidisciplinary institute that involves the Berkeley campus and the U.C. San Francisco Medical School. QB3 aims to bring leading scientists and engineers on the Berkeley campus together with medical researchers at UCSF Medical School to help solve important problems in biomedicine. Three faculty in the Chemical Engineering Department have appointments in QB3.

Several faculty in the department are working to develop materials that can function with precision. Such materials, particularly those that can carry out functions in response to changes in external stimuli, are important components of many emerging technologies. The way to make such materials is to learn how to manipulate molecular components such that the desired function is obtained. Strong and collaborative research programs exist in the department wherein synthesis, characterization, and theory are brought together to design new catalytic and polymeric materials as well as those pertinent to microelectronics and MEMS technologies. In this regard, graduate students in the department benefit from strong synergies with the Department of Chemistry as well as the Molecular Foundry at LBNL. The Molecular Foundry is a new national facility with the aim of developing "designer" materials by manipulating molecular-scale phenomena. Two centers of excellence—the Center for Catalysis and the Center for Biochemical Engineering—further foster collaborative research.

Chemical engineering draws from various areas and is perhaps the broadest of all engineering disciplines. Preparing students to meet today's challenges for energy-efficient processes, pollution abatement, and rapid translation of chemical and biological discoveries into products and processes requires faculty dedication to research and teaching. This kind of dedication assures that Berkeley graduates will continue to contribute to the solution of important societal problems.

Future chemical engineering students will need skills not even contemplated when the department was founded. The Berkeley Chemical Engineering Department has been traditionally at the forefront in new fields and will remain so through research that challenges the boundaries of contemporary science and engineering.

***Acknowledgments:*** *We thank all faculty colleagues in the department and Yvette Subramanian for helping us write this article.* ❒

# INTRODUCTION

# Strategies for Effective Teaching in Chemical Engineering

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My first formal introduction to effective teaching strategies in chemical engineering was a National Effective Teaching Institute that I attended in 1991. It was codirected by Richard Felder, James Stice, and Rebecca Brent, and has been held every year since 1991 just prior to the annual meeting of the American Society for Engineering Education (ASEE). Workshop participants are given the opportunity to gain firsthand knowledge of the elements of effective teaching, including lecturing, active and cooperative learning, course planning, and evaluation.

Of all the things I learned in the workshop, the most impactful was that the most widely used teaching method—lecturing, as traditionally practiced—is actually the least effective in promoting student learning and that students learn best by doing. My own experience confirms the numerous published demonstrations that the standard lecture format is less effective than a number of alternative teaching methods.[1,2]

Faculty interest in effective teaching has increased significantly over the past decade as a consequence of a variety of factors. Various constituencies, including employers, legislators, accrediting bodies, university administrators, and parents, have sought greater accountability for the educational training of skilled engineers equipped to solve 21st century engineering problems. The new Accreditation Board for Engineering and Technology (ABET) engineering criteria for accreditation that became standard in 2001 require engineering departments to demonstrate that their graduates have a command of engineering fundamentals as well as communication, critical thinking, and other lifelong learning skills.[3]

Faculty have responded to this increased focus on learning outcomes by re-evaluating how engineering is taught and by seeking ways to evaluate and improve teaching. It is increasingly recognized that traditional approaches to teaching often fall short of achieving the desired outcomes and that there are benefits in moving from a faculty-centered teaching model to a student-centered learning model.[4]

*Gilda Barabino is Associate Professor of Chemical Engineering at Northeastern University. She received her BS degree from Xavier University of Louisiana in chemistry and her PhD from Rice University in chemical engineering. She previously served as the Vice Provost for Undergraduate Education at Northeastern University. Her teaching and research interests are in biochemical and biomedical engineering, reactor design, and cellular and tissue engineering*

Venues for faculty to learn about effective teaching continue to increase as more workshops dedicated to teaching are offered by universities, professional organizations, government agencies, and private foundations, as universities establish or expand teaching and learning centers, and as the literature on teaching and learning continues to grow. Every five years, the Chemical Engineering Division of ASEE offers a Summer School for chemical engineering faculty. The purpose of the Summer School is to disseminate innovative and effective teaching methods to a wide spectrum of chemical engineering undergraduate programs.

During the 2002 Summer School, I organized a poster session devoted to effective teaching strategies. It was designed to provide a forum for the exchange of creative ideas and approaches to chemical engineering education and for sharing practices related to effective teaching. The poster presentations that were judged the best by an expert faculty panel in each of four categories (lecture-, laboratory-, and computer-based strategies, and strategies related to general approaches, learning styles, or outreach) are presented in this issue of *Chemical Engineering Education.*

Some strategies for effective teaching that are represented in the following set of papers include active and cooperative learning, project-based learning, the use of high school outreach to enhance engineering student learning, and the use of a focus topic such as racing cars or biochemical/bioprocess engineering to illustrate core chemical engineering fundamentals in an elective course.

My hope is that the papers presented in this special issue will serve to further promote the sharing and exchange of ideas that began during the Summer School, and to disseminate a set of interesting and innovative approaches and best practices in chemical engineering education. Readers are also encouraged to investigate the burgeoning body of engineering education literature and resources. Several resources are recommended below as a starting point for this investigation.

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*Chemical Engineering Education*

*Journal of Engineering Education*

***Magazines and Proceedings***

ASEE *Prism*

Proceedings of ASEE Annual Conferences

***Web Sites***

Richard Felder's home page at <http://www.ncsu.edu/effective_teaching>

Effective teachers are creative and use a range of pedagogies and learning strategies designed to focus on student learning and to consider student learning styles. They also view students as active participants in the learning process, and view assessment as a means of driving the learning process. The papers included in this series represent some examples of effective teaching strategies that have been used successfully in chemical engineering.

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### PAPERS IN THIS SERIES

***Lecture***

- "Water Day: An Experiential Lecture for Fluid Mechanics," *Ford*
- "Synthesis, Resourcefulness, and Effective Communication in Group Learning: Introduction to Biochemical Engineering," *Peeples*

***General, Learning Styles, Outreach***

- "Engaging the Imagination of Students Using Experience Outside the Classroom: A Course in Bioprocess Engineering" *Ostafin, et al.*
- "Incorporating High School Outreach into Chemical Engineering Courses," *Ross and Bayles*

***Lab***

- "Lab-Based Unit Operations in Microelectronics Processing," *Chang, et al.*
- "Passing It On: A Laboratory Structure Encouraging Realistic Communication and Creative Experimental Planning," *Moor and Ferri*
- "Incorporation of Experimental Design in the Unit Operations Laboratory" *Doskocil*

***Computer-Based***

- "Increasing Time Spent on Course Objectives When Using Computer Programming to Teach Numerical Methods," *Silverstein*
- "High Performance Engines: Fast Cars Accelerate Learning," *Han, et al.*

# WATER DAY
## An Experiential Lecture for Fluid Mechanics

LAURA P. FORD
*University of Tulsa • Tulsa, OK 74104*

Water Day is essentially playtime with water. Different stations are set up outdoors, and the students go from station to station experiencing and observing different basic fluid-flow phenomena. They see how water flows from holes in a tank, how a stream narrows as it falls and how a water stream can knock over a block. These demonstrations are not like the usual laboratory experiments with statistical data analysis; the students make only qualitative observations or rough estimations to get a feel for the phenomena.

Students receive the most benefit from the demonstrations when Water Day is held at the beginning of the semester. Knowing that the students observed the phenomena during Water Day, the instructor can refer to the different stations when the appropriate topic comes up in class. The experiments can be explored quantitatively in class examples or homework problems throughout the semester. For an extra-credit assignment at the end of the semester, the students can be given the original observation sheet with instructions to name the equation or concept that explains the observations seen on Water Day. This forces them to review the course material, which has now been touched upon three different times over about three months.

If the fluid mechanics class is a spring course, Water Day can still be held. Instead of being at the beginning of the semester, it usually occurs at the end of the semester when the weather is warmer. The benefit of being able to refer to the stations throughout the course is lost, but the students' observations can be used to review the entire semester.

I hold Water Day during a regular class lecture for my engineering science "Introductory Fluid Mechanics" course, which is taken by juniors in chemical, mechanical, and petroleum engineering. I encourage student participation with the promise of a perfect homework score for filling out an observation sheet, given to them at the beginning of the demonstration. Although I usually allot an entire lecture to Water Day, it is short enough to be held during half of a 75-minute lecture.

Water Day is held to provide a minimum experience level with fluid flow phenomena. It is especially beneficial for the international students, who make up 10-50% of our fluids enrollment, since many of them are from arid countries and did not have the chance to play with water hoses as children. The demonstrations ensure a minimum experience level for all students, and the course then builds on this experience.

Water Day also incorporates some pedagogical tools. It emphasizes sensing, visual, and active learning styles, which are often neglected in engineering lectures.[1] Holding a Water Day and referring to it during the semester appeals to somatic understanding, which relies on the sense of touch.[2,3] Somatic understanding can be gained by taking an object apart, by feeling the force required to deflect a water stream, and by making the water shoot far with a garden hose. It is the lowest level of understanding, but it gives the students a baseline from which they can develop the higher levels of understanding that we want. Water Day provides an opportunity for somatic understanding, and the rest of the course works takes this understanding to higher levels.

## GENERAL PREPARATION

Some assistants and special materials are necessary for holding a Water Day. The campus physical plant can help with hoses and a water supply, and teaching assistants for the class, or other graduate or senior students, can help man the stations. My current Water Day stations cover the continuity, Bernoulli, conservation-of-linear-momentum, and moment-

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of-momentum equations, the *vena contracta* effect, and relative and absolute velocities. The following supplies are needed for these stations:

- *Observation sheets*
- *Nozzles*
- *A tank with holes and plugs*
- *A jug with a hole in the lid*
- *A trash can lid*
- *A book or block*
- *A three-arm spinning sprinkler*

The materials are intentionally common and inexpensive. The experiments are described in detail below, and suggestions for other fluids topics are given later in this paper.

***Tank-With-Holes Station*** • To prepare for this experiment, something must be found to use as a tank. For classroom demonstrations, an 11-oz coffee can is suitable, and for Water Day, a 50-L carboy or a 2-L soda bottle will do well. Punch or drill at least four holes in the tank, keeping the diameter of the hole in proportion to the volume of the tank and making sure there are corks available to plug the holes. Some holes should be at the same horizontal level, and some of them should be at different vertical levels—a five-hole cross pattern works fine. During Water Day, plug the holes and fill the tank. For observation purposes, it is best to have the tank sitting on a cart or table rather than on the ground. Remove the corks and let the students observe the water flow. The observation sheet should direct the students to specifically observe

1. How the water flow from a particular hole changes as the water level in the tank drops *(They should see that the flow from a particular hole shoots a shorter distance from the tank as the water level in the tank drops.)*

***Figure 1.*** *Flow from the vertically-aligned holes in a tank.*

2. How the flows from the horizontal holes are the same or different *(They should see that the water streams from the horizontal holes shoot the same distance from the tank.)*
3. How the flows from the vertical holes are the same or different (see Figure 1) *(They should see that the water shoots further from lower holes than from the upper holes. This is true only if the tank is above a critical height from the ground, which is why the cart or table is useful.)*
4. How the diameter of a jet compares to the diameter of the hole *(They should see that the diameter of the jet is smaller than the diameter of the hole.)*

Observations 1 through 3 can be explained by applying the Bernoulli equation to flow from the surface of the liquid in the tank to the free jet at the hole. Observation 4 is an example of a *vena contracta.* In our course, this material is covered in the fifth week of class when we reach Section 3.6 of the textbook *A Brief Introduction to Fluid Mechanics.*[4]

Variations can be added to the main experiment. Instead of drilling the horizontal holes all the same size, make each one different. The students will be able to see that the jets all shoot the same distance (neglecting viscous effects) but that the flowrates are different. For another variation, try rounding the inside of one of the holes. The students should be able to see the difference in contraction coefficients between the square and the well-rounded holes.

***Garden-Hose Station*** • All that is needed for this station is a garden hose with no nozzle. Ask the students to

1. *Point the opening of the garden hose upward and note how far the water travels above the opening*
2. *Cover part of the opening with a thumb and note how far the water travels above the opening (see Figure 2, next page)*
3. *Experiment with covering the opening and noting the different distance the water travels.*

The students should be able to see that the water travels further when more of the opening is covered. This can be explained by assuming constant flowrate and applying both the continuity and Bernoulli equations. This problem is also addressed in the fifth week of our course and is covered explicitly in Problem 8.24 of the text.[4] For a variation of this station, include a flowmeter and consider the assumption of constant flowrate.

***Jug Station*** • For this station, a jug with a hole in the lid is needed—a one-gallon milk jug works well. Make a quarter-inch or smaller diameter hole in the lid (inserting a short section of a straw in the hole helps make the jet smoother), fill the jug with water, and turn it upside down, as shown in Figure 3. As the water drains from the jug, the students can observe the diameter of the jet as a function of the distance from the jug. The diameter of the jet should decrease as the stream moves further from the jug. This can be explained by applying the continuity and Bernoulli equations to two points in the jet. This material is covered at the same time as in the previous two stations and in Problem 3.24 of the textbook.[4] A variation of this station suggested by a reviewer is to change the viscosity of the water by adding sugar. At high viscosities, the flow should be slower and smoother.

***Trash-Can-Lid Station*** • For this station, an assistant, a trash-can lid, and a garden hose with a nozzle are needed. The student should hold the trash can lid perpendicular to the ground at all times and should be about 10 feet from the assistant. Using a nozzle, the assistant should form a narrow stream of water and aim it at the trash can lid (see Figure 4). The student holding the lid should be directed to observe the forces required to hold the lid in place as he moves the lid from perpendicular to the water stream to nearly parallel to the water stream. It seems to be easier to feel the difference in forces if the lid is kept perpendicular to the ground at all times (see Figure 5). The student should notice that more force is required to hold the lid in place when it is perpendicular to the water stream than when it is parallel. This can be explained by applying the conservation of linear momentum equation to the water stream. This material is covered in the eighth week of the course when we reach Section 5.2 of the text.[4] Problem 3.40 in *Fluid Mechanics*[5] addresses the perpendicular part of this station. A second part on the nearly parallel case could be added.

***Book-or-Block Station*** • A book or block, a garden hose, and a nozzle are needed for this station. If a book is used (telling the students it is their fluid mechanics book is particularly effective at the end of the semester), wrap it well in plastic bags so it doesn't get wet. Place the book or block vertically on its short side and adjust the nozzle to a narrow jet of water. Direct the students to observe what happens when they aim the jet at the book, starting at the bottom of the book and moving to the top. Nothing should happen when the stream is at the bottom, but the book will tip over as the stream is moved upward. This can be explained by applying the conservation of linear momentum equation to the water stream to find the force of the book on the water. This force is turned around to find the force of water on the book, and a moment balance is done on the book. This station is considered explicitly in Problem 5.30 of the text.[4] An interesting variation would be to knock over books of the same thickness but different weights or blocks of the same size but different densities.

**Figure 2.** *Water shooting from a garden hose with the opening partially covered.*

***Three-Arm-Spinning-Sprinkler Station***

For this station, a two- or three-arm spinning sprinkler is needed. Connect it to the garden hose and instruct the students to determine which direction the nozzles point (clockwise or counterclockwise), which direction the sprinkler rotates (clockwise or counterclockwise) when the water is turned on, and the absolute and relative velocities of the water jets. The students should be able to determine that the sprinkler rotates opposite to the direction

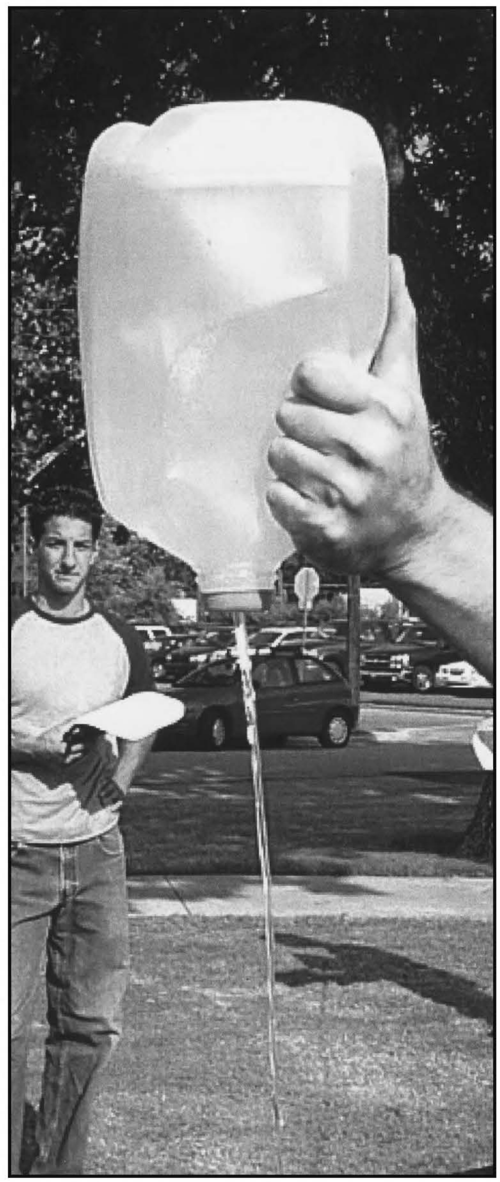

**Figure 3.** *Water flowing from an upside-down jug.*

the nozzles point and that the relative velocity (relative to the sprinkler) is normal to the nozzle exit area. They probably will not be able to determine that the absolute velocity (relative to a fixed frame of reference) is radial if the resisting torque is negligible. This can be explained by the moment-of-momentum equation, covered in the seventh and eighth weeks of the course, in Sections 5.1.3 and 5.2.4 of the text.[4] A variation would be to add a flowmeter and observe the rotation rate as a function of water flowrate.

***Other Stations***

Adding pressure gauges at various locations in the hoses could demonstrate pressure drop due to fittings

**Figure 4.** *Trash-can-lid station. Note that the student is tipping the lid towards the ground instead of keeping it perpendicular to the ground.*

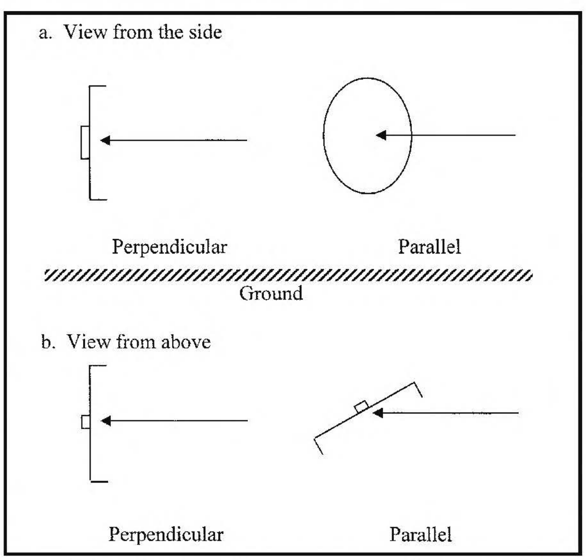


**Figure 5.** *Sketches of the trash can lid in positions perpendicular and parallel to the stream. Note that the plane of the lid remains perpendicular to the ground at all times.*

and friction. Other stations suggested by reviewers are observation of delta formation in a muddy or sandy parking lot, the location of eddies in a creek relative to flow disturbances, and vortex formation in a draining tub. With latex paint and a paint gun, they could see the effects of viscosity and particulates on fluid flow. Anything new the students can see or feel will help their understanding of the material later. The challenge in developing new stations is keeping them simple, safe, and inexpensive.

## OTHER APPLICATIONS OF WATER DAY

Water Day can be used with groups other than fluid mechanics classes. The idea for Water Day came from Dr. Christi Luks, who had done similar experiments with middle-school students at a Young Scholars Program and Engineering Summer Academy. Water Day could be used in an Open House or done when recruiting prospective freshmen. The stations could also be used with a freshman introduction-to-engineering class to whet their appetites for things they will understand later. Some of the stations are easily modified for use indoors, which expands their range of usefulness.

## EVALUATION

One of the pedagogical goals of Water Day is to include sensing, visual, and active learning in a lecture course that might not include them otherwise. Sensing is used in the trash-can-lid station when the students feel the difference in force, and visual learning is in all the stations. This watching is not "mindless" since the students must evaluate what they see and record their evaluations on an observation sheet (*e.g.*, they note that the stream narrows as it falls from the water jug). Active learning is included in the trash-can-lid and water-hose stations because the students must do something. Taken together, the stations add sensing, visual, and active learning to the course.

Another pedagogical goal is to provide an opportunity for somatic understanding as a baseline to build upon. Water day *is* experiencing fluid flow phenomena, so students leave with a minimum level of somatic understanding.

No formal assessment of Water Day has been done. Nearly 100% of the students participate since they are encouraged by the promised homework score. Informal feedback indicates that the students enjoy it. One comment from a group doing this at the end of a semester was, "Cool! You can see the *vena contracta!*" One student said that he liked having the experience to draw on later, *i.e.*, he liked having the somatic understanding to build on.

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# INTRODUCTION TO BIOCHEMICAL ENGINEERING

## Synthesis, Resourcefulness, and Effective Communication in Group Learning

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The current nature of engineering requires its practitioners to be comfortable using information from several fields to solve problems. Successful engineering design requires the use of several possible tools to view, decipher, and address problems of interest. Interdisciplinary efforts result in innovative solutions to many complex problems in the health and environmental sciences. These approaches also expand the current chemical process industries to include the most recent advances in fields such as biotechnology, nanotechnology, and "green" chemistry. Today's graduates must be equipped with tools that will enable them to evaluate complex, open-ended problems using their engineering perspective.

We must encourage students to develop an understanding of engineering problem solving and expose them to diverse areas where their skills may be applied. Tools that enable students to be effective in the global community include 1) an ability to deconstruct and solve complex problems, 2) an ability to research and find answers to original questions, and 3) an ability to effectively communicate new discoveries. These tools are formed by expanding laboratory opportunities for students, adding open-ended design projects to courses (including discussions of topical issues in coursework), and fostering individual investigations.

## INTRODUCTION TO BIOCHEMICAL ENGINEERING: A SYNTHESIS COURSE

As students reach their junior and senior undergraduate years, they are already well-versed in chemical engineering fundamentals and are beginning to apply them specifically in unit operations and process design. Critical aspects of learning can be addressed by immersion into unfamiliar territory where students are required to apply chemical engineering principles to solve new and unusual problems. The course "Introduction to Biochemical Engineering" (IBChE) represents an opportunity for this kind of engineering synthesis and design. Synthesis, the assembly of components to form a new whole, is demonstrated in biochemical engineering as students design products and processes based on combining chemical engineering with microbiology, molecular biology, and biochemistry.

Teaching a biochemical engineering course is not a novel concept. Several useful textbooks have been written that enable students to apply chemical engineering approaches to analyze, model, and apply biological systems.[1-3] Requiring biochemical engineering as part of the synthesis courses of the undergraduate ChE program has proven to be quite useful in meeting several education objectives. The explosion of information and expansion of molecular techniques in the biological engineering disciplines have also presented a challenge for instructors to keep pace and expand course resources beyond the classical texts to address bioprocess and bioproduct design on the molecular, cellular, and process levels. The challenge is in defining the key aspects of biological and biochemical sciences to which students should be exposed.

There is great interest in applying advances in the biological sciences to a wide range of interdisciplinary applications. Current chemical process industries are expanding to include the most recent advances in biotechnology for chiral molecule synthesis and environmentally beneficial catalysis. Biobased feedstocks and biological catalysts are being integrated into industrial processes for the manufacture of foods, pharmaceuticals, and commodity chemicals. Further, the advent of genomic information and advanced molecular analysis tools has stimulated great interest in bioinformatics, biomicroelectronics, and molecular medicine. In this context, it is difficult to strictly define the breadth of content encom-

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passed in biological engineering. There is great interest in elevating aspects of biology as an enabling science foundational to chemical engineering. Evidence of this interest is the number of chemical engineering programs that are pursuing research efforts in the biological sciences and are changing the name of their departments to encompass "biomolecular engineering." But the mechanism for including biology in the earlier stages of the chemical engineering curriculum has yet to be developed.[4]

For the purposes of exposing ChE undergraduates to the explosion of opportunities in the biological sciences, biochemical engineering is introduced as the application of ChE principles (including material and energy balances, thermodynamics, transport phenomena, and reaction engineering) to processes based on living cells or components of cells. The goal is to meet students where they are in terms of knowledge base and usher them into new territory where their unique contributions as chemical engineers can be established.

"Introduction to Biochemical Engineering" has been developed and improved to address critical learning goals for maturing ChE undergraduates. It also serves graduate students seeking exposure to the bioengineering field. In the course, students define biochemical engineering by doing research and self-learning about the impact of biotechnology in the technological, economic, societal, and global contexts. Open-ended design problems, group problem solving, written and oral presentations, and laboratory experiments based on current research significantly enhance the learning experience. A typical class includes ChE juniors and seniors, a few biochemistry undergraduates, and a few first-year graduate students from chemical and biochemical engineering and the chemistry departments. The diversity of the class participants often enables an interdisciplinary approach to group learning.

Published prerequisites for the course include organic chemistry and math through differential equations. Chemical engineering students are encouraged to take the course after having chemical reaction engineering and other fundamental ChE courses. ChE graduate students have taken the prerequisite materials and usually enroll at the same time as the core graduate ChE courses. Students from chemistry and biochemistry take the course with permission and awareness that additional review of ChE concepts may be required. Their experience with core biological and chemical concepts gives them an advantage in other aspects of the course, however. The result is a blended course where students with complementary skills work together to solve open-ended problems.

## LEARNING GOALS AND ELEMENTS

In order to guide students in the learning process and also to develop a basis for course assessment, several course learning goals were established. They related strongly to the educational outcomes of the undergraduate chemical engineering program[5] (see Table 1, next page).

Elements of the course were developed to accomplish course learning goals. They included

- *Introducing the biotechnology field with guided self-learning, web resources to enhance familiarity with field language*
- *Practicing problem-solving skills through in-class group assignments*
- *Providing hands-on learning experience through laboratory experiments*
- *Challenging students to perform a design project on a topical issue of their choosing, analyze current technological problems, and pose a solution*
- *Assigning written and oral report assignments to communicate learning experiences*

## RESOURCEFULNESS

Problem-solving skills for maturing engineers evolve from merely looking up answers to studying situations, reviewing necessary background information, posing hypotheses, and testing them to develop appropriate solutions. Students must learn to find answers to open-ended questions by applying an iterative design process.[6] This should be done throughout the curriculum and not be relegated to a capstone course. To facilitate the process within IBChE, students were assigned several tasks that required excursions into the world-wide web. Web links accessible from the IBChE course page[7] guided students to a variety of sites, including National Science Foundation Bioengineering and Environmental Systems, the Swiss Protein Database, and educational links for microbiology. Questions about the web information necessitated that the students review these sites. They took web-based quizzes developed on a password-accessible WEB Course Tools (WebCT)[8] account page.

For independent study, additional resources were provided on the IBChE course page in the form of supplementary web links. These resources included links to writing guidelines, to special biochemical engineering topics, to chemical reaction engineering topics, and to employment opportunities in bioprocessing and biotechnology fields.[7]

## GROUP ASSIGNMENTS

Within the IBChE course, students have several opportunities to work in groups through in-class problem solving, laboratory experiments, and design projects. Group sizes are adjusted depending on the size of the class and the distribution of graduate versus undergraduate or chemical engineer versus non-chemical engineer. Class sizes have ranged from 15 to 30 students, and group sizes have ranged from 2 to 5 students, depending on the assignment. Groups are assigned in a variety of ways, including random selection during class, sign-up sheets for laboratory time slots, and student self-selection. Typically, all the different methods for group assignments are used during a given semester.

## IN-CLASS GROUP PROBLEM SOLVING

Solving problems as groups served to encourage students to communicate with each other and to work together as teams to solve problems. This problem-based active learning mode

**TABLE 1**
**Course Outcomes Worksheet**

| *Course goals* | *Supports ABET Outcomes[5*]* | *Course Activity* | *Basis for Goal Assessment* |
|---|---|---|---|
| By the end of the course, the student will be able to identify enzymes and microorganisms used in bioprocessing technologies and to describe the basics of biological structure and function. | a(●);e(●) | Lectures; in-class examples; web resources; web quizzes; design project; lab experiment; exams; homework | Homework; lab and design reports; web quiz data; exams |
| By the end of the course, the students will be able to choose and apply the simple models of enzyme kinetics and cell growth that yield accurate results for the problem under consideration, including: the Michaelis-Menten equation with and without competitive inhibition and the Monod growth equation. | a(●);b(●);c(○); e(●) | Lectures; in-class examples; design project; lab experiments; exams; homework | Homework; lab and design reports; exams |
| By the end of the course, the student will be able to apply chemical engineering principles of kinetics, transport phenomena, and thermodynamics in the design and analysis of batch and continuous biochemical reactors | a(●);c(●);e(●); k(○) | Lectures; in-class examples; design project; lab experiment; exams; homework | Homework; lab and design reports; exams |
| By the end of the course, the student will have participated in group laboratory and design experiences and will have described this work in several written reports and one poster presentation. | a(●);b(●);c(●); d(○);e(●);g(wog●); h(○);i(●);j(○) | Lab experiments and design project | Lab and design reports; report grading handouts; design description homework; poster presentation evaluation forms |
| By the end of the course, the students will have been exposed to topical issues in biotechnology covering societal and and economic impacts of new technologies (*e.g.,* genetically modified foods, environmentally benign manufacturing, gene therapy). | d(●);f(○);g(w●); i(●);k(○) | In-class group issues discussions; written project reports (including iteration of introduction, economic societal impact); ventures in course web resources. | Design project part A; design description homework; web-learning assignments |
| By the end of the course, the student will have had opportunities to further his or her professional development through team experiences, studying ethical issues in biochemical engineering practice, practicing oral and written communication skills, and using modern computer tools. | g(●);h(○);i(●); j(○) | Ventures in course web resources, including employment links; poster presentations; homework; design project | Ethics links in assignments page; homework with data analysis; design and lab reports; web resource page |

○ denotes moderate contribution to the outcome
● denotes substantial contribution to the outcome

**Letters "a-k" represent desirable program outcomes for student attributes as described by the Accreditation Board for Engineering and Technology[5] and modified by the University of Iowa Chemical and Biochemical Engineering program as follows:*

**University of Iowa Chemical Engineering Program Outcomes**

a. Each graduate will have the ability to apply knowledge of mathematics, science, and engineering fundamentals.
b. Each graduate will have the ability to design and conduct experiments and to analyze and interpret experimental results.
c. Each graduate will have the ability to design systems, components, or processes to meet specified objectives in chemical engineering.
d. Each graduate will have the ability to work as a member of a multidisciplinary team and have an understanding of team leadership.
e. Each graduate will have the ability to identify, formulate, and solve chemical engineering problems.
f. Each graduate will have an understanding of professional and ethical responsibility.
g. Each graduate will have the ability to communicate effectively in written (w), oral (o), and graphical (g) forms.
h. Each graduate will have an education that is supportive of a broad awareness of the diversity of the world and its cultures, and that provides an understanding of the impact of engineering practice in the global/societal context.
i. Each graduate will recognize the need for and have the ability to engage in lifelong learning.
j. Each graduate will have knowledge of contemporary issues.
k. Each graduate will have the ability to use the techniques, skills, and modern engineering tools necessary for engineering practice.
l. Each graduate will have a thorough grounding in chemistry and a working knowledge of advanced chemistry, including organic and physical and inorganic analytical, polymer or biochemistry, depending upon their individual educational goals.
m. Each graduate will have a working knowledge of chemical process safety.

also increased student engagement in class activities.[9,10] Class diversity contributed to unique approaches to defining problems and making assumptions. Students were given textbook classical bioprocessing examples to discuss and solve during class time. They presented their work to the class, answering key questions about the specific problem. Key questions for discussion included, "What are the assumptions?" and "What is the strategy for solving the problem?" Group work was collected at the end of class and bonus points were awarded based on student participation.

## LABORATORY EXPERIMENT: USING AND EVALUATING ENZYMES

During the course, students were required to participate in an enzyme kinetics lab based on the characterization of enzyme activity for a thermophilic $\alpha$-amylase. This enabled incorporating research efforts from Peeples' lab into the teaching environment. After self-learning about enzymes through visiting sites such as the Swiss Protein Database,[11] the website of Novozymes[12] (a major enzyme company), and the websites of chemical vendors,[13] students learned about activities in the cloning, isolation, and characterization of thermophilic enzymes.[14] They were given a sample of amylase enzyme of unknown characteristics—source was either a commercial thermostable amylase (Sigma Chemical Co.) or a recombinant hyperthermophilic amylase from Peeples' research lab.

In the most recent course, students were asked to discuss how they would market such a product. After brainstorming ideas for enzyme characterization, they were instructed to collect data about the enzyme and to produce a product information sheet reporting its characteristics. This required writing a different type of document than is required in other laboratory courses. Students opted to study salinity, temperature, and pH effects as well as kinetic parameters. Working in groups of four to five, students collected data and reported their information to the class. Class data were pooled so that all of the students had all of the analyses. Each individual wrote a product description, which was then graded.

## DESIGN PROJECT AND EFFECTIVE COMMUNICATION

The aspect of the course that allowed the students to investigate the field of biochemical engineering and put bioengineering in an approachable context was the design project. It represents an important element in establishing the relevance of bioengineering to ChE students and comprises the major portion of the course grade. Students worked in groups of two to three on this semester-long project, and working within different teams from the lab assignment afforded them the opportunity to improve interpersonal communication.

Students were asked to investigate the economic, social, and technological issues surrounding a chosen topic in biochemical engineering. This form of case study exposed the class to more aspects of the discipline than could be covered in a traditional lecture format. Students completed several group reports and a poster presentation of their project to further widen the exposure of the entire class to a variety of case studies in biochemical engineering. As design groups progressed in their research of bioengineering during the course of the semester, each report served as a mechanism to iterate through the writing as well as to give feedback on the design process and focus to the area of bioengineering under study. The iterative nature of the design reports enabled faculty and teaching assistants to help students focus on and address important design considerations by the final report. Students were encouraged to take advantage of patent information, process reviews, and experts in the field through the research of their chosen topic. Assignments were focused on identifying the molecular, unit operations-level or process-level improvements. Publications from the College of Engineering Center for Technical Communications were distributed to help students properly reference source material.[15]

The first design assignment consisted of a brief abstract introducing the topic area. Students were required to choose an appropriate topic that was manageable within the context of an introductory course. Over several years, the projects have included tissue engineering, drug delivery, genetically modified foods, and gene therapy. A list of the topics that design students chose in the 2001 course offering is shown in Table 2. "Design Report A" focused on the economic and social issues surrounding the development or application of bioengineering technology, and "Design Report B" required synthesis and chemical engineering analysis. Students were asked to perform process or product design and analysis using biochemical engineering concepts. They were to decide on the level (molecular, unit operation, or process) where improvements to the technology could be made.

Given the ability to research and evaluate complex problems and to use this information in the synthesis of solutions, graduating engineers must be able to communicate ideas to diverse constituencies. In addition to the three written design project assignments, students also presented their work in a class poster session. Held at the end of the semester, it was a source of interaction between undergraduates, graduate students, and faculty. All were invited to visit the poster session and learn about the activities of the IBChE class. Students were required to evaluate other student posters and guests were also invited to rate poster presentations and to provide comments. Instructor and guest review, as well as student reviews, were used to compute the final poster grade.

## ASSESSMENT

Course learning goals, student performance, and the contribution of the course to the CBE program outcomes were assessed through analysis of course elements and class surveys. Based on the annual assessment, improvements were made to the content and delivery, and reassessment was carried out in subsequent offerings. Assessment tools included evaluation of student work, WebCT data (hits and statistics), and student surveys. Student work was assessed by developing metrics on the grading of all course elements and topic areas. Achievement levels included "Mastery" (>85%), "Intermediate Understanding" (>75%), "General Understanding" (>65%), "Novice" (>55%), or "Failure." The entire class obtained intermediate-to-advanced levels of understanding across the course.

In 2002, most of the class (93%) completed surveys addressing the learning goals and course elements. Through the surveys, students evaluated the priority warranted by, as well as their achievement of each learning goal. They were asked if the stated learning goals should be emphasized in the course and if they achieved those goals. The standard deviation in student perceptions reveal that there is not much statistical significance in the differences among some of the course elements. However, lower standard deviations reveal areas where there was strong student agreement regarding the course element. Students perceived their performance to be highest in goals 6 and 2, respectively (see Table 1), and their lowest areas of achievement to be on goal 3.

These scores appear to be improvements from the previous course offerings where students were less confident about their achievement of course learning goals. One reason for the increase in perceived achievement was the redefinition of course learning goals. For example, based on previous assessment (2001), "Goal 1" was written without a clear meaning and as a result students were not sure if the goal was achieved (4.3/6). The 2002 goal was rewritten to use more clearly active words describing the expectation of student behavior (see Table 3), and as a result, students expressed more confidence about the priority of the goal and their achievement of it (4.8/6)

In addition to surveying students regarding the learning goals, course elements were assessed by asking them, "What contributed most to the achievement of the course goals?" and "What contributed most to student learning?" The results are given in Table 4.

It should be noted that students perceived Goal 4, the inclusion of lab experiences and design projects, as a lower priority. At the same time, they recognized the group projects as a very important learning tool, contributing the most (5.00/6.00) to student learning. They regarded the lab experiment itself as one of the lowest contributors to student learning (4.67/6.00). Still, the narrower degree of deviation of responses reflects a more uniform agreement on the overall utility of group work. Absolute numbers for student achievement of course goals appear to improve over the three-year offering of the course. Within the ChE curriculum at the time of IBChE, students have typically taken numerous lab-intensive courses, including unit operations laboratory, chemical process safety with lab, and materials science lab. They have also had many lab experiences in the various chemistry requirements. Thus, the enzyme lab purely for the sake of offering experience is a lesser contributor. Students also found it challenging, and in some cases frustrating, to analyze data collected by the entire class, but the opportunity to push students beyond their comfort zone into a different type of writing and data analysis is an important aspect of the course delivery. Lessons can be learned about answering questions

**TABLE 2**
**Topics for Biochemical Engineering Design Projects**

| Topic | Description |
|---|---|
| Anthrax | Evaluation of *B acillus antrhacis,* treatment and prevention options |
| NatureWorks TMPLA | Evaluating the production of Cargill-Dow's polylactic acid-based polymer |
| PCR | The principles, application, and details of the polymerase chain reaction process as a new technology in waste-water treatment |
| pHBA Biosynthesis | Evaluating the production of p-HBA using genetically engineered *Pseudomonas putida* |
| Poultry Rendering | Studying the fermentation of poultry waste to produce protein meal |
| Protein Engineering | How mutation of the glucoamylase enzyme affects its binding characteristics |
| Starch Hydrolysis | Studying the effect of high-temperature enzymes on starches and understanding how the enzyme is used in the pulp and paper industry |
| Xanthan Gum | Studying the production of the polysaccharide by the bacterium, *Xanthomonas camplestris* |

**TABLE 3**
**Improvement of Course Learning Goal Clarity**

| | |
|---|---|
| **2001 Goal 1:** | *By the end of the course, the student will understand basic concepts regarding the behavior of enzymes and microorganisms used in bioprocessing technologies (e.g., food processing, pharmaceutical production, environmental remediation, and chemical synthesis).* |
| **2002 Goal 1:** | *By the end of the course, the student will be able to identify enzymes and microorganisms used in bioprocessing technologies and to describe the basics of biological structure and function.* |

and making decisions with less-than-perfect information. Perhaps one way to improve student perception of the lab experience may be to better articulate the specific learning objectives of the lab project.

Because the course goals were designed for contribution to program educational outcomes, as reflected in Table 1, the learning goals could be used to reflect the larger program goals. IBChE showed strong contributions in specific areas of communication, problem solving, and lifelong learning skill development. Based on the design of course elements and assessment of student performance, the goals of enhancing student communication and problem-solving skills, and improving laboratory skills and student familiarity with contemporary issues were met by improved offerings of IBChE.

## SUMMARY

While there is much activity in the area of including biological sciences earlier in the ChE undergraduate curricula, opportunities exist to use bioengineering as a point of immersion for engineering students. Enabling students to investigate this unfamiliar discipline and to apply ChE skills in synthesis can enhance the educational experience. Assessments showed the highest contributor to learning was the group-learning activities where students investigated and defined the aspects of biotechnology relevant to their interest. Course activities mapped well to the overall program objectives by enabling students to analyze problems by using ChE principles to synthesize solutions to problems in a new discipline. Further, using a variety of additional course elements, including in-class problem solving, lab experiments, and traditional lectures, homework, and tests could be integrated with the independent learning process to facilitate development of critical skills for a lifetime of engineering exploration.

**TABLE 4**
**Assessment of Learning Goals and Course Elements[1]**

***Student Perceptions of Course Learning Goals***
*(Out of 6 points, 1=low priority, 6=high priority)*

| | 2000 Priority | 2000 Achievement | 2001 Priority | 2001 Achievement | 2002 Priority | 2002 Achievement |
|---|---|---|---|---|---|---|
| 1 | 4.8 | 4.0 | 5.0±0.92 | 4.3±1.2 | 5.0±1.2 | 4.8±1.2 |
| 2 | 5.2 | 4.9 | 5.3±0.93 | 5.1±1.0 | 5.3±0.91 | 5.1±1.1 |
| 3 | 4.9 | 3.7 | 5.1±0.71 | 4.0±1.2 | 5.2±1.1 | 4.1±1.4 |
| 4 | 4.4 | 4.7 | 4.7±1.0 | 4.9±1.1 | 4.6±1.4 | 4.7±1.2 |
| 5 | 4.7 | 3.9 | 4.9±1.0 | 4.3±1.5 | 4.7±1.3 | 4.7±1.2 |
| 6 | 4.8 | 4.2 | 5.0±0.86 | 4.5±1.2 | 5.4±0.96 | 5.2±0.93 |

***What contributed most to achievement of course learning goals?***
*(Out of 6 points, 1=low priority, 6=high priority)*

| | 2000 | 2001 | 2002 |
|---|---|---|---|
| Group projects | 5.1 | 4.7±0.80 | 5.4±0.79 |
| In-class problem solving | 4.2 | 4.2±1.4 | 5.2±0.58 |
| Homework | 4.8 | 4.8±0.56 | 4.8±1.1 |
| Lab experiment | 4.3 | 4.3±1.2 | 4.7±1.2 |
| Recall of facts | 4.5 | 4.5±0.87 | 4.4±0.79 |

***What contributed most to student learning?***
*(Out of 6 points, 1=low priority, 6=high priority)*

| | 2000 | 2001 | 2002 |
|---|---|---|---|
| Group projects | 4.4 | 4.4±1.0 | 5.0±0.74 |
| Homework | 4.9 | 4.9±0.72 | 5.0±0.95 |
| Lectures[2] | N/A | N/A | 5.0±1.0 |
| In-class problem solving | 4.2 | 4.3±1.4 | 4.8±1.1 |
| Lab experiment | 4.0 | 4.0±1.1 | 4.7±1.2 |
| Recall of facts | 4.0 | 4.5±1.3 | 4.3±0.78 |

[1] *Standard deviation from class surveys available for 2001 and 2002, 15 students*
[2] *Survey updated in 2002 to include student evaluation of lectures*

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# A COURSE IN BIOPROCESS ENGINEERING

## Engaging the Imagination of Students Using Experiences Outside the Classroom

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Bioprocess Engineering has the potential to become one of the leading chemical engineering fields due to the explosive discoveries that are occurring and continue to occur in the field of life sciences. Since the rate of progress is so accelerated in this field, we must train future engineers to be willing to go beyond the conventional classroom education with initiative, motivation, and creativity.

We have developed a course that engages students' imaginations and participation outside the classroom, that offers real-life experiences through field trips, and that provides a chance for students to express their enthusiasm by publishing their own newsletter. Through these activities, students find that although life sciences is not an exact science, it is filled with tremendous need for challenging and novel conceptual development, which can be exciting to pursue through quantitative numerical analyses and expression.

In the chemical engineering department at the Notre Dame University, which has no formal bioengineering degree program, the second-semester senior/graduate-level bioprocess engineering course attracts students with various backgrounds. By the time they have completed the course, some will have established a strong foundation for embarking on graduate research, while others will have acquired sufficient practical knowledge to become entry-level bioprocessing engineers.

To fulfill the educational goals outlined in the ABET assessment criteria, this course introduces essential biology, biotechnology, and computational concepts while providing an environment in which the student can improve their skills in design, analysis, problem solving, teamwork, and communication. In order to develop a fast-paced, attractive, and self-motivated course, the leading roles for learning are shared between the students and the instructor. The students attend traditional lectures on the fundamentals of bioprocessing and are then asked to take the initiative in using the laboratory learning modules, in organizing a field trip to a local bioprocessing factory, and in publishing a newsletter on bioprocess engineering. They are evaluated based on their performance in all of these aspects, and the course is improved by assessing the results of a standard student Course Evaluation and additional questionnaires.

## OBJECTIVES OF COURSE

Recent advancements in molecular biology demand a new way of thinking in bioprocess engineering. During the last decade, explosive amounts of information have become available in the life sciences and it has become almost impossible for engineering students to know all there is to know about the field. In order to introduce such a wealth of information in one semester to students with little biological background, while maintaining an emphasis on traditional bioprocessing, there must be a carefully crafted set of course objectives. We have identified the following goals:

- *Students should know the structures, natural habitat, and industrial use of various microbes. Since most of the bioprocessing topics discussed in class will be*

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related to microbes, students should have a good understanding of the subject area.*

- *Students should have a good grasp of the analysis of microbial cultures and be able to describe quantitatively their growth and scale-up.*
- *Students should be able to design bioreactors for different microbes when provided with sufficient knowledge about the growth culture supply, gas supply, release of waste products, and heat transfer.*
- *Students should be familiar with microbial product recovery and purification. They need to know the common methods used in product recovery.*
- *Students should be made aware of genetic engineering methods to design microbes to achieve improved product yield.*
- *Students should have some laboratory experience in microbial culturing and enzyme kinetics with sufficient computational, statistical, large-scale bioprocessing, and error analysis skills.*
- *Students should learn to work as a team, improve their communication skills, and be aware of the outside activities related to their fields.*

The course syllabus that reflects such goals is shown in Table 1, and a list of useful texts is given in Table 2.

In order to accomplish these goals, two general postulates were introduced to set the direction of the lecture section of the course. First, biological phenomena and concepts were deductively introduced in the class.[1,2] By approaching the subject from organisms to molecules, it was possible to focus continually on the theme of bioprocess engineering, while introducing the subjects of molecular and cellular events as needed. Future engineers must be trained to direct process development and to pioneer new discoveries in biology and genetics by bringing traditional engineering functions to bear in this novel field. Bioprocessing in a cell can be described in terms of various linked cellular "unit operations" (organelles) in which internal functions are driven by molecular-scale bioprocessing units (proteins and nucleotides) within the cell. This approach differs from the order of presentation typical in many bioprocess engineering textbooks, which start with an in-depth description of the chemical basis of biological systems and enzyme kinetics before introducing the cell, growth models, and unit operations. The choice between the two approaches may well be decided by the number of credit hours students are allowed to take in biology.

**TABLE 1**
**Course Syllabus**

| | |
|---|---|
| **Goals** | By the end of this course, you should be able to<br>• Identify basic structure and types of microbes found in nature and used in industry<br>• Culture microbes—sterile method<br>• Design and operate bioreactors<br>• Harvest and characterize microbial products<br>• Describe intercellular function and structure models of cell growth<br>• Describe the strategy of genetic engineering and molecular cloning to improve product yields<br>• Describe metabolic engineering with solid understanding of enzyme kinetics and its historic evolution<br>• Communicate with the others and work as a team |
| **Text** | Required: none<br>Supplemental Reading: Hand-Out Materials |
| **Class** | Tuesdays and Thursdays 9:30 - 10:45 |
| **Instructor** | Agnes E. Ostafin, Assistant Professor<br>182B Fitzpatrick Hall<br>Phone 631-3798, e-mail: aostafin@nd.edu<br>Office hours: By appointment |
| **Grades** | Grades will be based on your performance in<br>• Take-home exam (30%)<br>• Homework problems, including interactive exercises with reports (55%)<br>• Field trip with a follow-up lab (5%)<br>• Participation in publishing Bioeng. Newsletter (10%) |
| **Course Outline** | I *Introduction to Bioprocessing: Concept through Application*<br>II *Traditional Bioprocessing*<br>a. Biological cells, bioenergetics, and cell metabolism<br>b. Microbial growth and modeling<br>c. Bioreactor design<br>d. Recovery and Purification of products<br>III *Enzymes and Applications*<br>IV *Contemporary Bioprocessing*<br>a. Genetic engineering<br>b. Metabolic engineering<br>c. Nonconventional systems |

**TABLE 2**
**Source Textbooks Used in Course**

- *Bioprocess Engineering,* W. Veith; Wiley Interscience, New York, NY (1994)
- *Bioreaction Engineering Principles,* J. Nielsen and J. Villadsen; Plenum Press, New York, NY (1994)
- *Cell and Molecular Biology,* 2nd ed., G. Karp; Wiley, New York, NY (1999)
- *Biochemical Engineering Fundamentals,* J. Bailey and D. Ollis, McGraw-Hill, New York, NY (1986)
- *Bioprocess Engineering Principles,* P. Doran; Academic Press, San Diego, CA (1995) (Out of print)
- *Fundamental Laboratory Approaches for Biochemistry and Biotechnology,* A. Ninfa and D. Ballou; Fitzgerald Science Press, Bethesda, MD (1998)
- *Bioprocess Engineering,* 2nd ed., M. Shuler and F. Kargi, Prentice Hall International Series in Physical and Chemical Sciences, Englewood Cliffs, NJ (2002)

The second postulate used in course development was that while traditional bioprocess engineering addresses the issues of development and optimization of organism growth and product recovery, contemporary bioprocess engineering must also address the issues of engineering new organisms to better suit the purpose. The impact of recent advances in genomics and proteomics is quickly coming to bioprocess engineering and must be used by bioprocess engineers. For this, discussions of proteins, DNA, enzyme kinetics, and other biochemical processes both inside and outside the cell are critical.

## ACTIVITIES OUTSIDE THE CLASSROOM

While classroom instruction continued, the students initiated activities outside the classroom to enhance their understanding of concepts and their knowledge of real-world applications. Active participation of the students made this course a more exciting learning experience.

***Take-Home Examination*** • A take-home examination was given about midway into the semester to test the students on their ability to model and design fermentation processes. They should show good grasp of microorganisms and their regulated growth. Students appreciated the opportunity to express their knowledge in a relaxed environment.

***Regular Homework*** • Traditional problem-solving homework exercises were assigned to develop and test student comprehension of the various analytical approaches used in this field.

***Interactive Homework*** • In addition to traditional problem-solving homework, interactive modules were developed in order to engage student participation in the learning process. Rather than providing students with a set of numbers to plug into equations and submitting the computational results as homework, we arranged opportunities for them to find these numbers experimentally. We hoped the students would have a better feel for the significance and the range of errors that come with these numbers and how they would affect the final outcome if they were provided with interactive homework.

Relying on the laboratory instruction provided, students performed two laboratory experiments outside the regular classroom hours to generate data. These data were subsequently used to answer the homework problems. Students were divided into groups of 3-4 team members and used the learning laboratory modules. Each module was a mobile unit equipped with analytical instruments to conduct a specific laboratory experiment. Consulting with the graduate teaching assistants, students planned and set up the experiments by themselves, arranging their work schedule as demanded by the experimental procedures. With proper management of student schedules and the learning modules, this flexible arrangement could accommodate 22 students to complete the two experiments described below before the end of the semester. A high degree of student initiative was the key to the success of this arrangement.

• **Growth Analysis of *E. coli*:** Students had already been exposed to the growth analysis of bacteria in the lecture. The objectives of this experiment was to 1) learn the use of a pH meter, a spectrophotometer, and a centrifuge, 2) learn sterile techniques, 3) numerically analyze growth of bacteria, and 4) determine the mass transfer of glucose to the organism. Using a well-established method[3] in microbiology, the teaching assistant provided the original colony of *E. coli* to the students and they cultured bacteria in Luria-Bertani liquid culture medium[4] while intermittently determining the growth spectrophotometrically. A similar experiment was conducted with glucose, observing the rate of its uptake with Benedict solution.[5] Students reported quantitative kinetic analyses with degrees of errors on the lag phase, exponential growth phase, declining phase, stationary phase, and death phase during bacterial culture. The rate of transfer of glucose to the organisms was also reported. Most of the teams were able to obtain reliable data, but some failed and had to borrow data from colleagues. This highlighted the need to perform careful, well-recorded experiments and encouraged students to work together to achieve the long-term goal. The entire process took a little over two weeks, during which the students expended a similar number of hours as they would have spent doing regular homework.

• **Collision and Diffusion Limited Enzyme Catalysis:** Through this experiment the students also become familiar with the use of a pH meter and spectrophotometer. In addition, they learn how to run a LabView module, to understand the importance of pH in enzyme kinetics, to construct the three basic plots used in enzyme analysis (Lineweaver-Burk Plot, Eadie-Hofstee Plot, and Hanes Plot), and to understand the effect of collision frequency and kinetic energy of collision on the rate of enzyme catalysis. After becoming familiar with the conventional enzyme kinetic study in a buffer, the students performed a similar experiment in glycerol to mimic real-world bioprocessing where diffusion-limited reactions would take place in non-Newtonian fluids. Since all the reagents were prepared in advance, well-coordinated teams completed the experiments in two sessions of 2-3 hours.

First, students carried out the enzyme kinetics analysis of urease in water, using urea as the substrate, to understand the importance of buffered solution for enzyme kinetics. The rest of the experiments were conducted in HEPES buffered solution at pH 9.0. The rates of reactions were determined using Berthelot color assay[6] and the concentrations of the enzyme and substrate were adjusted to obtain the constants for the

Michaelis-Menton model at room temperature. This was a relatively simple system and the students were able to obtain data with a relatively small range of standard deviations.

In the second part, similar experiments were performed in a different concentration of glycerol to demonstrate the effect of increasing viscosity of the solvent on the enzyme reaction. The students were asked to explain the significance of high viscosity solvent on enzyme kinetics and its effect on the various constants.

The students considered this type of homework as somewhat taxing, but in general appreciated the firsthand experience in wet biochemical experiments.

***Real-Life Bioprocess Manufacturing and Laboratory Practice*** • About halfway into the semester, a mandatory 3-hour tour to a local microbrewery was scheduled.[7] The students experienced scaling up of laboratory procedures, integration of chemical and mechanical engineering in flows of liquids and a number of regulatory systems, and communication between the administrative personnel, engineers, and technicians. The students embarked on a small-team project to brew three types of bottled beer, starting with the kits purchased from the brewery. Brewing took up to four weeks, and the grade was judged by student participation as recorded by the TA. In general, the excitement level for this module was highest, and an increase in registration was noted in the following year, with specific requests for a repeat of this module.

***Publication of Bioengineering Newsletter*** • A major semester-long team project, the Bioengineering Newsletter, was assigned as the final project for the course. It provided an opportunity for the students to practice long-term team-based project execution and negotiation skills, to use written and verbal communication skills, to develop better literature review techniques, and to become aware of current events in the area of bioprocessing. The entire class of 22 individuals comprised the publication staff of the newsletter. Class members were assigned specific roles and responsibility levels, such as editor, writing team, design and layout team, financial team, and printing and distribution teams. Each responsibility level was given a list of duties, and team leaders were told to report regularly on their progress to their immediate senior in the publishing-team hierarchy. General guidelines and a timeline were provided, and the team leaders were asked to set and enforce deadlines for their own teams. The goal was to produce the final publication on time.

In order to keep some control over the progress of the project throughout the semester, each team leader was expected to provide copies of their regular reports to the instructor and to the editor, indicating the accomplishments of their team for the preceding reporting period and reporting any difficulties that may have arisen. The editor was asked to provide a final comprehensive report on the project on the activities of each team and suggestions for the future. The concept of multi-layered reporting within a large team, although realistic, is sometimes difficult to achieve in the classroom since some students may be reluctant to assess the performance of their peers or to pay strict attention to deadlines. When a very detailed calendar of events was provided, there was more compliance with the structure.

Each student was asked to write a one-page single-spaced article with references and properly sourced graphics relating to a subject relevant to bioprocess engineering. The writing team was to provide a specific theme for that year's newsletter along with a list of suggested topics for the students to write about. Students were free to choose any topic, but if it was not on the list, they had to obtain approval from the writing team. Eventually, students reached a consensus and instructor intervention was minimal.

The design and layout team was responsible for creating the electronic publication using Microsoft Publisher. This group defined the manuscript size and graphical elements, and provided a mock-up to the editor, who proofread the copy before printing. The financial team raised money to cover the cost of printing by soliciting donations from student engineering organizations on campus, such as AIChE, SWE, MEP, and various departments. Excess funds were used to provide pizza and drinks for the inevitable last-minute "push to publish" just before finals week. Each member of the class and each financial donor received a paper copy, and five went to the instructor. Distribution of printed newsletters takes place during finals week. Wider distribution was achieved through website dissemination at <http://www.nd.edu/aostafin/ben1>.

## STUDENT PERFORMANCE EVALUATION

Students were evaluated based on

- Their ability to comprehend and express bioprocess engineering subjects quantitatively: *take-home examination (30%)*
- *Problem-solving homework (30%)*
- Taking initiative in conducting two experiments and the ability to analyze the results quantitatively: *Interactive homework (25%)*
- Ability to apply knowledge to the real world: *site visit and follow-up experiments (5%)*
- Communication skills and ability to work as a team:

*Continued on page 207.*

# INCORPORATING HIGH SCHOOL OUTREACH INTO ChE COURSES

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Three years ago, an undergraduate-level Introduction to Biomedical Engineering elective was created at the University of Maryland, Baltimore County (UMBC). One goal of the course was to include a group project that allowed an opportunity for the students to delve deeply into an area of interest that was not covered in the lecture material. A second objective was to provide a forum for the students to hone their presentation and group interaction skills.

We decided to try something new and different that would challenge the students in a way they had not yet experienced. The idea was to integrate a high school outreach presentation into the course that required the students to participate in problem-based learning. In addition, using the high school setting for the presentation challenged the undergraduates to present highly technical material to an audience with little technical knowledge. We believe this latter skill is critical for success in the "real world." Based on the success of the outreach projects in the elective course, the idea was also tailored to a required course in heat and mass transfer.

## THE PROJECTS

While the content of the projects varies between the two classes, many aspects of the exercise are the same. The presentations are planned for a high school class period that lasts for approximately 45 minutes. In most cases, presentations are given to an upper-level science or math class. Typically, a segment of the presentation is in a lecture format to introduce students to the topic. Interactive components are critical to the success of the presentations, however, so lecture time is kept to a minimum. Exercises to get the high school students involved are an important part of the project and have encompassed such ideas as games ("Who Wants to be a Biomedical Engineer?", "Engineering Jeopardy"), skits ("The Doctor, the Scientist, and the Engineer"), demonstrations (geyser eruption, air freshener diffusion, conduction and convection experiments, electroplating), and puzzles. Student participation is encouraged by using small treats (approved by the teacher) for those who volunteer answers or participate in activities in front of the class.

At the end of the presentation, the group members give the high school students information on their backgrounds, how they chose engineering as a career, and any summer industrial or research experiences they have had. The undergraduates also describe their future plans, if known. The high school students are then given time to ask career-related questions. Before concluding, a survey is performed to help the group determine the effectiveness of its presentation. Finally, information related to the presentation topic is left in the classroom for any student who wants to learn more. Examples of "leave behinds" are bookmarks with definitions and web addresses, a bulletin board that stays up in the classroom, informational CDs, and web sites with links related to the projects.

## ORGANIZATIONAL DETAILS

In each class, the projects carry significant weight in the final course grade (15% in Heat and Mass Transfer and 40% in Introduction to Biomedical Engineering). The projects last

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for a full semester and points are distributed throughout the semester for reaching milestones leading up to the actual outreach presentation. Groups are chosen by the students within the first week of class, and project topics are assigned. Groups contain a minimum of three students and a maximum of four, depending on the class size (we have integrated these projects into classes with up to 25 students). We found it very important for each group to have at least one member who attended high school in the U.S, and it was also helpful if at least one group member had a car. All group members are required to spend equal time leading the presentation.

In the Introduction to Biomedical Engineering course, topics that are current or emerging research areas in which chemical engineers participate are chosen. Examples include tissue engineering, bioinformatics, biosensors, metabolic engineering, and controlled release. In this case, the projects are an exercise in problem-based learning because the outreach topics are not covered in the course content.

In the Heat and Mass Transfer course, the projects must include demonstrations and activities that demonstrate the fundamentals of transport phenomena. Part of one class period at UMBC is taken to demonstrate what the projects could include. The following are example demonstrations.

- The session is begun by asking the students to discuss how they can tell when air pressure changes. *(Possible answers may include flying in an airplane, going up a mountain and feeling your ears pop, etc.)*
- The students are divided into pairs and given a straw, two pieces of string, and two balloons. Ask them to blow up the balloons to equal sizes and tie them to the ends of the strings. The trailing ends of the strings should then be tied to the straw, so that the two balloons are near each other on the straw, but not touching. One student in the pair will be told to hold the straw and the other student will blow so that his/her breath goes directly between the balloons. Ask the students to predict what will happen. *(The students usually expect the balloons to separate further, but the opposite is true...the balloons move together! Blowing between the balloons creates a stream of air that is moving faster than the surrounding air. The pressure between the balloons is lower than the pressure of the air surrounding them, so they come together.)*
- The students are given a clear plastic cup filled with water, along with two straws (one 3-inch and one 4-inch straw), and are challenged to blow across the top of a straw in the water and cause water to come out of it. *(In order for the water to spray out of the straw that is in the water, the students must put the 3-inch straw into the water in such a way that it does not touch the bottom of the cup, and then take the other straw and hold it near the opening and perpendicular to the top of the straw that is being held in the water. Blowing through the longer straw across the top of the immersed straw causes a spray of water to come out of the straw in the water. The faster the blast of moving air from the student's mouth, the lower the pressure exerted around the blast. When the blast flows across the top of the lower straw, the pressure on the liquid in that straw is reduced, and since elsewhere on the water's surface the air pressure is atmospheric, the water is pushed upward through the upright straw toward the low-pressure area. When the water gets into the air stream, it is pushed and scattered by the quickly moving air.)*
- Give the students a Ping-Pong ball, two small paper cups (2 to 3 inches tall), and some masking tape. Ask them to tape the cups onto the top of a table, one behind the other, four inches apart. Put the Ping-Pong ball in the first cup and challenge the students to get it out of the first cup and into the second cup—neither the cups nor the ball can be touched by any solid or liquid. *(Blowing across the top of the cup will produce lift on the ball and it will pop up out of the cup when the air speed is high enough. Controlling the ball's motion to get it to land in the second cup is not easy!)*
- Give the students a round piece of cereal and a bendable drinking straw and challenge them to get the cereal to hover above the straw. *(Bend the straw to a right angle and insert it into the mouth like a pipe. Take a deep breath and, with the cereal held above the straw opening, gently and with control, blow air at the cereal. Let go of the cereal once you start blowing. This takes practice! The cereal will stay roughly at the same height because forces upward [the air stream] and downward [gravity] on the cereal are balanced. This is more easily demonstrated using toy blow pipes or with a hair dryer and a Ping-Pong ball—the angle of the air dryer can be varied to further demonstrate the effect of velocity, air pressure, and gravity.)*

These are just a few examples of hands-on experiments that can be used to demonstrate Bernoulli's principle (which the heat and mass transfer students have studied the previous semester in fluid mechanics). Then, the students are encouraged to explain what math and science skills they learned in high school to study Bernoulli's principle and how it relates to industrial applications (design of pumps, airplanes, etc.)

The first milestone of a project is to find a high school classroom that is within 30 miles of campus for the presentation (5% of the project grade). In general, the UMBC students find schools and classes on their own, with some choosing to return to a group member's own high school. Other common choices include schools that are near UMBC or that target a specific demographic (such as an all-girls school or a predominantly minority inner-city school). To date, presentations have been made in six different counties in the greater Baltimore area. A compiled list is kept of classes we have previously visited, along with contact information to be given to groups that encounter difficulties finding a venue for the projects.

To meet the first milestone, groups must turn in the name of the high school, the course name and time, the teacher name and contact information, the number of students enrolled, and the grade level of the students. We have found high school teachers to be quite accommodating and enthusiastic about our participation in their classrooms.

Within the first month of the semester, the groups are required to meet with the professor for a preliminary meeting (5% of the project grade). At this meeting, the group must present preliminary ideas for the presentation and have a general idea of the information they will present. Each group must turn in one typed page outlining their ideas. We have found this initial part of the project to be very challenging for the students because it requires significant independent reading and synthesis of information. The topics assigned are purposefully broad so that this step requires a significant effort.

At this point, students must make choices as to what material would be both interesting to high school students and at an appropriate level. Approximately two weeks later, the students are required to have a second meeting with the professor (5% of the project grade) to present a full outline of the project presentation, including specific details about what material will be presented and how it will be presented. The plan at this point must incorporate feedback given after the preliminary meeting.

Approximately two weeks before the outreach presentation takes place, at least one member of the group is required to visit the school classroom to meet the teacher, verify the date and time for the project, and to assess if the room is adequate for the planned exercise (5% of project grade). We have found this step to be critical for a successful outreach project.  It was added after the first year of the projects when we experienced several classrooms that were not adequate or appropriate for our presentation. Examples of classrooms that were inadequate or inappropriate included classrooms without screens for the projection of the presentation, open classrooms that made hearing difficult, lack of seating for all the observers, and lack of lab space for the demonstration.

At least two weeks before the presentation date, each group is required to present the outreach project to the professor (5% of the project grade). This presentation is expected to mimic exactly what is planned for the high school classroom, to be carefully timed, and to include any props, games, and handout material. The groups must also turn in the "leave behind" information that has been developed, along with a copy of the student and teacher surveys they plan to use for assessment. This meeting typically results in significant feedback on content level, clarity of explanations, and quality of presentation materials (overheads, slides, etc.). In addition, the meeting commonly identifies any problems that arise with the organization of planned activities or games. At the end of the practice presentation, groups are either given permission to go ahead with their presentation or are required to practice again in front of the professor.

The outreach presentations are typically held within the last several weeks of the semester and account for 60% of the project grade. The UMBC students are asked to dress in typical "everyday" clothes for the presentation to help the high school students relate to them. In the Introduction to Biomedical Engineering course, one lecture is cancelled for each outreach presentation.

In addition to performing an outreach project, all students are required to attend one other outreach presentation as observers. We have found this to be especially helpful for students who are nervous about presenting in front of a group or who did not attend high school in the United States and are unsure of what to expect. The student groups are solely responsible for running the project presentation. The professor does not participate, instead observes and evaluates the presentation. See Table 1 for a typical evaluation sheet.

Assessment is a vital aspect of the project (15% of grade). Each group must collect survey information from

**TABLE 1**
**Sample Outreach Project Evaluation**

Date ______________

Group Members

______________________________________

School

______________________________________

Duration

______________________________________

# High School Students in Attendance

______________________

| | Poor 1 | 2 | 3 | 4 | 5 | Excellent |
|---|---|---|---|---|---|---|
| Clarity of speech - overall | 1 | 2 | 3 | 4 | 5 | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| Volume of speech - overall | | | | | | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| ______________________ | 1 | 2 | 3 | 4 | 5 | |
| Organization | 1 | 2 | 3 | 4 | 5 | |
| Flow | 1 | 2 | 3 | 4 | 5 | |
| Group participation | 1 | 2 | 3 | 4 | 5 | |
| Student participation | 1 | 2 | 3 | 4 | 5 | |
| Slides/Overheads | 1 | 2 | 3 | 4 | 5 | N/A |
| Game | 1 | 2 | 3 | 4 | 5 | N/A |
| "Leave behind" | 1 | 2 | 3 | 4 | 5 | |
| Professionalism | 1 | 2 | 3 | 4 | 5 | |
| Ability to relate to audience | 1 | 2 | 3 | 4 | 5 | |
| Enthusiasm | 1 | 2 | 3 | 4 | 5 | |
| Technical content | | | | | | |
| Technically correct | 1 | 2 | 3 | 4 | 5 | |
| Clearly explained | 1 | 2 | 3 | 4 | 5 | |
| Appropriate to topic | 1 | 2 | 3 | 4 | 5 | |
| Appropriate level | 1 | 2 | 3 | 4 | 5 | |
| Terminology | 1 | 2 | 3 | 4 | 5 | |
| Held student interest | 1 | 2 | 3 | 4 | 5 | |

both the high school teacher and the students. All teacher surveys must include the question "Would you be willing to have another group perform an outreach project in your class in future years?" The response to that question is turned in to the professor for use in building a list of contacts for groups in future years that may have difficulty finding a classroom.

The remainder of the survey is not turned in, but rather serves as feedback for the group. Information from the survey is expected to be incorporated into the group's self-assessment statement to provide support for conclusions that are drawn. The self-assessment statement is a critical assessment of the efficacy of the outreach project (three typed pages maximum, one statement per group, with signatures of each group member). The statement must address several issues: What was done well? What could have been done better? Was the presentation effective? How do you know? What would you do differently if you were to do it again? How well did your group function together? How could you improve the way your group functioned? What overall grade would you give yourself?

Points are distributed for "accuracy" of the assessment as judged by the professor and for writing clarity (not for strength of the project itself). For example, a project with major difficulties that were accurately assessed would receive a low project score, but a high score for self-assessment. We believe this element of the project is critical because it forces the students to begin self-evaluation. The professor's evaluation of the project is given back to the students after the self-assessment is turned in so the students can gauge how well they identified their own strengths and weaknesses.

We have estimated that we spend approximately 2 to 3 hours per group in order to implement this program. This time investment has certainly been worthwhile considering the positive feedback we have received from the high school teachers and students and the UMBC participants.

## OUTCOMES

We have witnessed several desirable outcomes from our outreach presentations. In nearly every case, the level of enthusiasm of UMBC students has been very high. They have been highly motivated to put on an interesting presentation and participation within the groups has been surprisingly uniform. We have witnessed only a few cases where one or two group members performed all the work. To the contrary, since each member is required to spend an equal amount of time leading the presentation, in most cases all group members have contributed equally to the project. The comments relating to the projects on the end-of-semester course evaluations have been overwhelmingly positive.

The initial reaction to the project at the beginning of the semester has typically been, "This will be really easy," followed shortly by, "This is going to be really hard!" In particular, the students have been challenged by learning a new topic on their own, narrowing the topic, and choosing what material to present. In addition, it has been challenging for them to determine the level of their audience and to tailor a presentation to that level. While these skills can be critical in the "real world," they are often overlooked in the undergraduate experience. We believe the outreach format can successfully target and enhance these skills.

Since each group is required to develop its own survey, no standardized results can be reported here. Each group did have to survey the teachers and students on the effectiveness of their presentation, however, and in all cases the surveys indicated the students' understanding of the topic had significantly improved. They also indicated that they had a better understanding of what chemical or biochemical engineers do.

An unexpected outcome for the UMBC students has been an increased pride in what they are doing and a sense of accomplishment. As a result of returning to the high school setting, many students have an increased awareness of how much they have learned and how far they have come during their undergraduate experience. They often speak with pride about their impending graduation and future plans for work or graduate school. In one case, at the end of a presentation three group members described their plans to pursue PhD degrees (two at M.I.T. and one at Georgia Tech). Quite unexpectedly and without prompting, the class of thirty high school students stood up and applauded. After the presentation, the group members expressed pride at what they had accomplished and expressed an understanding for the first time that they were role models for the high school students.

Providing role models to high school students has been an ongoing goal for the outreach projects. In our experience, the high school students have been very interested to learn more about the experiences of the undergraduates. In particular, UMBC attracts a significant pool of highly talented minority students (graduating classes in chemical engineering have averaged 47% minority students and 47% women in the last three years). We believe that these students in particular project powerful images to young high school students. It is not unusual to hear the high school students comment, "You don't look like engineers." We believe that this type of direct contact can powerfully combat stereotypical images of the engineering profession.

## ACKNOWLEDGMENTS

We would like to thank Dr. Michael Sierks, Arizona State University, for his input into the initial concept for the outreach projects. ❒

# LAB-BASED UNIT OPERATIONS IN MICROELECTRONICS PROCESSING

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The semiconductor industry has grown rapidly in the last three decades, and chemical technologies have played a central role in its continuing evolution. Historically, chemical engineering has focused on petrochemical and bulk chemical production, but more and more chemical engineers are working in the microelectronics and related industries. The most recent AIChE placement survey shows that the number of BS graduates placed in the electronics industry has increased since 1998 from 7.0% to 15.9% in 2001 (it decreased dramatically last year to 4.2% due to the economic slowdown).

The percentage of ChE graduates with advanced degrees hired into the semiconductor industry is even larger. For example, more than 25% of PhD graduates have been hired by the electronics industry since 2000.[1] Chemical engineers have the advantage of a solid background in chemical kinetics, reactor design, transport phenomena, thermodynamics, and process control that allows them to meet the challenges in microelectronics processing.

***The most recent AIChE placement survey shows that the number of BS graduates placed in the electronics industry has increased since 1998 from 7.0% to 15.9% in 2001***

Many chemical engineering pioneers in this field have recognized this symbiotic relationship[2-4] and a number of schools have started incorporating microelectronics processing into their curriculum. For the most part, however, the material tends to be presented in specialized, elective courses without a laboratory component. One common approach to provide hands-on experience is to have students make a transistor in a lab typically offered by the electrical engineering department. Students go through a series of microfabrication processes (either hands-on or observed) to build a complete integrated circuit, or a set of test transistors.

While this lab can be an exciting and successful approach to introduce the students to the field of microelectronic processing, there are some limitations. First of all, it is often taught with a cookbook approach, and second, there is limited time devoted to each process, so process analysis is usually ignored. The resulting device functionality supersedes the process engineering. Finally, not all schools have the necessary resources to offer this lab to their chemical engineering undergraduates.

A complementary approach is to incorporate the unit operations in microelectronics processing into the existing chemical engineering curriculum. An example of such an approach is the incorporation of thermal oxidation of silicon into the unit operations lab at Georgia Tech.[5] This approach can provide students with depth as well as breadth by presenting these unit operations in the context of core chemical engineering science.[6,7]

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Development of programs in this area has led to innovative and improved education practices.[8-10] A successful example is the curriculum developed by the Chemical and Materials Engineering Department at San Jose State University. The essence of their project is to abandon the traditional laboratory cookbook instruction method and create a team-oriented and open-ended laboratory where students develop the types of skills they will later use in industry. The content of their laboratory includes having students make a field effect transistor and perform open-ended experiments to improve the process.[10]

While the approach at San Jose relies on coordination between students in three different engineering disciplines (electrical, material, and chemical), at Oregon State University (OSU) we are implementing the same type of learning environment solely within chemical engineering. In this way, we can leverage off the fundamental research in microelectronics processing to develop unit operations accessible to undergraduate students based on their core engineering science background.

Integration of unit operations into microelectronics has occurred in conjunction with a transformation in the senior unit operations laboratory that began during the 2000-2001 academic year. A newly created endowed chair, the Linus Pauling Engineer, was hired from industry to identify and incorporate the highest priority professional practices in the senior lab. She serves as "project director" for this class that helps graduates become prepared for industrial practice. Professional practices are incorporated into the lab through lectures, classwork assignments, and homework assignments. Eight lectures cover project management, meeting skills, technical writing, oral presentations, safety, rational management processes (situational, problem, decision, and potential problem analysis), personality self-assessment, and conflict resolution.[11] All students complete writing assignments and oral presentations to practice the professional skill as well as to demonstrate technical understanding of the unit operation. The instructor, the student, and the student's peers assess each student's work process skills, safety performance, and team behavior.

## INTEGRATION OF MICROELECTRONICS UNIT OPERATIONS INTO THE CHE CURRICULUM

Hundreds of individual process steps are used in the manufacture of even simple microelectronics devices, but the fabrication sequence uses many of the same unit processes a number of times. A list of unit operations that are common for the fabrication of microelectronic devices, along with the curricular material related to each topic, are given in Table 1. These unit operations rely on core chemical engineering science.

We are developing unit operations modules for integration into the chemical engineering curriculum and unit operations laboratories at OSU, including plasma etching, chemical vapor deposition (CVD), spin coating, electrochemical deposition, and chemical mechanical planarization (CMP). These unit operations contain complex systems that involve interaction of many physical and chemical processes. Fortunately, there have been extensive research efforts in these areas, and many of the fundamental mechanisms have been elucidated. For example, plasma etching processes have been modeled based on the fundamental transport and reaction processes occurring within the glow discharge to understand issues of etch rate, selectivity, uniformity, and profile.[12-15] Similarly, chemical vapor deposition reactors have been modeled in analogy to porous catalysts,[16] incorporating transport and reaction processes.[17-20] Control schemes have been based on the fundamental CVD reactor models.[21] The fluid dynamics of photoresist spin coating has been modeled and studied experimentally to predict coating thickness and uniformity as a function

**TABLE 1**
**Unit Operations in Microelectronic Device Fabrication**

| *Unit Operations* | *ChE Core Courses* |
|---|---|
| Bulk Crystal Growth from Melt | Fluid Dynamics; Heat Transfer; Mass Transfer; Thermodynamics; Reaction Engineering; Process Control |
| Surface Reactions<br>Cleaning and Oxidation | Kinetics; Fluid Dynamics; MassTransfer |
| Etching<br>Plasma Etching, Wet Etching | Mass Transfer; Kinetics; Reaction Engineering; Process Control |
| Thin Film Deposition<br>• Physical Vapor Deposition<br>• Chemical Vapor Deposition<br>• Electrochemical Deposition | Kinetics; Fluid Dynamics; Mass Transfer; Heat Transfer; Thermodynamics; Electrochemical Engineering; Reaction Engineering; Process Control |
| Lithography<br>• Photoresist spin coating<br>• Photoresist baking<br>• Photoresist exposure and development | Fluid Dynamics; Mass Transfer; Polymer Rheology; Kinetics; Process Control |
| Doping and Dopant Redistribution<br>• Ion Implantation<br>• Thermal Diffusion | Mass Transfer; Heat Transfer; Process Control |
| Planarization<br>• Chemical Mechanical Polishing | Fluid Dynamics; Mass Transfer; Electrochemical Engineering; Process Control |

of spin-speed, fluid properties, and spin duration.[22-25] Similarly, fluid-dynamics-based models of chemical mechanical polishing are being developed.[26-28]

We are synthesizing the research results in the literature and applying them to the five unit operations discussed above to make them accessible to undergraduate chemical engineers. At the same time, we are reinforcing the fundamental engineering science taught in the curriculum. To accomplish this objective, we are developing both *lab based* and *classroom based* instruction.

Integration into the lab occurs through the two required unit operations laboratories (ChE 414 and 415) as well as an elective, Thin Film Materials Processing. The first quarter of the two-quarter lab sequence is highly structured and focuses on the students completing three unit operation experiments. We intend to have each student complete at least one microelectronics unit operation during this rotation. The second quarter of the senior lab course builds on the work done in the first quarter. The focus is on working independently, developing a project proposal, completing experimental work, and writing a final technical memorandum that includes recommendations for future work. The microelectronics unit operations are designed to be flexible enough so that each year the group of students has a new, unique, and creative experience. The first four unit operations were integrated into the second-quarter lab in the spring of 2002 and are described below. The unit operations experiment in chemical mechanical planarization was added in the spring of 2003.

Students who are interested in pursuing high-tech careers can obtain a transcript visible microelectronics or materials science and engineering option in the chemical engineering department. In either of these options, Thin Film Materials Processing is required. Starting in the winter of 2003, the thin films course was expanded from 3 to 4 credits to enhance the laboratory component and in the lab the students rotated through six experiments. Three experiments—plasma etching and spin coating, silicon nitride deposition, and copper electrodeposition—are based on the unit operations mentioned earlier. Students also study wet and dry silicon oxidation, have a vacuum components lab, and undergo a "virtual" lab based on the semiconductor device applets developed by Wie and coworkers at SUNY, Buffalo.[29]

In the processing labs (plasma, CVD, electrodeposition, and oxidation), students are introduced to the unit operations. For efficacy, these labs are conducted in a well-prescribed manner where the process parameters and lab procedure are given to the students. Each group runs the process at different parameter settings, and once the entire class has rotated through a given unit operation, the students are presented with the data collected from the entire class for analysis.

For example, the silicon nitride deposition is operated at three temperatures and three flow rates ($NH_3$ rich, stoichiometric, and $NH_3$ lean). Students measure growth rate, film thickness (from which they calculate den-

**Reactor Design**
**ChE 432 Detailed Design Project - LPCVD Silicon Nitride**

Spring, 2002

**Introduction**
This project is designed for senior students in ChE 432 who are interested in experiencing a detailed design/simulation project in microelectronics processing. The topic selected is LPCVD (Low Pressure Chemical Vapor Deposition) that has been used for the deposition of silicon nitride on silicon wafers in the process for producing ICs.

**Requirements**
Students who work on this project are required to

1. Propose a design idea for a piece of equipment that handles 200 silicon wafers of 300mm in diameter
2. Develop a model to simulate the performance of the equipment
3. Determine proper operating conditions, *i.e.*, temperature distributions, operating pressure, feed rates, and reaction time for controlling the deposit thickness at 1000Å with variations across wafers and from wafer to wafer within ±3%.

***Figure 1.*** *The CVD senior design-project assignment.*

**TABLE 2**
**Implementation Grid of Microelectronics Unit Operations and ChE Classes**

| *Course* | *Plasma Etching* | *Chemical Vapor Deposition* | *Spin Coating* | *Electro-chemical Deposition* | *Chemical Mechanical Polishing* |
|---|---|---|---|---|---|
| Materials Balances | | X | | | X |
| Energy Balances | | | | | |
| Chemical Process Statistics | X | | | | |
| Thermodynamic Properties & Relationships | X | | | X | |
| Phase and Chemical Reaction Equilibrium | | X | | X | X |
| Applied Momentum and Energy Transfer | | | X | | |
| Chemical Engineering Laboratory I | | X | X | X | |
| Chemical Engineering Laboratory II | X | X | | X | X |
| Chemical Plant Design I | | | | | X |
| Chemical Plant Design II | | X | | | |
| Chemical Reaction Engineering | X | X | | X | |
| Thin Film Materials Processing | X | X | X | X | X |
| Polymer Engineering and Science | | | X | | |

sity), and index of refraction for their particular run. Then they look at the entire data set of the (nine) groups in the class to explore the effect of temperature and concentration on nitride deposition.

The vacuum lab gives students experience with constructing a vacuum system and shows them the basic components in any vacuum system, including pumps, pressure measurement, mass flow control, and different types of flanges. The virtual lab provides a workshop on carrier physics, crystal structure, and integrated circuit processing with subtractive pattern transfer. For more detail, go to <jas2.eng.buffalo.edu/applets/>.

Classroom examples are developed based on the labs as well as the research literature. Each of the four unit operations listed above will include at least two example exercises or homework problems to be integrated into a core chemical engineering science or design course. By integrating the technical content in this manner, the future process engineers in this industry will be able to draw upon core fundamentals as they go about problem solving. A grid of target courses for classroom integration is given in Table 2. Those marked with an "x" represent targeted courses. For example, the design problem offered in Process Design II in the spring of 2002 is shown in Figure 1.

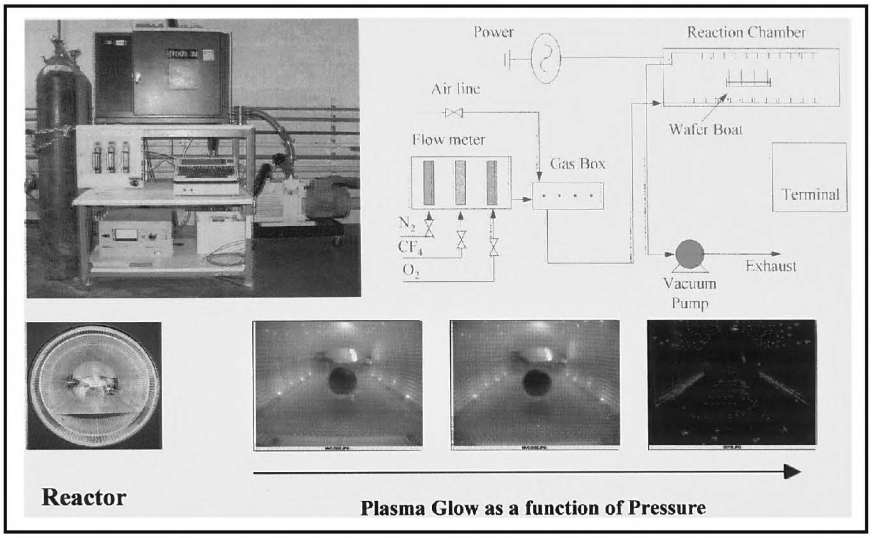



***Figure 2.*** *Plasma barrel etcher and schematic.*

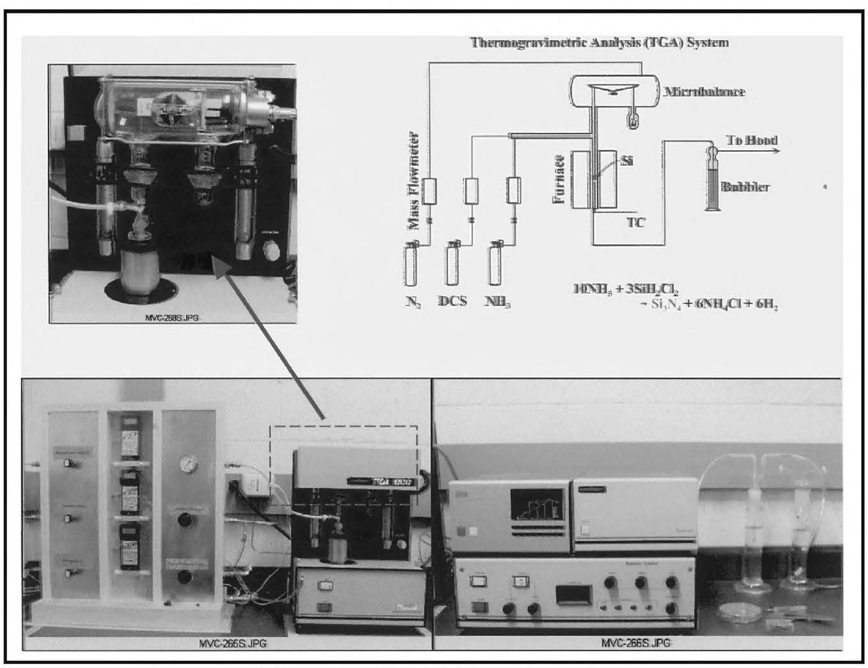



***Figure 3.*** *Silicon nitride CVD reactor and schematic.*

## ■ *Plasma Etching*

Glow discharge plasmas are used for a variety of surface manufacturing applications, especially in integrated circuit manufacturing where up to 30% of all process steps involve plasmas in one way or another. A plasma barrel etcher has been incorporated into the projects in the second-quarter lab and the thin film course. This plasma barrel etcher unit and supporting systems were donated by Intel (see Figure 2). In the barrel etcher, ion bombardment is suppressed since the substrate holder is contained within a Faraday cage. Thus, the etch rate depends on the concentrations of free radicals that react at the substrate surface. Uniform etching only occurs when mass transport to the surface is much greater than the inherent reaction rate. By measuring the etching rate as a function of radial position, the relative importance of mass transfer to surface reaction can be backed out. The variation of etch rate as a function of the sample radius allows students to interpret etch data in terms of fundamental chemical engineering principles (*e.g.*, transport and reaction). Industrially, obtaining a uniform etching rate is also a central problem in plasma etching reactor design.

Other examples of student lab experiments include: finding optimal process settings for etching polyphenylene oxide materials using $SF_6$ and $O_2$ feed gases by using Design of Experiments (DOE) and analyzing the problem using a well-mixed reactor model; the effects of wafer spacing on etch rate; the effect of the number of substrates, *i.e.*, loading, on etch rate; and transient analysis of temperature effects on the etching rate.

In the spring of 2002, two groups of three students each were given an assignment to develop a process that minimized interwafer, as well as wafer-to-wafer, variation in etching rate. This lab included several processes to pattern and etch a wafer, including cleaning, spin coating, photolithography, and plasma etching. Additionally, students developed their own artwork to serve as a mask in photolithography. The experimental design focused on etching parameters, however, while the other processes were unchanged. One group did a 2x2 design in which they varied pressure and wafer spacing while the other group varied power and spacing. Thickness measurements before and after etching were made using a profilometer. The plasma reactor does not have temperature control. Thus the temperature rises as power is input during the etch process. This facet provided a good opportunity to use chemical engineering analysis to understand the system. The group was advised to record temperature during the process, but needed faculty help to develop an averaging method based on the Arrhenius expression for the activated process. The plasma lab analysis can be found at <http://che.oregonstate.edu/research/LBUOMEP/>.

## ■ *Chemical Vapor Deposition*

In this module, the gas-solid reaction kinetics are elucidated through real-time rate measurements using a modified thermogravimetric analyzer (TGA)(see Figure 3). Students can measure an increase in mass of the silicon wafer sample specimen (about 10 mm by 20 mm) with time, resulting from the deposition of silicon nitride at different reactant concentrations and reaction temperatures at atmospheric pressure. Inert argon is mixed with the two gaseous reactants (ammonia and dichlorosilane). Since the reaction is at atmospheric pressure, as opposed to vacuum, students must account for the effect of resistance to diffusion through the gas film on the silicon surface and find ways to eliminate the mass-transfer effects. In this context, they were asked to discuss the difference between the low-pressure CVD and atmospheric-pressure CVD. The kinetics obtained using the modified TGA were integrated into the senior capstone design course via designing a CVD reactor and simulating its performance for achieving uniform film thickness. Students were challenged to develop a simple mathematical model that incorporates the fluid flow, diffusion, and reaction that take place simultaneously. Students used their model to predict the growth of silicon nitride films on two hundred 300-mm wa-

a

b

**Spin Coating of Photoresist—Fluid, Mass, and Heat Transfer Problems**

Spin coating of photoresists is found in most photolithography steps in microelectronics processing. One general formulation of photoresist involves a low molecular weight polymer dissolved in a low boiling point (high vapor pressure) solvent at various concentrations (typically 60-80wt% polymer). The photoresist is spun onto a *silicon wafer* (currently 6-, 8-, or 12-inch nominal diameter) at various *spin speeds* for various *spin times*. The material properties (such as the viscosity) change with time as the solvent evaporates. Typical coating thickness values after spinning are 1-5μm, with residual solvent in the film. Residual solvent removal is achieved by a high-temperature "baking" step. There are several interesting and challenging transport problems that can be derived from this process that are suitable for undergraduate courses. These problems are not "plug and chug" but rather require that the students reason through the physical situation and apply simplifying assumptions to arrive at reasonable *models* (see two recent textbooks by Middleman[3,34,35] for examples).

**Fluid Mechanics Problem** • In the industrial setting, the coating process typically begins by dispensing a "puddle" of liquid at the center of a rotating wafer. The puddle very quickly spreads to the edges of the wafer. The spreading of a "viscous drop" has been presented by Middleman.[34, p. 272] The analysis most relevant to the spin coating problem presented here was first studied by Emslie, et al.,[22] where the author assumed that the film was initially at a uniform thickness across the entire wafer and that the fluid was Newtonian and nonvolatile. These assumptions led to a rather simple model for film thickness (H) in terms of spin speed ($\omega$), spin time (t), initial film thickness (Ho), density ($\rho$), and viscosity ($\eta$): $H = Ho\,(1 + 4\rho\omega^2 Ho^2 t/3\eta)^{-1/2}$. The students can be given typical values of **spin speed** (1000-5000 rpm), **spin time** (30-120 sec), **initial film thickness** (Ho ~ 100μm), **density** (800 - 1000 kg/m$^3$), and **viscosity** (10 - 1000 mPa-s) to generate curves of film thickness (H) vs. time (t). These calculations can be used to point out the relative importance of the various parameters in a spin coating application.

**Mass and Heat Transfer Problem** • The transient mass transfer problem for the rate of removal of solvent from the film during the spin coating process is a difficult problem to solve. Once again, the students are challenged to make simplifying assumptions, as was done with the fluid mechanics problem, to arrive at models that can be tested. In addition to the information given above, the students are told that there must be **90% removal of the solvent** in the spinning step. One approach to solving this problem is to start with the assumption as was made above of a uniform initial coating thickness (Ho ~ 100μm). The problem then reduces to an unsteady-state mass transfer problem, similar to solvent evaporation from a polymer film described in Middleman.[35, p. 128] The students must identify the simplifying assumptions of no internal convection, one-dimensional diffusion (thin film), and rapid exterior convection due to the high speed spinning, and *comprehend the limitations of these assumptions*. For instance, if the film is spinning at high speed and thinning, how can there be no internal convection? The residual solvent removal in the "baking" step can be modeled in a similar manner.

***Figure 4.*** *(a) Spin coater, and (b) spin coating classroom example.*

fers, varying with temperature-profile settings, reactant feed rates, and operating pressures.

## ■ Spin Coating

Spin coating has come into widespread use in the microelectronics industry for coating the photoresists used to define patterns in the films on a silicon wafer. It will also be used in future technologies as polymers become incorporated as dielectric materials. The underlying principles of spin coating (fluid flow, fluid properties, surface phenomena) and the process itself make it a natural for inclusion in the chemical engineering curriculum. The precursors to coating, surface wetting, and adhesion are also classical problems. The spin coating of solid substrates with various viscous liquids and surface wetting phenomena (surface tension, contact angle, viscosity) is done using a "state-of-the-art" programmable laboratory spin coater from Specialty Coating Systems (SCS Model P6700) (see Figure 4a) and highly polished oxide-coated 6-inch wafers. Examples of engineering projects include: experiments on viscous, Newtonian liquids to test the Emslie model and compare data to published spin coating results for Newtonian liquids;[22] coating photoresist on silicon wafers as the first step in the photolithography process.

This unit process has been used as a project in several outreach activities. Classroom examples for momentum, heat, and mass transfer are given in Figure 4b.

## ■ Electrochemical deposition

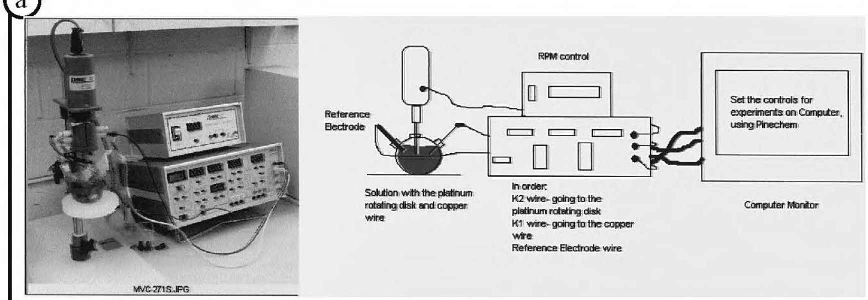
The electrochemical deposition system includes a computer-controlled bipotentiostat, PineChem software, rotator, electrodes, and a standard voltammetry cell (see Figure 5a). A variety of experiments could be designed using this system. Examples of such experiments are

- *Diffusion coefficient determination by rotating electrode cyclic voltammetry*
- *Measurement of the kinetics and the flux of copper ions to an electrode surface by means of rotating ring-disk electrode*
- *Study of mass transfer using rotating electrodes*
- *The effects of additives on deposition rates*
- *Leveling effects of additives*
- *Superfilling phenomena*
- *Resistive seed effect*

In the spring of 2002, the student team was taught how to use this system by going through a "cookbook" experiment using cyclic voltammetry and the rotated disk electrode to characterize the redox reaction of potassium ferricyanide solution. After the training, they were asked to propose an experimental plan using this setup. They decided to study the copper mass transport using different copper electrolytes ($CuCl_2$ and $CuSO_4$) and the influence of a sulfur-containing additive (thiourea). The experiments were performed using acid copper solutions prepared from $CuCl_2$ and $CuSO_4$ with and without thiourea. The electrochemical reactions were characterized by sweeping the voltage and measuring the current. The boundary layer thickness was controlled by the rotating speed of the working electrode and the Levich equation was used to determine the diffusivity.

A classroom example based on copper electrodeposition is given in Figure 5b. In addition, many interesting laboratory problems on copper plat-

a




b

**ChE 312 Phase and Chemical Reaction Equilibrium**

Electroplating is used to deposit the copper metal lines in integrated circuit processing. In this case, dissolution of a copper anode is used to provide cupric ions for reaction, *i.e.*, the solid copper-cupric ion reaction is used both at the anode to generate cupric and at the cathode to grow the resulting film. Please calculate the minimum electrode potential to achieve copper growth for the following cell

$Cu(s)|CuSO_4(l, 0.1M)||CuSO_4(l, 0.01M|Cu(s)$

using (a) ideal solution model, and (b) modified Debye-Hückel theory

A number of concepts in chemical reaction equilibrium can be taught through this classroom example, including

- How to write electrochemical reactions
- How to incorporate the concept of electrical work into the equilibrium formulation. How to calculate the electrochemical potential from the Gibbs energy
- How to estimate activity coefficients for ionic species in an electrolyte solution (Debye-Hückel theory)

***Figure 5.*** *(a) Copper electrodeposition reactor and schematic, and (b) electrodeposition classroom example.*

ing can be found in a manuscript by Talbot.[30]

■ ***Chemical Mechanical Polishing***

The experimental setup of a bench-scale CMP module is shown in Figure 6a. The setup is adopted from the research literature,[31-33] which has been useful in understanding the reaction mechanisms during CMP. In this setup, the copper CMP will be studied in a three-electrode electrochemical cell by using a copper-plated rotating disk electrode. The polishing downward force will be measured by a balance, which supports the entire electrochemical cell. The DC electrochemical measurement will be carried out by using a potentiostat. A variety of experiments can be designed to study the copper CMP process. For example, the effect of $HNO_3$ or $NH_4OH$ on the chemical etching mechanism, the effects of additives (*e.g.*, inhibitor, oxidizer), the relation between downforce, and removal rates through the Preston equation. The Preston equation[31] relates removal rate to driving force in the same way that mass transfer coefficients relate mass transfer to driving force. Studies on the bench-scale system will be scaled up to the industrial-scale system shown in Figure 6b.

## OUTREACH

Three modules, including plasma etching, spin coating, and copper electrodeposition, were implemented in the outreach programs that are currently in place in the chemical engineering department: 1) Summer Experience in Science and Engineering for Youth (web site at <http://www.che.orst.edu/SESEY/>), and 2) the Saturday Academy and Apprenticeships in Science and Engineering program (web site at <http://www.ogi.edu/satacad/ASE/index.html>). Each of these programs has a somewhat different focus, but share several common underlying themes: exposure of high school students to careers in science and engineering through research experiences and other opportunities that are typically not available to them in the high schools; recruitment and retention of underrepresented groups (girls and ethnic minorities) into science and engineering; and a goal of increasing the technological literacy of high school students so they can be empowered to make educated career choices.

## ASSESSMENT PLAN

The measurable student outcomes for each unit operation will include

- The students will demonstrate communication skills. *For example, they will be required to master written and oral reports.*
- The students will demonstrate technical synthesis in each of the unit operations. *For example, in CVD they will use kinetic data in reactor design problems.*
- The students will demonstrate professional practices. *For example, they will be required to demonstrate project planning before performing experiments.*

Each of these outcomes will be assessed by three methods:

- Student self-assessment and peer-assessment, *e.g.*, survey of effectiveness of educational materials.
- Evaluation of student performance by instructors.
- Feedback from industrial constituency, *e.g.*, survey of student performance from industrial employers.

## SUMMARY

The integration of microelectronics-based unit operations into the chemical engineering curriculum at Oregon State University has been presented in this paper. We are developing both lab-based and classroom-based instruction. Five new unit operations are being implemented in the senior lab, including plasma etching, chemical vapor deposition, spin coat-

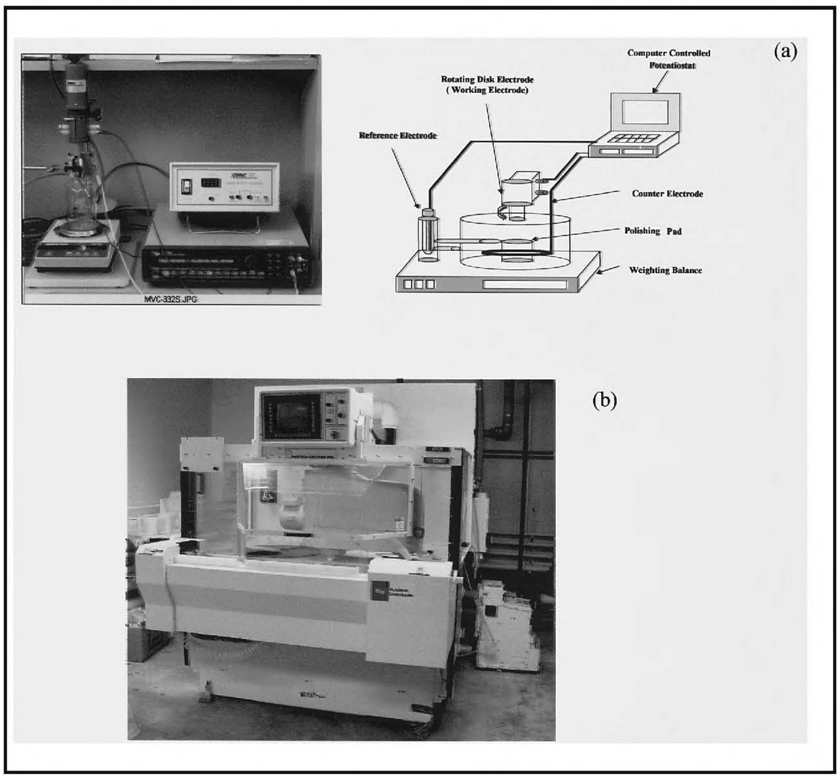



***Figure 6.*** *(a) Bench-scale CMP and schematic (b) industrial-scale CMP.*

ing, electrochemical deposition, and chemical mechanical planarization. These labs are also included in an elective course, Thin Film Materials Processing. Classroom examples are being integrated into chemical engineering core courses. In addition, the students are learning professional practices that include effective oral and written communication, project planning, time management, interpersonal interaction, teamwork, and proactive behavior. These modules are also being used effectively in outreach programs.

## ACKNOWLEDGMENTS

The authors are grateful for support provided by the Intel Faculty Fellowship Program and the National Science Foundation's Course, Curriculum, and Laboratory Improvement Program under grant DUE-0127175. We also acknowledge the Dreyfus Special Grants Program (SG-97-075), OSU Precollege Programs, Kelley Foundation, and Bridges Foundation for their support of the outreach program Summer Experience in Science and Engineering for Youth, and Pete and Rosalie Johnson for the endowment of the Linus Pauling Engineer. SEH America graciously donated the highly polished and oxide-coated 6-inch silicon wafers. Helpful discussions with Emily Allen of San Jose State University and Chuck Croy of Intel Corporation are greatly appreciated. The authors would also like to acknowledge the reviewers for the critical reading and suggestions they made regarding this paper.

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# INCORPORATING EXPERIMENTAL DESIGN INTO THE UNIT OPERATIONS LABORATORY

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Typically, the unit operations laboratory is one of the least-liked classes in the chemical engineering curriculum at the University of Missouri-Columbia. Unfortunately, many students view laboratory experiments as unfocused and haphazard investigations of various types of equipment that provide mere busy-work during their demanding course load. Although the concepts investigated are useful for all students, most of them think that the circumstances behind the investigations are not representative of those typically encountered in industry. In an attempt to provide the students with a more industrially meaningful experience when performing an experiment in this class, design-of-experiment (DOE) techniques have been combined with one classic unit operations experiment to present a more "real-world situation" to the student.

DOE is the application of screening designs and statistical sampling to obtain a desired result, such as minimizing the number of experiments necessary to obtain the answer to a problem or minimizing the variance of estimated coefficients obtained through regression to a model that predicts the output from some system. The first result above affects quantity of effort, which is directly related to cost, while the second affects accuracy of the result. Therefore, DOE is useful in industrial settings as a powerful tool that effectively reaches a compromise between cost and accuracy so an informed decision can be made.

A designed experiment tests how changes made to chosen input variables for a process or system affect some output response. Experimental design methods play an important role in process development and improvement. In-depth knowledge of the process is not required to make improvements in the process when using this approach—a statement that was confirmed in class by multiple students who had industrial co-op assignments where such experiments were performed.

## TEACHING OF EXPERIMENTAL DESIGN

Three class lecture periods are scheduled for teaching the basics behind an effective DOE approach, including statistical and error analysis, blocking, replication, randomization, screening designs, full- and half-factorial experimental design, and central composite design. The material is elementary enough that each student can easily understand how DOE works and complements the coursework covered by students who have taken the elective course "Experimental Design and Statistical Quality Control for Chemical Engineers." Additional material detailing the experimental design approach and factorial analysis can be found in the text by Box, Hunter, and Hunter [1] used for this course as well as in other widely used sources.[2,3] For the sake of those who are unfamiliar with DOE principles, however, and to adequately introduce the material used for the sample analysis for the experiment presented later, the class material covered for a three-factor, two-level, half-factorial experimental design is discussed below.

In many cases, a large number of variables exist that can have an effect on a system. The main effect is a change in the response that results from a change in level from a low value to a high value of the variable and is calculated as the average of the difference between all the responses at the high value of a variable and those at the low level of that variable.

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As seen in Figure 1, the eight trials indicated by all the gray and black points are required to perform a two-level, three-factor, experimental design that effectively models the main effects and interaction effects associated with changes to the three-input variables. Equations can be written to calculate the main effects and interaction effects between variables when three or more variables are being investigated. The greater the magnitude for a calculated main or interaction effect, the more significant the effect on the response that factor exhibits.

When a large number of potential input variables exists, the system has high variability, or additional factor levels need to be studied due to nonlinear relationships, the number of experiments that are required to completely understand the system can become quite large, causing a large time commitment for optimization of the system being investigated. Experimental design techniques can be used to maximize the amount of information obtained from a reduced number of experimental trials. When high accuracy is not necessary, a half-factorial experimental design can be performed, which requires half the amount of the $2^n$ trials ($2^{n-1}$) needed for the full-factorial experimental design. Therefore, for the half-factorial three-factor, two-level design, four trials are performed at operating conditions indicated by the black points in Figure 1 or at the complementary half-fraction conditions indicated by the gray points. Conducting trials at either of these sets of four operating conditions gives a balanced design necessary to determine the optimum. The equations used to calculate the main effects for the three input variables become

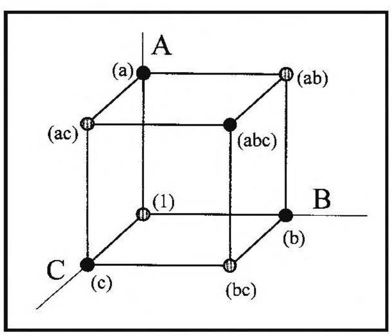


*__Figure 1.__ Geometrical representation of three-factor, two-level experimental design strategies. A full-factorial experiment is achieved using trials performed at all the black and gray points, while a half-factorial experiment is achieved by performing trials at either the black or the gray points. Letters in parentheses indicate results obtained for an output response from a trial performed at a high value for each variable indicated and a low value for any variable not indicated. For example, trial (ac) indicates the output response measured when factors A and C were set at their high (+) value and factor B was set at its low (-) value.*

$$\text{Main Effect of Variable A} = 2\beta_1 = \left\{\left[\frac{(ab)+(ac)}{2}\right]-\left[\frac{(1)+(bc)}{2}\right]\right\}$$
$$\text{or}\left\{\left[\frac{(a)+(abc)}{2}\right]-\left[\frac{(b)+(c)}{2}\right]\right\} \tag{1}$$

$$\text{Main Effect of Variable B} = 2\beta_2 = \left\{\left[\frac{(ab)+(bc)}{2}\right]-\left[\frac{(1)+(ac)}{2}\right]\right\}$$
$$\text{or}\left\{\left[\frac{(b)+(abc)}{2}\right]-\left[\frac{(a)+(c)}{2}\right]\right\} \tag{2}$$

$$\text{Main Effect of Variable C} = 2\beta_3 = \left\{\left[\frac{(ac)+(bc)}{2}\right]-\left[\frac{(1)+(ab)}{2}\right]\right\}$$
$$\text{or}\left\{\left[\frac{(c)+(abc)}{2}\right]-\left[\frac{(a)+(b)}{2}\right]\right\} \tag{3}$$

The coefficients for all interaction effects are set to zero in the process model. When performing a half-factorial experiment, interaction effects must be assumed to be negligible since Eqs. (1) through (3), which are used to determine the main effect for each of the three input variables, are identical to the equations used to determine the interaction effect between the other two variables. Proving that these equations are indeed the same makes an excellent exercise for those students who have not had any previous experience with DOE.

For this design's mathematical model, the origin for the model is relocated to the center of the investigated three-dimensional volume pictured in Fig. 1 and measurements for factors A, B, and C are normalized so that a value of +1 for A, B, or C corresponds to that factor's value at the level where the factor was the maximum value investigated, and -1 corresponds to that factor's value at the level where the factor was the minimum value investigated. Therefore, the model becomes

$$\text{Output Response} = \beta_0 + \beta_1 A + \beta_2 B + \beta_3 C + \text{error} \tag{4}$$

where $ß_0$ is the average of the four completed trials and the error is determined from replicates of trials completed at the conditions of the new origin or at the conditions of at least one of the four completed trials (see Box, Hunter, and Hunter for more in-depth analysis[11]). This relationship can also be determined via multilinear regression analysis conducted using various statistical and mathematical software.

## GUIDELINES FOR EFFECTIVE INCORPORATION OF DOE

Not all laboratory experiments are adequate candidates for successful incorporation of the DOE approach. When determining if a current experiment has the potential for inclusion of the DOE approach, the following factors should be considered:

- Experimental trials should not take a significantly large amount of time to complete. One or two trials should not take the entire laboratory period unless multiple days will be given to complete the necessary trials.
- Effort required to convert the system to perform additional trials with the new input variables should be minimized to keep the students interested in the process.
- A variety of potential input variables should exist such that each student group can potentially investigate different variable combinations and avoid repetition. Including variables that have little-to-no effect on the process keeps the exercise realistic.
- A maximum, minimum, or discontinuity in the output response should not exist when each input variable is changed over the range of values given to the students when only two-level design strategies are used. Students may become confused in their analysis when these types of behavior exist within the range being studied, especially if the result contradicts theory.
- When time does not permit a full-factorial experiment to be performed during the assigned laboratory time, interaction effects between variables should be small or negligible. Since this is an introductory exercise for the students, strong interaction effects should not complicate the analysis.
- A highly variable system requires a sufficient number of trials to adequately determine the error. If only a limited number of trials can be performed, however, the trials should be highly reproducible so that experimental errors are minimized. In the case discussed here, performing trials for determining the error component to the model is not possible during the allotted laboratory time; therefore, students are required to speculate on the error component in their report.

It is of the utmost importance that, when incorporating the DOE approach into a current experiment in the laboratory, the original technical objective of the experiment must still be achieved while meeting each of the conditions listed above. Otherwise, the equipment may be viewed as a "black box" for generating data and the original focus of the experiment is replaced by a focus on DOE analysis.

## EXPERIMENTAL SETUP

A unit operations experiment titled "Residence Time Distribution for Stirred Tanks in Series" was chosen for incorporating the DOE approach into the curriculum. A diagram of the apparatus used for this experiment is shown in Figure 2. It consists of three Plexiglas stirred tanks in series, where the tank outlets are overflows to the next tank or to drain. The third tank can be physically changed between two different tank sizes (3.70 or 7.15 L). Stirring speed is adjusted using speed controllers, which control the percentage of power supplied to each motor used for stirring the solution in each tank.

At the start of the experiment, tank #1 contains an initial salt concentration (Morton, kosher). Each tank is fitted with a 10 kΩ thermistor conductivity cell (Cole-Parmer Model #U-19500-00) connected to a digital readout (Cole-Parmer Model #U-19300-00), which is used to measure and display the conductivity near the outlet of each tank. Conductivity is measured on a scale of 0-10 mS and is correlated to the salt concentration using a student-generated calibration curve obtained prior to performing the first trial. The concentrations determined from the time-dependent conductivity measurements are used to determine the mean residence time for each tank in the series.

Distilled water is fed from a large feed tank to the bottom of tank #1 using a pump. A rotameter located between the pump and tank #1 is used to regulate the flow rate of distilled water to the system. A "T" configuration of valves located prior to the entrance of tank #1 allows for the option to bypass the series of tanks in order to establish a consistent flow rate prior to introduction to the tank. A LabView-based data acquisition "virtual instrument" (VI) is used to display to screen and record to file the conductivity measurements as a function of time. Data analysis used to determine mean residence time is performed using the material in Chapter 13 of

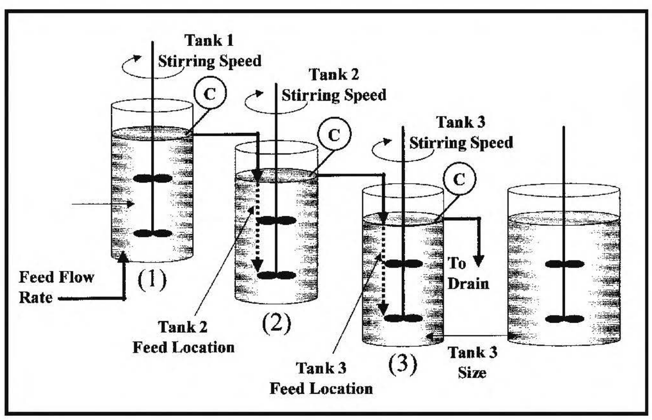


*Figure 2. Diagram of the apparatus for the "Residence Time Distribution for Stirred Tanks in Series" laboratory. The eight potential input variables that could be investigated are indicated in the figure. The symbol "©" indicates the location of conductivity probes in the stirred tanks.*

*Elements of Chemical and Reaction Engineering* by Fogler[4] and will not be presented here.

## INCORPORATION OF EXPERIMENTAL DESIGN

The original objective for this lab experiment was to determine the residence time distribution (RTD) for each tank in the series from *one* set of experimental data, which on average takes between 30 and 45 minutes. The objective for the lab experiment was modified to incorporate experimental design into the procedure so students perform additional analysis on how changes to various input variables affect their specific output response. The students were also able to see how these changes affected the mean residence time and the residence time distribution for the four trials investigated, which remains the main objective for the experiment. In this way, students play an active role in determining the direction in which the experiment proceeds, while the original technical objective of the experiment is still achieved.

Since the results from this experiment are typically presented in an oral presentation, the objective for each group performing the experiment is different, to avoid duplicate presentations and keep the students involved in the presentations. Examples of two objective statements given to groups are:

> ***Objective 1:*** *As the head engineer at Max Product Chemical Company, you are required to determine which operating conditions would allow for the shortest amount of time for the maximum product concentration to be released to the downstream separator (from tank #3). To accomplish this, an initial product concentration is flushed from a CSTR (tank #1), using distilled water, into a second, and ultimately, a third tank before heading to the separator located in a remote part of the plant. For this experiment, you will use salt to simulate the product as it travels through the series of stirred tanks. Note: The initial salt concentration in tank #1 can be varied.*

> ***Objective 2****: As the lead engineer in the chemical waste group at Enviromate Industries, you are required to determine which operating conditions would allow for the lowest maximum concentration of a toxic substance to be released from the plant (from tank #3). To accomplish this, the waste stream undergoes dilution in a series of three tanks. For this experiment, you will use salt to simulate the toxic substance as it travels through the series of stirred tanks. Note: The initial salt concentration in tank #1 is a constant.*

The premise of the experiment is that, as engineers working for a particular industry, each lab group is given a 3-hour time frame (*i.e.*, one laboratory period) in which the process equipment is available for their investigations. This period of time is meant to simulate plant downtime that is scheduled for them to obtain the necessary data from the trials to reach their assigned objective. Each group must choose three factors from the list of eight potential variables given in Table 1 in which adjustment within the given high and low limits might bring about some desired output response. Students are encouraged to review the theory and follow their own curiosity when making their choices. For example, many groups have performed experiments with the tank #2 stirrer speed set to 0 in order to investigate nonideal mixing, a behavior that is not typically covered in lectures. Since this condition is not covered in the lab procedure either, this leads them to seek additional sources to help explain their results. The students are actively involved in the design of the experiment, so they learn more about the process they are investigating.

Since the experiment is performed in a fixed three-hour time period, students are unable to perform a complete two-level full-factorial experiment in the allowed timeframe and must perform a half fraction of the two-level full-factorial experiment (a total of four trials), making relevant assumptions concerning interaction effects in order to rank the effectiveness of the three chosen parameters toward achieving the desired response.

**TABLE 1**
**Operating Conditions Available for Potential Input Variables for the "Residence Time Distribution for Stirred Tanks in Series" Experiment**

| *Input Variables* | *Original Operating Conditions* | *Low Level* | *High Level* |
|---|---|---|---|
| Feed flow rate | 0.3 gal/min | 0.3 gal/min | 0.5 gal/min |
| Initial salt concentration | 6 g/L | 4 g/L | 6 g/L |
| Tank #1 stirring speed setting[a] | 20 | 20 | 50 |
| Tank #2 stirring speed setting[a] | 10 | 0 | 10 |
| Tank #3 stirring speed setting[a] | 40 | 20 | 40 |
| Tank #2 feed location | Bottom of tank | Bottom of tank | Top of tank |
| Tank #3 feed location | Top of tank | Bottom of tank | Top of tank |
| Size of tank #3[b] | 3.70 L | 3.70 L | 7.15 L |

[a] *Setting based on power-regulated percentage applied to stirrer motor.*
[b] *Tank is physically changed between two different sizes.*

The high and low levels for the potential input variables are indicated in Table 1. The groups are required to keep the input variables that were not chosen at the settings indicated by the original operating conditions.

Before developing a design, the students inspect the experimental setup to familiarize themselves with the equipment. Each lab group is required to complete an experimental design to present to the instructor prior to being cleared to perform the experiment. The presentation is required to provide an exact list of the factors that will be investigated and why, plus provide an order in which the experimental trials will be performed so a well-developed plan is specified.

Each group submits a one-page summary of their design, which typically includes a figure, and responds orally to questions concerning their design approach. Incomplete or unorganized presentation materials are to be updated and resubmitted for approval. Any failure to successfully present a design strategy before the allotted laboratory time results in forfeiture of the group to perform the experiment at that time and a penalty in their grade for having to reschedule time for performing the experiment.

## EXAMPLE SOLUTION

Sample "Objective #1" (given previously) was investigated. The feed flow rate (variable A), tank #1 stirring speed (variable B), and tank #3 volume (variable C) were chosen as the three input variables to be investigated to minimize the time needed for the maximum concentration to leave tank #3. The output response that was measured was time measured in seconds. Table 2 gives the experimental conditions and output responses for a half-factorial experiment that was performed for trials represented by the gray points given in Figure 1. Using Eqs (1) through (3) to solve for the main effect for each variable gives $\beta_1 = -78.5$, $\beta_2 = +11.5$, and $\beta_3 = +41.0$. Taking the average of the time needed to reach the maximum concentration in tank #3 for the four trials gives a value for $\beta_0$ of +362. Therefore, by plugging in the determined coefficients into Eq. (4), the model for determining the time in which the concentration in tank #3 is a maximum becomes

$$\text{Time (in seconds)} = 362 - (78.5 \cdot A) + (11.5 \cdot B) + (41.0 \cdot C) \qquad (5)$$

For this particular investigation, the allotted time did not allow for replicates to be performed, so the error term could not be determined. Students are required to address this issue when they are only able to complete four trials during the laboratory period.

Ranking the chosen input variables in terms of importance shows that, over the given range available for each variable, changes in the feed flow rate had the greatest effect on the output response, while changes in the stirring speed for tank #1 had the smallest effect. Increasing the size of tank #3 and the stirring speed for tank #1 had a positive effect on the time, while increasing the feed flow rate had a negative effect on the time. Therefore, the model equation given in Eq. (5) clearly shows that, in order to reduce the time required to elute the salt from tank #3, the system should be operated at a high level for the feed flow rate, while operating at a low level both for the size of tank #3 and for the stirring speed in tank #1. It is important to note that these optimum operating conditions were determined without obtaining data from that specific set of operating conditions.

By looking at the experimental residence times determined for each of the experimental trials investigated, given in Table 2, one sees that the ordering of the residence times follows that of the elution times for these trials. Therefore, the original objective of determining the residence time distribution for the system of three tanks in series remains intact and the role of residence time can be used in the analysis of the objective.

**TABLE 2**
**Experimental Conditions and Output Responses for Half-Factorial Experiment Investigating Feed Flow Rate, Tank #1 Stirring Speed, and Tank #3 Volume**

| *Trial* | *Feed flow rate (gal/min)* | *Tank #1 stirrer setting* | *Tank #3 volume (L)* | *Elution time[a] (s)* | *Residence time for system[b] (s)* |
|---|---|---|---|---|---|
| (1) | 0.3 | 20 | 3.70 | 388 | 544 (586) |
| (ab) | 0.5 | 50 | 3.70 | 254 | 357 (352) |
| (ac) | 0.5 | 20 | 7.15 | 313 | 454 (461) |
| (bc) | 0.3 | 50 | 7.15 | 493 | 714 (769) |

[a] Time needed to reach a maximum concentration in tank #3.
[b] Theoretical residence times are indicated in parentheses.

## STUDENT EVALUATION

Student comments on year-end course evaluations have been positive for using DOE in the unit operations laboratory. Overall, they found the "Residence Time Distribution for Stirred Tanks in Series" lab performed from a DOE approach to be of industrial importance, especially those who had used DOE techniques in earlier co-ops and internships without exactly knowing that they were using these techniques. Course evaluations indicated that the DOE approach used in the laboratory was "interesting" and "useful." In fact, one group immediately applied their new knowledge of experimental design in a subsequent lab experiment.

In informal discussions, students expressed their enjoyment of the opportunity to choose their own pathway for the experiment based on the outlined conditions set forth by the specific objective. The report grades associated with analysis and discussion of the results for this experiment were consistently one of the highest of the semester, presumably due to the students being more actively involved in the up-front preparation of the laboratory procedure followed to achieve the objective and the subsequent analysis.

Future assessments will quantify the success of this approach by surveying the students on the following goals, where students

- *Recognize applicability of DOE in other labs and, most especially, its potential usefulness in future career endeavors.*
- *Have a better understanding of how to efficiently optimize a system.*
- *Appreciate how DOE can enhance the understanding of how changes to input variables affect a process.*

## CONCLUSIONS

Incorporation of design-of-experiments techniques in the undergraduate unit operations laboratory provides students with an industrially useful approach to test how improvements can be made to an existing system without intimate knowledge of how the process works. Incorporation of DOE into current laboratory experiments is relatively simple, provided the experimental trials do not require a significant amount of time to perform or modify from trial to trial and that the original objective of the laboratory is not diminished. Students are receptive to performing experiments using DOE since the industrial significance of this approach is high and has the potential to be used in future career endeavors.

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# PASSING IT ON

## A Laboratory Structure Encouraging Realistic Communication and Creative Experiment Planning

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One of the difficulties of structuring a laboratory class is how to leave problems open-ended while at the same time provide the students with enough information so they know what is expected of them and how to get started. The key goal in our effort to achieve such a balance was to create a setting where students would have

- *A realistic communication experience, including both memo writing and oral presentation*
- *The opportunity to plan sequences of experiments, including the use of statistical design of experiments*
- *An opportunity to design their own studies*

Our basic approach was to have student groups write memos to each other and to build on each other's work. This was done in the context of a one-semester unit operations laboratory course that begins with simple unit operations and builds to running and simulating distillation. It is the middle semester of a three-semester sequence of laboratories. The first laboratory is a series of bench-top heat, mass, and momentum transport experiments that includes instruction and practice in some basic statistical analysis, laboratory planning, and formal report writing. In the second laboratory, the subject of this paper, students work in our unit operations laboratory, which includes pilot-scale chemical process equipment. It includes simple systems for investigating the operation of pumps, flow in pipes, heat exchangers, and flow in packed beds, building to eventually operating and analyzing two distillation columns. Also included are experiments that teach students how to calibrate and use a gas chromatograph and experiments that measure vapor/liquid equilibrium using an Othmer still.[1]

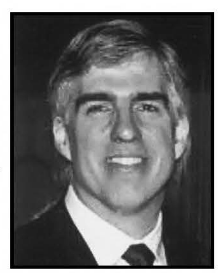
This sequential approach has been used for the last three years. There have been some variations in the details of the structure in various semesters. The specifics described here were used for the spring 2001 semester. In that semester, we ran three sections of laboratory with three groups of three students in each laboratory section. We have also used a similar setup with four groups per section.

## SEQUENTIAL STRUCTURE

The semester was organized into three distinct parts: 1) a three-week introduction to sequential experimental design using a fluidized-bed coating experiment, with the students working in small groups, 2) a seven-week set of simple unit operations experiments, where the small groups pass on their results, and 3) a four-week distillation section where larger groups work on distillation experiments, simulation, and presentation. Table 1 shows the experimental schedule for the laboratory. The three parts of the laboratory are described below.

### *Introduction to Sequential Experiments*

The initial block uses a fluidized-bed coating process based on a design from Rowan University.[2] A washer is heated

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with a heat gun and dipped in a fluidized bed of colored polyethylene powder, which melts to form a coating on the washer. The main experiment is to examine the impact of preheat temperature and dip time on coating thickness. This is measured by the change in weight of the washer. The first week is devoted to detailed experimental familiarization. Students are presented with a laboratory plan that instructs them to determine the practical operation limits of the process (*e.g.*, what is the temperature range that will produce coatings and is achievable with this equipment?), to spot check the calibrations (*e.g.*, test the thermocouple reading in ice water and/or boiling water), to develop a procedure including a written standard operating procedure (SOP), and to test the reproducibility of the system by completing three to five coatings at the same conditions. This week helps students get used to the idea that we will not be telling them all the details of how to run the equipment and shows them how they can approach a new process.

In the second week the students are expected to design and complete a $2^{4-1}$ fractional factorial experiment examining the impact of preheat temperature, dip time, washer size, and fluidization air-flow rate.[3] During this week, students are learning about fractional factorial experiments and the important idea of screening variables to determine which ones can be safely ignored.

In the third and final week of the block, students design and complete a two-variable central composite design.[4] Here they are developing a detailed second-order empirical model of the coating process. This three-step sequence allows them to get used to the idea that experiments can build from one to the next. This sequence gives them some ideas for their own sequential experiments in the next part of the laboratory and an introduction to some important statistical experimental designs. To make some of the logistics of the laboratory work, the third week of the initial block is actually interleaved with the second part of the laboratory.

***Simple Unit Operations Experiments***

Students carry out seven simple chemical engineering unit operation experiments. This is the heart of our building approach. There is only one apparatus of each type, so each group is working on a different experiment in any given laboratory session. The experiments are broken into two groups: one group of four experiments (Block II) and one group of three experiments (Block III). Experiments from a given group are run every other week to allow time for memos to be passed from one group to the next (see Table 1, particularly the every-other-week arrangements of Blocks II and III). A brief description of the seven setups is given in Table 2 (next page).

Students are given a simple introduction to each experiment. These introductions present the general nature of the unit operation, list the capabilities of the equipment, and reference sections in their texts where they can find additional information. Table 3 (next page) is an example experiment handout.

There are three groups in a section, so each experiment is run three times. The first week an apparatus is used and students are required to complete familiarization runs examining calibrations, limits of operation, procedure, reproducibility, and an initial base experiment. A memo to the instructor and to the next group that will use the equipment is due one week after the laboratory. The interleaving of experiments allows two weeks between runs so that the subsequent group has time to plan experiments based on the first group's runs. The second group to use an apparatus generally uses the most obvious capabilities of the equipment. This week ends up being the experiment we had students run when they did not pass information. They pass their results to a third group and it is responsible for finding ways to explore creative new ideas based on the previous two groups' work.

During this part of the course, each group is required to orally present their results twice. The presentations

**TABLE 1**
**Overall Laboratory Schedule Showing Interleaving of Experimental Blocks**

| *Week* | *Block* | *Group 1* | *Group 2* | *Group 3* |
|---|---|---|---|---|
| 1 | I | Fluidized Bed - familiarization and characterization | | |
| 2 | | Fluidized Bed - fractional factorial design | | |
| 3 | II | Flow in pipes and valves | Pump Performance | Heat Exchanger |
| 4 | I | Fluidized Bed - central composite design (Response Surface Methods) | | |
| 5 | II | Pump Performance | Heat Exchanger | GC |
| 6 | **III** | **Mixing** | **Packed Bed** | **Othmer Still** |
| 7 | II | Heat Exchanger | GC | Flow in pipes and valves |
| 8 | **III** | **Packed Bed** | **Othmer Still** | **Mixing** |
| 9 | II | GC | Flow in pipes and valves | Pump Performance |
| 10 | **III** | **Othmer Still** | **Mixing** | **Packed Bed** |
| 11 | IV | Total Reflux Distillation | | |
| 12 | | Simulation of distillation | | |
| 13 | | Continuous Distillation | | |
| 14 | | Presentations, Evaluations, Clean Up | | |

are video taped and the students are required to review the tape and complete a simple self-evaluation.

The process of transferring memos from one group to another is facilitated by using a web-based document storage and transfer area, which is part of the Blackboard 5 software system[5] we use at Lafayette College. We use Blackboard's group function to set up a group for each laboratory section. Students can then upload their reports to their section's file exchange area and download other students' reports.

We use several mechanisms to ensure the planned experiments are safe and reasonable. Each group is required to submit a pre-laboratory report to the instructor two class days before the laboratory. It must include an experimental plan with a complete run list, a review of the safety issues and precautions, and an SOP they will follow. The instructor reviews these reports before the laboratory meets. An instructor is also present when the experiments are run (we are an undergraduate institution and do not have graduate TAs to assist).

Some institutions may need to run more than the three or four groups that are usual for our laboratories. Having two sets of groups that are running out of sync could double the number of groups per section. One set of groups could be running the Block II experiments while another set of groups is running the Block III experiments—the next week they switch. The two sets of groups essentially function as two sections within one time block. This type of arrangement could accommodate up to eight groups per section.

***Distillation Experiments***

The last four weeks of the term the students are reconfigured into two larger groups to run experiments on our two distillation columns. In this block, each group builds on its own work. The first week they become familiar with the equipment and run it in total reflux. The second week is held in the computer laboratory and the students use the process simulator, ChemCAD,[6] to model their distillation column. They compare their results from the previous week to simulation results and predict how their column will perform in continuous operation. The third week they run the columns in continuous operation, and during the final week they deliver an oral presentation of the results of their distillation studies.

## RESULTS AND DISCUSSION

A first indication of the success of this approach was the positive performance of students in the laboratory. Providing students with only a simple introduction to the laboratories, such as is seen in Table 3, students succeeded in developing and planning these laboratories themselves.

The students' efforts during the third week of a laboratory were particularly encouraging. For time-consuming experiments such as the Othmer still, this structure allowed students to accumulate a significant body of data. For the fluid-flow experiments (pump performance, pipes/valves/fitting, and mixing), many students chose to explore the impact of different viscosities. They were able to adjust viscosity using propylene glycol antifreeze solutions. Some students compared measured pump efficiency to the temperature gain in the system for the pump experiment. For the packed bed, one group completed experiments examining the impact of temperature on the pressure drop.

In some cases, students' suggestions have led us to improve the capabilities of the laboratory. Recently, one student wanted to look at the impact of impeller diameter on pump performance. This led us to purchase a new centrifugal pump with interchangeable impellers. While this was an additional expense, it improved our facilities and made them more flex-

**TABLE 2**
**List of Experiments in Simple Unit Operations Blocks II and III**

**Flow in pipes and valves**
This is a simple fluid-flow apparatus consisting of a feed tank, pump, rotameter, and piping network. The piping network has a number of segments where pressure drop can be measured, including an orifice meter with interchangeable plates, two valves, a straight run of pipe, and a run of pipe with two elbows.

**Pump Performance**
This apparatus consists of a turbine pump and a centrifugal pump piped in parallel and instrumented to measure inlet and outlet pressure, total flow, and the power drawn by the motor.

**Mixing**
This apparatus includes three mixing tanks of various sizes with removable baffles. We use a fully adjustable laboratory mixer with torque and speed readouts. Three different types of impellers are available. The mixing of solid particles was examined.

**Heat Exchanger**
This apparatus consists of a small shell-and-tube heat exchanger with temperature sensors on all inlet and outlet streams. A steam injection heater is used to provide hot water. Simple three-way valves are used to reverse which stream is on the tube side and which stream is on the shell side. Both flowrates can be varied.

**Packed Bed**
A pilot-scale absorption bed, packed with half-inch Intalox saddles, is used for this experiment. In this laboratory, students are simply looking at the pressure drop at various air and liquid velocities. In addition, they are introduced to the concept of flooding.

**GC**
This experiment uses a Varian 3000 gas chromatograph. Students are expected to learn how to operate the equipment and to develop a calibration curve for methanol/water mixtures.

**Othmer Still**
This bench-scale equilibrium still is used to develop vapor liquid equilibrium information for the methanol/water system.

**TABLE 3**
**Example Laboratory Handout**

**Heat Exchangers**
Heat exchangers transfer heat from one fluid to another. They are essential to the operation of most chemical plants. In this equipment we will see how a simple countercurrent heat exchanger functions under various conditions and compare the results to usual design correlations.

**Equipment and Capabilities**
The heat exchanger setup has a cold tap-water feed and hot-water feed. Each stream can be fed to either the shell side or the tube side. Temperature sensors allow monitoring of both inlet and both outlet temperatures.

With this apparatus you can
- Estimate the overall heat transfer coefficient for both flow configurations (hot-water shell side and hot-water tube side)
- Look at the variation in heat transfer coefficient for various flow rates of each fluid and both flow configurations
- Look at the effect of hot stream temperature on heat transfer
- Estimate the time constant of the heat exchanger

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**Specific Requirement**
Each group should measure the overall heat transfer coefficient for several conditions and compare the result to coefficients estimated by standard correlations.

**TABLE 4**
**Results of Quantitative Questions in Survey**
*Students were asked to rate how much they agreed with the statement on a scale of 1 to 5 (5 being "strongly agree"). Results are for responses from 26 students (out of 27) who took the class.*

| | *Mean* | *Standard Deviation* |
|---|---|---|
| During Laboratory II, my ability to write a memo that clearly communicated my results to my peers improved | 4.5 | 0.65 |
| As a result of my experience in Laboratory II, I feel better able to contribute to a sequential experimental study | 4.1 | 0.63 |
| I am better able to use statistical methods to plan engineering experiments. | 3.8 | 1.07 |
| My ability to prepare and present my own experimental work improved over the course of the semester | 4.2 | 0.59 |

ible for future years.

At the end of the term, a random sample of junior-year chemical engineering students was interviewed as part of our ABET assessment process. The interviews were about their entire experience as chemical engineering students and were conducted by professors who were not their instructors. One of the questions asked was, "How have your experiences this year developed your ability to solve engineering problems?" As students responded to this question, one of the primary areas of discussion was the value they saw in this particular laboratory. They expressed satisfaction at being able to design their own experiments and felt that writing memos to each other gave them a realistic experience.

To further assess student response to this course, the students completed a written survey one year after they had been in the class. Table 4 lists the results for quantitative questions. They were asked to rate on a 1-to-5 scale how well the statement reflected their experience. Students generally felt the laboratory contributed to their ability to write memos, to their ability to contribute to a sequential study, to their ability to use statistical methods to plan experiments, and to their ability to present their work. Scores were highest for writing and lowest for statistical design of experiments. These low scores are a result of a small number of students who rated this area low. They expressed a desire for a separate course in statistics. The impact of these few students can also be noticed in the higher standard deviation.

In addition, several open-ended questions were asked that required a written response. Two of these questions are shown in Table 5. Most students mentioned some form of communication skills as both a key goal and as what was most helpful to them. For both questions, many mentioned the use of sequential experiments and statistically designed experiments. It is interesting that a quarter of the class cited the open-ended nature of the experiments as a help to their learning but seem to have missed that this was one of our goals. Almost all students mentioned at least two of the items as helpful. The results presented here are categorizations (a content analysis) of the students' written responses. That the categories correspond for the two questions shows that the communicated goals of the class and the resulting learning were connected.

Many of the specific responses to the question concerning what the students found helpful were very encouraging. Some of the things they noted were

- *The openness and freedom to design experiments that investigated your personal area of interest*
- *The ability to work on a piece of equipment that I have never seen before and learn its functionality by setting up an experiment and seeing it through.*
- *Having to force myself to answer engineering questions*

**TABLE 5**
**Response to Two Qualitative Questions**
*This table summarizes a content analysis of students' written responses to two questions.*

| *Values are the percent of respondents who included the areas below in their discussion of these two questions* | *Questions:* *What did you see as the key educational goals of the laboratory?* | *The aspects of the laboratory that were most helpful to my educational experience were...* |
|---|---|---|
| Communication skills | 68 | 63 |
| Planning sequential experiments | 55 | 33 |
| Statistical design of experiments | 50 | 17 |
| Understanding of important unit operations | 41 | 21 |
| Ability to work in teams | 14 | 4 |
| Understanding distillation | 14 | 4 |
| Ability to handle open-ended problems | - | 25 |
| *Number of students responding to question* | *22* | *24* |

*rather than following a set recipe.*

- *I actually realized the importance of all the background work I had done for the previous two-and-a-half years.*

One particularly encouraging comment that appeared was

- *At no other point at Lafayette was I able to understand and experience truer "engineering."*

In this survey, we also asked, "If I could change one thing about the structure of Laboratory II, it would be..." Twenty percent of the respondents indicated they would change nothing. Twenty-three percent found some problems with the structure. They noted that they had difficulties if the previous group did a poor job or was late with its report. Two students went so far as to request that we be stricter with our deadlines. The major drawback and difficulty of this structure is the dependence of students on each other's work. Instructors can work to make sure the previous group is on time and that the quality of its work is taken into account when grading reports, but we believe this interdependence among the students is a realistic and helpful experience.

Since this survey was taken, we have made the report deadlines stricter, including a strict 10%-per-day late penalty. This has essentially eliminated late reports. Students are also given a grading sheet that lists the key items we will be looking for in each report. This has led to more consistent student memos. Finally, student memos are graded considering how they have improved upon previous work.

## CONCLUSIONS

The key aspects of the approach we are using are

- It allows students to build on each other's experiments
- It provides only minimal information on how to run the equipment and leaves that as the first job to be done (which develops independent thinking by requiring students to develop their own SOPs)
- It provides students with an example of a sequence of experiments, including how to get started with a new piece of equipment
- It requires students to communicate their results via memos between the groups.

This approach provides a setting for realistic communication, experience in working on realistic sequences of experiments, and an opportunity for students to design their own studies. Student feedback and instructor observations support that these goals are being met. Student response is generally positive, as seen by the responses in general department interviews and in assessment surveys. A key to success is to manage the process so that students are not unfairly impacted by deficiencies in previous groups.

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## A Course in Bioprocess Engineering

*Continued from page 183.*

*participating in publishing a Bioengineering Newsletter (10%)*

### ASSESSMENT

This course has been taught only once under its present title, "Bioprocess Engineering"—in the spring of 2002. Assessment of whether or not the learning goals were achieved in this class was determined through exit surveys and teacher course evaluations. Some examples of questions that were asked of the students were

- *Did they feel the amount of learning they experienced was better, as good as, or less than in other core engineering courses?*
- *Did they think this course helped them to see where key issues of transport, thermodynamics, and reaction kinetics play a role in biological systems?*
- *Did they feel confident in their ability to begin employment in a field related to bioprocess engineering?*

The responses were divided: about 2/3 of the class participants responded positively to the course and felt it was a good introductory course to enable their further advanced studies in this area, while the other 1/3 did not find the course particularly beneficial. Some commented that the course was "very interesting," "tied in concepts previously learned in other courses in bioprocessing," and "the homework laboratories made the corresponding parts of the lecture more colorful." Because there was no formal text for the course, some students "had difficulty in finding additional information to solve some homework problems." A reserve list of library texts covering the course material was always made available in the Engineering Library, but access to on-line resources may be a more effective way to disseminate these materials.

### CONCLUSIONS

To our surprise, most of the ambitious goals set for the course were accomplished. Such excellent accomplishments were due to the students' willingness to participate in the outside classroom activities. We could have done even better if more students had had some university-level biology background.

The student engineers adapted well in the conceptual and computational analyses in the classroom dealing with the biological system, but some had difficulty in growing microbial culture. This was quite understandable, and the Department of Chemical and Biomolecular Engineering is moving toward requiring one semester of biology for all engineering students in the future.

Many students who took the course were excited about the prospect of molecular-biology driven bioprocess engineering and appeared to have enjoyed the less stressful approach to the subject, although it was a demanding course. We intend to improve the quality of the course by analyzing formal and informal assessments of the course. In the future, it would be advisable to solicit an external evaluation of the course.

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## ChE letter to the editor

To the Editor:

The recent article (Pitt, M.J., and J.E. Robinson, "Using a Commercial Movie for an Educational Experience," *Chem. Eng. Ed.,* **37**(2), 154, 2003) on the use of movies for educational experience is interesting, and may I suggest another possible movie for study...*The Man in the White Suit.* A brilliant young polymer chemist, working unofficially in a corporate research laboratory, develops a fabric that "never gets dirty, never wears out." At first this is seen as a blessing, but very soon it is seen as a threat to the entire textile industry, and attempts are made to suppress it.

Although *The Man in the White Suit* was made as a comedy, it says much about the role of industrial research and its economic and social impact. In some ways it is very dated, as it was made over fifty years ago; but today's students who see it could be asked to explain how it is dated and also to identify the aspects that are still highly topical. When I first saw it as a teenager, it reinforced my interest in applied chemistry, and that eventually led me to chemical engineering.

**Malcolm Baird**
*McMaster University*

# HIGH-PERFORMANCE ENGINES

## *Fast Cars Accelerate Learning*

*"FEEL THE NEED FOR SPEED? If you think the sound of an F-1 engine cranking up to 18,000 rpm coming out of turn 8 at Hockenheim is up there with Vivaldi and Mozart, you're probably going to like this course. If you know there is no such thing as too much horsepower and torque under your right foot, this may just be the course for you. If you would rather go to an Auto Show than go to a casino to gamble, hop aboard. If you think that a car is really for getting between Bernalillo and the main campus, there are probably other courses you would enjoy more."*

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The "High-Performance Engines" (HPE) course at The University of New Mexico integrates problem-[1,2] and simulation-based[3-5] learning approaches. The course encourages students to synthesize core chemical and mechanical engineering principles (*e.g.,* thermodynamics, transport phenomena, kinetics, catalysis, mechanics, and dynamics) to analyze historically famous racing engines. With independent analysis based on computer simulations, the students in groups of 3 or 4 get to understand engineering innovations that lead to the engines' superior performance in auto racing. The analysis transforms abstract engineering concepts into concrete, object-oriented outcomes.

The students also discuss the design parameters (*e.g.,* compression ratio, intake manifold geometry, and valve timing) to improve engine performance. The groups compete through modeling and simulation to achieve the best improvement. The educational competition augments students' interest in the course subjects and promotes their active participation.[1]

**The format of the HPE course is a problem-based learning environment centered on case studies of specific engines, many with great historical significance.**

To compare the improvement, students rely on WAVE, an engine design software provided by Ricardo Software. It enables custom engine design and performance simulation by simultaneously solving momentum, energy, and mass balance equations. Since auto manufacturers such as Ford Motor Company use the software to design production engines, the software training advantageously increases students' career potential in automotive design engineering.

The course also prepares a group of University of New Mexico students for the collegiate Formula Society of Automotive Engineers (FSAE) Competition.[6] The participating

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students optimize the competition car design by using WAVE. Figure 1 illustrates how the course exploits the racing engines as the centerpiece to integrate core chemical and mechanical engineering concepts while promoting active learning and preparing our students for the national FSAE Competition.

## COURSE DEVELOPMENT

A technical elective course such as High Performance Engines provides a convenient venue to explore problem-[1,2] and simulation-based[3-5] learning. These learning approaches have been proven to promote active student participation and enrich students' learning experience.[7] We introduced the course in the fall of 2001 and taught it again in the fall of 2002 to the upper division students in the departments of chemical engineering and mechanical engineering.

During the conception of the course, our strategy was to exploit high performance engines as the centerpiece to draw students' interest and integrate the two learning approaches around a central topic. If the course became successful, we anticipated that it might lead to additional courses that explore the rest of the automobile.

Our first task was to identify the potential audience and to promote the course. We advertised that the course would be about what makes automobiles go, and in particular, what makes them go *fast*. We also placed the focus of the course squarely on high-performance internal combustion engines. Although much more goes into an automobile or a racecar to make it perform well (*e.g.*, transmission, suspension, steering, tires, brakes, many forms of electronic instrumentation, and controls), our perception was that the high-performance engine would be a good place to start. After all, the engine is the power source, or more precisely the "transformer," of chemical energy into mechanical energy.

The HPE course appeals largely to students who view cars as more than just transportation and who regard an engine as the soul of an automobile. Since the course is geared toward car enthusiasts, these students are highly motivated to learn the subject matter. The course also reflects local history and general public interest. Albuquerque is the hometown of the legendary auto racing family, the Unsers. Auto racing is a tradition in Albuquerque and has a loyal following, including Formula 1 (F-1) and National Association for Stock Car Auto Racing (NASCAR) circuits. Because the University of New Mexico serves largely in-state students deeply rooted in the local community, the HPE course certainly appeals to a wide audience, including some of the alums who wish to return for continuing education.

With the target audience clearly identified, our intention was to help students see how fundamental engineering principles come to life in internal-combustion, spark-ignition engines. The engine operation and design require integrative understanding of thermodynamics, transport phenomena, kinetics, catalysis, mechanics, and sound wave dynamics. Students get to capitalize on the application of these engineering fundamentals to engine operation and design and see how they come to life. The course relies heavily on computational tools and information technology for modeling, simulation, visualization, and design of historically famous racing engines.

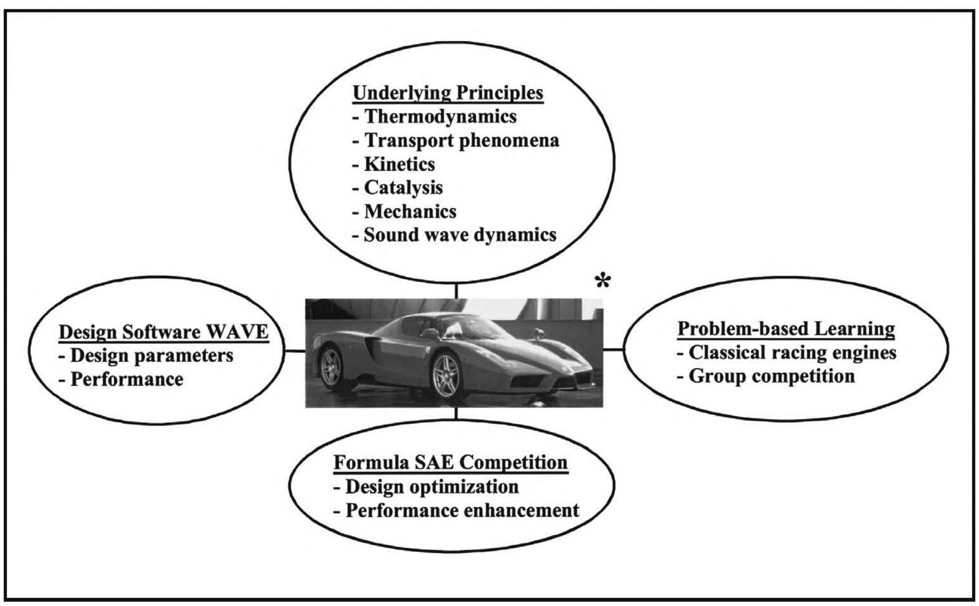


***Figure 1.***

*A conceptual diagram of the HPE course that exploits students' interest in concrete objects to integrate core chemical and mechanical engineering principles via problem/simulation-based, active learning while preparing them for national FSAE competition. (Picture of Ferrari FX is available via <http://www.ferrari.com>).*

## TEXTBOOKS

We chose Lumley's *Engines: An Introduction*[8] and Heywood's *Internal Combustion Engine Fundamentals*[9] as the main textbooks for the course. Lumley's book surveys the relevant topics of engine operation and carries enough depth for the students with limited hands-on experience in auto engines. This simplicity allows students with very basic mathematics to appreciate the engineering fundamentals behind engine operation. Overall, Lumley's book is an excellent option to broaden the potential audience by lowering the barriers for those who may not have extensive knowledge of auto engines. It also uses the Stanford Engine Simulation Program (ESP) available via <http://esp.stanford.edu>. This freeware lets students explore the engine's operating characteristics and thermodynamic performance as a function of geometric parameters of engines. The program is a straightforward and effective way to visualize methods for improving engine performance. We discuss other software tools later in this paper.

In comparison, Heywood's textbook thoroughly discusses operating principles with in-depth rigor. The topics in both books range from ideal models of engine cycles, to engine breathing, to engine heat transfer, to engine operating characteristics. These topics naturally lead to a discussion of subjects that are largely familiar to chemical and mechanical engineers, such as pressure vs. volume (P-V) diagrams of ideal Otto cycle, flow separation, thermal boundary layer, combustion, and mechanical vibrations and balancing. We added Heywood's book as a response to improve the course, based on a student survey conducted in the fall of 2001. The students expressed a need to see more rigorous analysis of engine operation in addition to the cursory demonstrations in Lumley's book.

## ENGINEERING TOPICS FOR CLASS DISCUSSION

The first topic discussed in HPE is the Otto engine cycle. Although the ideal Otto cycle is reviewed in numerous engineering thermodynamics courses, students often fail to appreciate its engineering significance. Our goal is to relate the P-V diagram to tangible engine performance so that students depart from abstract understanding of the diagram. We achieve this realistic understanding by first visualizing how each stroke (*i.e.*, intake, compression, ignition, expansion, blowdown, and exhaust) corresponds to the piston position between the top dead center (TDC) and the bottom dead center (BDC) of the cylinder, as illustrated in Figure 2.

We simultaneously introduce students to a concept of mean effective pressure (mep) as an artificial measure of thermodynamic performance of an engine. The mep value is intimately related to the P-V diagram. The product of mep and total engine displacement ($V_d$) is work done by the engine per power cycle, and the product is simply the shaded area carved out by the piston trajectory in the P-V diagram.

The power generated by the engine, a number that we all look at before purchasing a vehicle, is merely a product of the work produced per power cycle and the engine speed (N) in revolutions per second. This proportionality explains precisely why the brake horsepower (bhp) increases more-or-less linearly with the engine speed, often given in revolutions per minute (rpm), until the engine breathing becomes the limiting factor at high rpm.

This example demonstrates how an abstract concept can come to life by associating it with concrete objects and visualization. We expand on this approach with subsequent course materials by leading the students to make such associations. For instance, students directly relate intake manifold tuning, intake runner design, intake/exhaust valve size and number, intake/exhaust valve lift and overlap control by cam, and super/turbo charging to the engine performance figures. Making such connections requires fundamental understanding of sound-wave dynamics, turbulence and combustion, continuum fluid flow, mechanics, and advanced thermodynam-

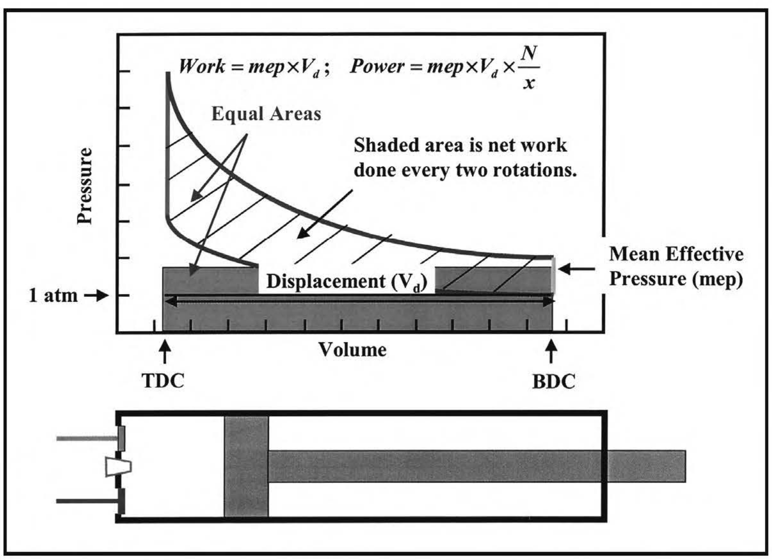


***Figure 2.*** *P-V diagram of ideal Otto engine cycle. Mean effective pressure (mep) is an artificial measure of an engine's thermodynamic performance intimately related to the P-V diagram. The generated power is simply a product of mep, total engine displacement ($V_d$), and engine speed (N) in revolutions per sec divided by the number of cycles per power stroke (x).*

ics. When the abstract engineering concepts are closely linked to tangible parts and concrete engineering outcome (*e.g.*, horsepower and torque), students become capable of retaining the learned information, and their desire to understand the engineering subjects remains strong throughout the course.

> *The course encourages the students to synthesize core chemical and mechanical engineering principles (e.g., thermodynamics, transport phenomena, kinetics, catalysis, mechanics, and dynamics) to analyze historically famous racing engines.*

## LOGISTICS OF THE COURSE

The instructors formulate the case studies that will be the focus of class discussion. These case studies require students to investigate the engineering topics mentioned previously. The instructors act primarily as *facilitators* to provide some degree of continuity and structure for the course. They essentially provide a forum for the extensive participation of students in this learning process.

Each case study starts with a brainstorming session moderated by the instructors. Students identify relevant engineering topics and areas that they wish to focus on. From time to time, the instructors themselves may be resources of knowledge in helping to explain concepts, but the faculty do not lecture in the conventional manner. They are, however, responsible for introducing modeling software (*e.g.*, ESP, WAVE, and Working Model 2D) and ensuring that students have adequate access to running these codes. The faculty members are expected to seek productive feedback from the students and to act on the feedback to improve the course.

Finally, the faculty evaluate student learning based on measures that truly reflect what students have gained in knowledge and competence. Some of the evaluation criteria are

- *The team's understanding of newly acquired concepts*
- *The depth and diversity of learning resources provided by the students*
- *The students' active participation during each case study*
- *Thorough documentation of quoted references*

Students are expected to have taken engineering thermodynamics before enrolling in the HPE course and instructor approval is required for those who have not taken it. Students are expected to attend all classes and to be thoroughly prepared.

At the beginning of the course, students form teams of 3 to 4 members each, and all activities during the semester are team-produced. Students can name their teams, for instance, after F1, IRL, and NASCAR race teams and compete during each case study. They are expected to participate extensively and fully in all aspects of working out the cases. This may include initial brainstorming sessions, concept identification, problem solving, and resource discovery. Teams are responsible for developing their own case study with guidelines provided by the faculty.

Although no one taking this course should be concerned about his or her grade, for the record, the grade is based on classroom participation, creative contribution to analyzing case studies, production of creative materials and learning resources, and the quality of case studies on performance engines, each of which is approximately equally weighted. For instance, students can bring real mechanical components to class, such as superchargers or camshafts, to demonstrate their working principles relevant to the corresponding case studies. Such participation reflects not only initiative, but also the students' creative approach to classroom presentation.

Since individual performance needs to be weighed appropriately in addition to the overall team performance, each team is responsible for a self-assessment of the performance of each team member. The grade for each student is based on overall team performance, peer evaluation, and self-assessment. The evaluation metrics chosen for the HPE course is available from <http://www.departments.bucknell.edu/projectcatalyst/Finalized%20Materials%20for%20CD/cats.htm>. the "Peer Rating Factor"[10] on this website is particularly useful in formulating the evaluation metrics.

## CASE STUDIES AND GROUP COMPETITION

The case studies used in the course are based on historically famous racing engines with significant engineering innovations of the period. These engines provide very successful examples of excellent engineering design. The posed problems generally require analyzing engine design parameters and their impact on performance. A few case studies are listed here as examples.

► **1954 Jaguar XK 3.4 L Inline Six**

1. *Provide additional background information and reference(s) for the XK engine.*
2. *Estimate the indicated mean effective pressure for*

*this engine.*

3. *Estimate the peak power.*

► **Honda RA122E/B 3.5-Liter V12**

1. *Provide additional historical and technical information on the Honda engine.*
2. *Estimate cylinder wall, piston crown, and exhaust valve temperatures as a function of engine speed (rpm).*
3. *Estimate the cycle-averaged heat loss rate in the given engine as a function of engine speed (rpm).*
4. *Discuss how the thickness of the cylinder wall and piston crown affects the heat loss.*
5. *Show semi-quantitatively how the exhaust valve diameter would affect valve temperature.*
6. *Provide an alternate way of estimating the cycle-averaged gas temperature and the exhaust gas temperature.*

► **Timing and Camshaft Design of 1989 Mustang GT**

1. *Provide nomenclature for main parts of the camshaft.*
2. *Relate cam profile and phasing to valve actuation and ultimately engine performance.*
3. *Select a commercially available cam for the 1987 Mustang and provide reasons for selection.*
4. *Use available software to simulate the engine performance.*

The third case is a primary example that can easily lead to group competition to produce the best performing engine. The group competition brings *fun* back to class, while at the same time promoting students' active participation.[1] "Who can produce an engine for the best quarter-mile time?" has proven to be an all-time motivator.

For those instructors who wish to implement a case study strictly limited to chemical engineering principles, the key points of the second case study are discussed in detail for illustration. The Honda F-1 engine case study focuses on heat transfer from the engine cylinder to the surrounding environment when chemical energy is released from the combustion process. The students are encouraged first to gather relevant information on gasoline, such as average molecular weight, specific gravity, heat capacity, and heat of combustion. For instance, one can assume complete combustion of octane to estimate the upper limit on the released chemical energy

$$C_8H_{18} + \frac{25}{2}O_2 \xrightarrow{\Delta H_c} 8\,CO_2 + 9\,H_2O \qquad (1)$$

For the adiabatic complete combustion, the students can calculate the exhaust gas temperature within the cylinder. The adiabatic gas temperature translates to the first estimate on the actual exhaust gas temperature since in the real situation, the released heat flows from the exhaust gas to valve assembly, cylinder wall, and piston head. The instructors must simultaneously guide the students to recognize that the amount

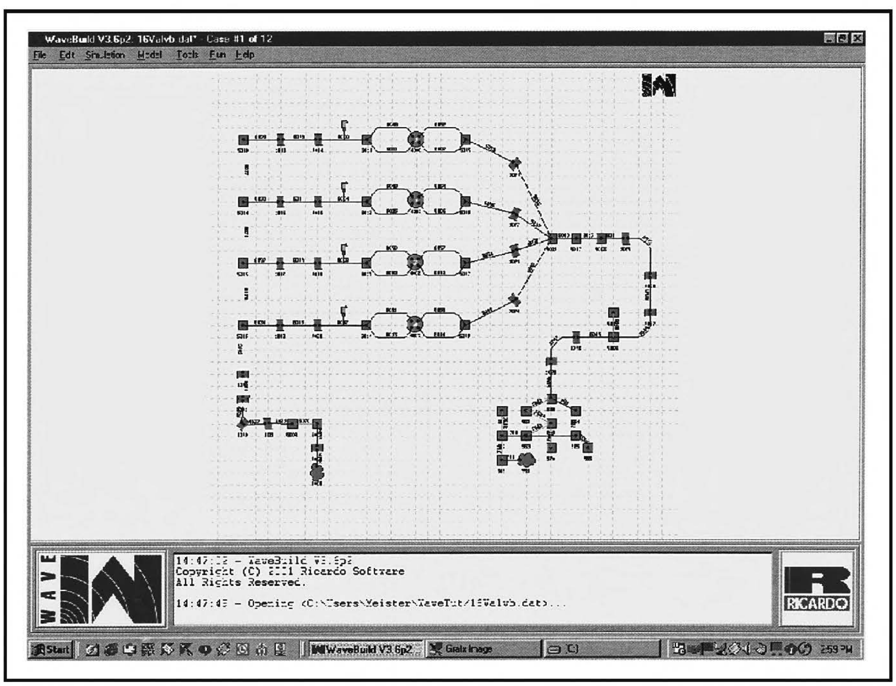


**Figure 3.** *Screen Shot of WAVE simulation software. The image shows modular components of a four-cylinder engine with complete intake and exhaust systems.*

***The course appeals largely to students who view cars as more than just transportation and who regard an engine as the soul of an automobile. Since the course is geared toward car enthusiasts, these students are highly motivated to learn the subject matter.***

of released chemical energy per unit time increases as the engine speed increases and that the heat transfer coefficient ($h_e$) for the turbulent flow of gasoline and combustion products in the cylinder also increases with increasing engine speed. That is, the increasing engine speed equals increasing Reynolds number (Re) for the working fluid in the cylinder, which in turn increases $h_e$ according to

$$\frac{h_e b}{k_g} = 10.4\left(\frac{Gb}{\mu_g}\right)^{0.75} \tag{2}$$

where b, $k_g$, and $\mu_g$ denote cylinder bore, thermal conductivity of working fluid, and viscosity of working fluid.[8] G is defined as $\dot{m}_a / A_p$, where $\dot{m}_a$ and $A_p$ denote mass flux per unit time through the cylinder and piston area. $Gb/\mu_g$ essentially equals Re. The heat transferred from the working fluid to the surrounding mechanical parts by forced convection is subsequently conducted through mostly metal engine components. In the case of the cylinder wall, the heat is finally transferred to the cooling jacket, whose temperature can be fixed for the purpose of calculations at a cycle-averaged temperature. By equating the heat flux from the convective heat transfer to the heat loss by conduction to the surrounding engine components, one can determine the surface temperature of valve assembly, cylinder wall, and piston head.

The remaining task is to account for the heat loss to the surroundings. The initial approximation on the exhaust gas temperature by adiabatic combustion no longer holds true. Thus, the students need to solve reiteratively for the exhaust gas temperature, which in turn affects both convective and conductive heat transfer. The students can consider additional complexity of heat conduction based on the varying cross-sectional areas of engine components available for the conductive heat transfer.

## LEARNING TOOLS

We introduce a number of software tools in the course. Although the effectiveness of introducing more than one software tool in a semester is still in debate, students often find their favorite from a selection of available tools, depending on their level of willingness to learn increasingly more complex software. For instance, ESP allows students to quickly grasp the key design parameters to improve engine performance with much ease and simplicity. For this reason, ESP is introduced in the early stages of the course.

The next software that we have considered introducing is Dyno/Drag 2000 by Motion Software, Inc., which contains an extensive list of commercially available engines and their components to simulate engine performance. The level of complexity comparatively increases from ESP to Dyno/Drag 2000. Dyno/Drag 2000 tests students' ability to choose the "right" components based on sound engineering decisions.

In comparison, WAVE (manufactured by Ricardo Software) is the most comprehensive and flexible software for simulating engine performance by simultaneously solving momentum, energy, and mass balance equations with a Wiebe-based combustion model. The software requires approximately a month of training to bring students to the point of simulating their own engines. Figure 3 shows a screen shot of WAVE simulation that students initially work on as a part of the training. The image illustrates four cylinders placed in the center with a full intake system on the left and a full exhaust system on the right. The user can specify details such as choice of fuel, exact geometry and operating temperature/pressure of all components, intake/exhaust valve lift as a function of crank shaft angle, rate and amount of heat release during combustion, and even complex muffler arrangements. Because some auto manufacturers use WAVE to design and optimize production engines, this training improves students' potential to pursue a career in auto design and manufacturing.

The last tool introduced is Working Model 2D by MSC Software. This tool allows students to construct moving components of an engine such as the cam and analyze their dynamic mechanical behavior. The exposure to mechanics helps students see that constructing a working engine requires more than understanding its thermodynamics, transport phenomena, and combustion.

The software tools additionally benefit the students who belong to the FSAE team. Using WAVE, these team members optimize their racecar design. The design rules of FSAE competition[6] are comprehensive, including chassis rules, crash protection, safety rules, and power-train restrictions. Among these rules, the design constraint of a 20.0-mm-diameter intake flow restrictor is the most limiting factor for engine breathing and hence, for its performance. The team members have been using WAVE to optimize the intake manifold to overcome this constraint and to maximize the engine

*Continued on page 219.*

# Increasing Time Spent on Course Objectives by USING COMPUTER PROGRAMMING TO TEACH NUMERICAL METHODS

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The chemical engineering curriculum is a crowded agenda, with students needing to allocate limited time resources to focus on educational objectives. A typical curriculum includes instruction in numerical methods, and programming assignments are one way of ensuring that students understand the methods underlying modeling calculations. Developing applications from "scratch" requires too much time spent on tasks not central to course objectives, however, leaving too little time for the engineering problem. An innovative approach to this problem, "Template-Based Programming," minimizes time spent on the elements of programming outside of course and assignment objectives.[2]

Template-based programming (not to be confused with the software engineering term "template") provides the student with a fully functional application, in all respects but one—the subroutine containing models and numerical methods is deliberately empty, with variables necessary to communicate with the user exposed and well defined for the student. The student is required to write only the codes necessary to implement the model and appropriate numerical methods. This enables students to focus on the assignment objectives without unnecessarily concentrating on the use of syntax and structures not germane to the engineering assignment.

## BACKGROUND

Newly graduated chemical engineers will potentially be called upon to perform a wide range of tasks involving computers. They will need to use current technologies requiring little programming skill, but they may also be called on to develop models and simulations that require some ability to develop procedural computer code. At times this will involve legacy codes, often in FORTRAN, dating back several decades. Sometimes this will require working in modern environments, such as writing complex procedural scripts in MATLAB, or integrating spreadsheet calculations with procedures written in Visual Basic.

***Template-based programming provides a means for incorporating computer programming into courses while minimizing time the students spend on programming tasks unrelated to the course objectives.***

The limited space available in the curriculum for computer training must be used to provide as broad a base as possible to enable graduates to adapt to the specific computing-related requirements of their employer as rapidly as possible. At the same time, it must be recognized that most chemical engineers are not expected to be applications developers,

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writing complete user-friendly programs from "scratch."

To maximize the value of each course in the curriculum, the integration of programming must be directed toward meeting educational and program objectives as defined by the individual department or program. Accreditation Board for Engineering and Technology (ABET) accredited curricula require that students learn "appropriate modern...computing techniques."[2] In most cases, chemical engineering programs have addressed that criterion in part by incorporating a programming course.[3] The most common language used is FORTRAN, with C, C++, and Visual Basic taught in many other programs.[3,4] Teaching procedural elements of scripting languages, such as those in MATLAB, Maple, and Mathematica, is proving to be an increasingly popular option among chemical engineering programs.[4]

The decision on how to incorporate programming into the curriculum should take into consideration why programming is important to chemical engineers. A CACHE Corporation survey[5] provides some interesting insight. Of the practicing chemical engineers surveyed, 92% never use FORTRAN or another computer language in their work. Furthermore, 86% of employers did not expect literacy in different computer language paradigms. Faculty members revising chemical engineering curricula to meet the needs of industry will find it challenging to determine the computing skills that should be taught as part of a core curriculum.[6] When the requirements of the ABET Engineering Criteria 2000 (EC2000) are also considered, the need to specifically address programming and computer use in the curriculum is even more pronounced.

Since there appears to be little need for practicing engineers to program, we must ask why we teach programming in most chemical engineering curricula. The most likely answer seems to be, because developing a program requires that the program author break down a complex problem into a logical series of steps in a syntactically rigorous language, with a flow of logic that should reflect the mental discipline an engineer should be capable of to solve challenging problems. Programming concepts are expected to strengthen two key facets of engineering education—problem formulation and problem solving,[7] although some studies indicate this may not be the case.[8] It can also be argued that programming languages are "a novel formal medium for expressing ideas about methodology,"[9] and thereby strengthen the communications component of the curriculum.

General purpose mathematical software (such as MATLAB, Maple, Mathematica, or MathCad) has been adopted by many chemical engineering programs with the intent of teaching students problem-solving skills requiring computer usage. Typically, this requires some degree of programming. The benefit of this approach is that the "overhead" of applications development is handled by the host application. One difficulty with this approach is teaching numerical methods with these packages when the program already has most numerical methods incorporated directly into the software. In this case, use of a high-level programming language may be more appropriate. In all cases, the opportunity for sufficient instruction of students in the software or programming language they are expected to use is critical.

Applications development requires that all details regarding a program be addressed, including memory management, user interfaces, buffer protection, graphics, file management, and operating system integration. Engineering students should be focused on the problem, addressing numerical methods, model accuracy and assumptions, stability, limits of applicability, communicating the model and results, and integrating the results with reality. The method described herein enables focus on the topics important to

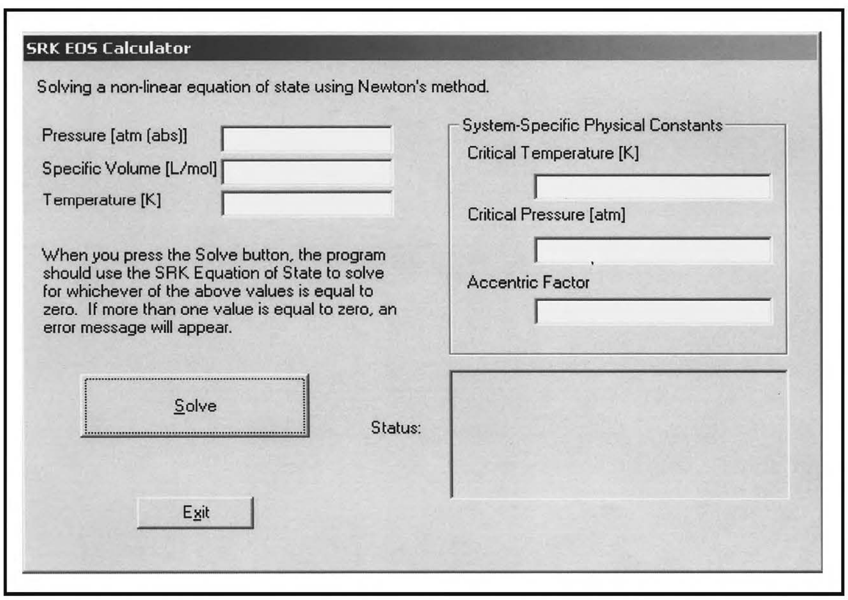


***Figure 1.*** *The user interface resulting from compiling and executing the template. The program is fully functional, except that it does not calculate anything when the button is clicked. Error messages regarding user input are still displayed, even without the student code.*

chemical engineering students.

## TEMPLATE-BASED PROGRAMMING

The template-based approach begins with a fully functional application. The student is provided with the complete workspace for the integrated development environment (IDE) under which they have previously worked in their programming course. Immediately after loading the template, they can compile and run the program, which will appear as in Figure 1. One key element is, however, missing. When the "solve" button is pressed, nothing is returned. That button calls a subroutine that, while fully commented and linked to the application, is devoid of executable code. The student is expected to write all necessary code to provide the subroutine with the functionality required by the assignment. A typical subroutine is shown in Figure 2 . All variables needed as input for the routine are exposed by global variables, as is the variable declared to store the result calculated by the students, which is returned to the application interface.

The result of the assignment is an attractive, uniform, fully functional, stand-alone application that students can then use for solving additional problems. Time spent on non-objective activities, such as preparing "FORMAT" statements or reading and writing to files has been minimized or eliminated. The high-level programming language has been used in such a way that it shares many of the benefits of math packages, including the ability to assume that I/O management, memory management, and the user interface are taken care of without need for consideration by the subroutine programmer.

## IMPLEMENTATION

Use of these templates develops along the same lines as other course material. First, expected outcomes for the assignment were derived from the course objectives. An assignment was developed and application constructed sans components required for the student to develop to achieve the expected outcomes.

Students were required to take a FORTRAN course to fulfill programming requirements until a policy change at the University of Kentucky (UK) in 2001 allowed them to take a course in Visual Basic to satisfy that requirement. To maximize the value of the student's previous training, early uses of this approach were coded in Compaq's Visual FORTRAN environment. Most recent uses of this approach have been assigned with a student option of using FORTRAN or Microsoft Visual Basic.NET templates. In all cases, students have been given the option of writing their own program from scratch, using any programming environment. The assignment is typically rather detailed, since some significant instruction is required to get started using the template because students have never had to work within someone else's application prior to this assignment.

## RESULTS AND DISCUSSION

Students did not write routines to collect model parameters from a console or data file, design structures to pass data between routines, or format numerical output and send it to the console or to a file. They gained no experience in inheritance, encapsulation, polymorphism, or GUI programming. They did design a model, specify required input and output, write subroutines and functions involving the model and a numerical method, debug their code, validate the model, and verify the numerical method. They focused, thereby, on the course objectives—modeling chemical processes or performing engineering calculations, selecting and implementing numerical methods, and practicing fundamental logic and problem-solving skills.

An additional benefit of the approach includes ease of grading. Since all students started from a common set of variables, the code was easier to trace. The results presented in the form of screen captures were consistent and easier to follow.

Template-based programming has been applied in two courses so far: Process Principles, the sophomore material and energy balance course, and Process Modeling, a junior-level course in modeling principles and numerical methods.

The class size in all courses in which this approach has

```
SUBROUTINE SRK()
!Routine to actually run the SRK EOS calculations
!
! It obtains values of 3 of 4 variables (PVT) and Tc,Pc,and the accentric factor
!from the dialog box
! It must provide a value of the missing variable while not changing the variables
!provided
! Minimal error checking is performed
! The following two statements incorporate this file into the overall project
use dfwin
use SRKGlobals
!**************************************************************************
!The following global variables are available to you.
!double precision     Pressure        Pressure given in the dialog box
!double precision     Volume  Specific Volume given in the dialog box
!double precision     Temperature     Temperature given in the dialog box
!double precision     TCrit   Critical Temperature given in the dialog box
!double precision     PCrit   Critical Pressure given in the dialog box
!double precision     Omega   Accentric Factor given in the dialog box (may be =0)
!You must assign a value to whichever variable from amongst  Pressure, Volume,
!Temperature was =0

!You will need to create some variables for use within your subroutine

!You may choose to create another subroutine INSIDE THIS FILE to handle equation
!solving

!You will need to first figure out what to solve for,and then branch to actually
!solve for that unknown
!That gives you three cases,one of which is trivial. For the other two, you will
!need to use Newton's method
!Remember to calculate the SRK parameters which you will use in all three cases.
!You will likely need to declare other variables to complete your program

!YOUR CODE STARTS HERE



!YOUR CODE ENDS HERE
END SUBROUTINE SRK
```

***Figure 2.*** *Typical student subroutine template.*

been applied has been ten or less. The UK engineering programs in Paducah are an extension of the main campus in Lexington. Students pursue a BS in chemical engineering under what is currently a curriculum identical to that of the Lexington program. Chemical engineering courses at UK Paducah are taught by UK faculty stationed in Paducah, with the remaining courses taught by Murray State University and Paducah Community College.[10] ABET accreditation is expected in July 2003.

The first use of template-based programming was in Process Modeling. One of the objectives for this course is that students "use computer software and programming languages to solve complex mathematical systems." Two assignments were given. The first was a simple determination of the machine epsilon, the smallest difference between two numbers that the computer can distinguish. The purposes of the assignment were to reinforce the idea of inherent limitations of computer calculations, to reintroduce computer programming to the students (who had not programmed during the 1 - 2 years since their programming course), and to familiarize the students with the template-based approach. The second project was an implementation of Gauss-Siedel elimination to solve for a solution to a system of linear equations.

The first time this course was taught at the Paducah campus, students were unable to complete the epsilon calculation due to difficulties with passing variables to subroutines, with using DO loops, with reading and writing input and output, and other serious programming deficiencies. The options left to the instructor were to reteach these topics every time the modeling course was offered, to eliminate the programming task, or to develop a method that would allow students to focus on the skills they needed to retain.

The second time the course was taught, templates were used. Students were surveyed regarding their perception of their programming skills and the utility of the template-based approach.[1] Table 1 summarizes the results. Students demonstrated improvement in perception of their individual skills in various programming concepts after the template-based assignment in all cases except for the question about basic mathematical operations and on the question regarding DO loops. The second project required a sequence of nested DO loops that tested their understanding of this construct, which was not as strong as they had previously perceived. Other results of the survey indicated more time was spent on engineering objectives than would have been spent without the template.

The students were enthusiastic about this approach, stating that they were more confident about starting to program since the "busy work" had been completed for them. The visual nature of the output was more satisfying than the console-based output of programs they had written previously. Students from the previous section of the course expressed envy that students using templates did not have to struggle through the issues they did with fundamentals of applications development.

**TABLE 1**
**Summary of Survey Results**
*("1" - student strongly disagrees: "5" - strongly agrees)*
*(Courses: CME200-Process Principles; CME420-Process Modeling)*

| | *Initial Survey CME200* | *Post Project Survey CME200* | *Initial Survey CME420* | *Post Project Survey CME420* |
|---|---|---|---|---|
| I am comfortable writing programs using FORTRAN | 2.8 | 3.0 | 1.8 | 2.5 |
| I understand how to use variable arrays in FORTRAN | 3.6 | 3.9 | 1.3 | 2 |
| I understand how to use if-then-else structures in programs | 2.7 | 3.4 | 2.8 | 3.5 |
| I understand the use of DO loops and how they are terminated | 3.6 | 3.8 | 3.3 | 3 |
| I understand the use of comparison operators in FORTRAN | 3.3 | 3.5 | 3.3 | 4 |
| I can perform mathematical operations on variables in a FORTRAN program | 3.3 | 3.8 | 3.3 | 3.3 |
| Using a template allows me to focus more on the engineering problem compared to writing a program from a blank file | N/A | 4.5 | N/A | 3.8 |
| The time spent programming was reduced by using the template | N/A | 4.3 | N/A | 4.3 |
| After having worked through the issues involved in starting to use the template, the template was easier to use than writing a program from a blank file | N/A | 4.1 | N/A | 4.5 |

The biggest improvements observed by the instructor were the reduction in time spent during office hours instructing students in programming fundamentals and the fact that all students turned in programs that met instructional objectives. Students spent far less time working on the programs using the templates than before, but the time they did spend was quality time, focused on the assignment objectives.

The second course in which this technique was applied was Process Principles in the fall of 2001 and 2002. During coverage of equations of state, students were required to solve the Soave-Redlich-Kwong equation of state for an unknown PVT variable using Newton's method. Again, students had issues with the numerical method, but not with the programming technique. In part, this was due to the freshness of the programming course in these sophomore's experience, but students still expressed a preference for working from a template instead of writing a program from a blank file. Submitted results were of superior quality compared to those of an assignment in the fall of 1999 that required complete development of an application to solve a similar problem.

Surveys were again conducted involving students in both sections of Process Principles in which templates were implemented. Table 1 summarizes those survey results. The key finding of the survey is confirmation that students again perceived that they spent more time focused on meeting course expected outcomes while practicing and improving their programming skills.

The template-based approach is flexible, readily applied not only to the Compaq Visual FORTRAN IDE and the Microsoft Visual Basic.NET environment, but applicable within MATLAB and other packages. In the fall of 2002, the Process Principles class had a group of students, half of whom had instruction in FORTRAN, and the other half a course in Visual Basic. Templates for both languages were made available and were used by students. The complete templates, including the code for the user interface, also serve as an example for students interested in developing their own applications for research or personal use.

There are some difficulties associated with the use of templates. The primary issue in implementing them is actually developing a reliable, debugged interface. With Compaq Visual FORTRAN, the interface development requires understanding of Microsoft Windows GUI development concepts, which is not part of the typical chemical engineering professor's background. More recent FORTRAN environments (Leahy Fortran.NET, for example) make this process much simpler. When students work under different languages or environments, multiple templates may be required, as they were during the fall 2002 offering.

The implementation of templates will benefit from some technical improvements. The subroutine should be encapsulated as an object, so that the student does not directly modify any variables from the host routines. Another alternative would be having the students develop the core of a dynamic link library that compiles independently from the application and may be called from a variety of other programs. Process simulators and data acquisition systems can also be integrated with the templates to further develop the student's computing skills.

To simplify adoption of this approach, the author has made templates freely available for download.[11] Other faculty who wish to share their templates with the engineering community at large are invited to submit their templates to the author for inclusion in a web-accessible library.

## CONCLUSION

Template-based programming provides a means for incorporating computer programming into courses while minimizing time the students spend on programming tasks unrelated to the course objectives. It allows the student to model processes and apply numerical methods in a logical manner, breaking down complex procedures into syntactically rigorous steps, resulting in a usable application. It also capitalizes on the programming courses students take early in the curriculum.

Templates have been successfully incorporated into two courses at the University of Kentucky's extended campus in Paducah, with very positive results, particularly with respect to time spent on engineering tasks as described in the course objectives. It is a flexible approach, as demonstrated by use with both FORTRAN and Visual Basic, and can be applied to many other languages or computing environments. Stable and robust template development does require substantial time, but results in a more efficient educational experience for the student.

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## High Performance Engines

*Continued from page 213.*

performance of Yamaha R6.

In addition to the software tools, we use WebCT, a web-based teaching tool. It enables prompt distribution of course materials, fast real-time communication with students via chat rooms, immediate feedback on student evaluation, and compilation of research topics and information relevant to the discussion topics. Although creating and improving a WebCT site requires more hours of preparation than conventional lectures, it proves an effective medium to keep the course more accessible and malleable for improvement.

### COURSE OUTCOME ASSESSMENT AND STUDENT EVALUATION

We expect the students to be able to perform the following tasks during the course of the semester:

- *Construct ideal Otto as well as nonideal P-V diagram describing each stroke of the internal combustion engine*
- *Identify key elements that contribute to the nonideality and how the nonideality impacts engine efficiency*
- *Recognize the importance of engine breathing and propose the methods of improving engine breathing based on full understanding of fluid mechanics*
- *Compare supercharging and turbocharging to natural aspiration and draw the piston trajectory on the P-V diagram*
- *Perform convective and conductive heat transfer calculations to approximate the temperature of mechanical components surrounding engine cylinders*
- *Design and virtually build a mechanically stable camshaft/valve assembly, using Working Model 2D*
- *Design a working 4- to 8-cylinder engine, using WAVE, and baseline the performance compared to commercially available production engines*

The majority of students are capable of performing the above tasks, evidence of which is based on their classroom presentation and full discussion of case studies, including the mathematical calculations. The narrow final grade distribution, ranging from 80% to 96% in cumulative scores based on the evaluation criteria described previously, support that the student groups collectively meet the expected course outcomes better than the majority of engineering classes.

The latest student course evaluation (Fall 2002) rates the course at 6 on a scale of 1 through 6, where 6 is the most favorable rating. The main categories of evaluation are course content, instructors, and effectiveness in learning. Overall, students enjoy the introduction to industry-developed software such as WAVE, the seminar format of the course that gets everyone involved, and the assignments that lead to good discussions. Students request lessening the gear head talk, however, and increasing the availability of instructors to answer the questions in regards to the case studies.

### SUMMARY

The format of the HPE course is a *problem-based learning environment* centered on *case studies of specific engines,* many with great historical significance. Students and faculty jointly explore the fundamental chemical and mechanical engineering aspects that govern the operation of the internal combustion engines, leading to an understanding of how engines work, how to model them, and how to design them for maximum performance. While engineering rigor is not sacrificed, the course is about applying good engineering and its tools to high-performance engines, and in the process, making engineering fundamentals come to life.

This course is not primarily about plugging numbers into formulas, although students do some extensive calculations at times, but rather about understanding, through implementation of computing and information technology for modeling, simulation, visualization, and design. The set of resources compiled over the semester, with contributions from all faculty and students, represents a rich legacy that will be useful to those who have taken the course as well as students who follow.

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# *Random Thoughts . . .*

# THE INCONTROVERTIBLE LOGIC OF THE ACADEMY

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I've spent decades at one academic institution and regularly visit others, but I still sometimes have trouble understanding academic institutional logic. Whenever my bewilderment reaches a critical point, I like to check in with my old grad school buddy Kreplach, who always seems to be on top of everything. I ran into him at a conference the other day.

*"So, Kreplach—I hear your Engineering School has raised the first 10 million dollars in its latest fund drive."*

*"Right—our* 'Forward to the Future' *campaign is off and running. We're going for 150 million big ones."*

*"But last month you told me that you just finished raising 50 million in your* 'Tackling Tomorrow's Technology Today' *drive and you haven't spent all of* that *money yet."*

*"Right again...so what's your problem?"*

*"Why do you need another 150 million?"*

*"So we can build new state-of-the-art bionanoinfotechnology facilities."*

*"I thought you already had them—wasn't your biotech center built just last year?"*

*"Well sure, but what we've got now doesn't have nearly enough room to put in the labs and offices that the new graduate students are going to need."*

*"What new graduate students?"*

*"The ones we're going to go after with those 60K fellowship programs that will come out of the 150 million."*

*"Sixty thousand? But that's more than we pay our new assistant professors."*

*"Yep, same with ours, and with that kind of money we should be able to pull a bunch of hotshot undergrads away from Stanford and MIT."*

*"That would be nice, but don't you and your colleagues already have as many graduate students as you can handle—can you just keep on adding new ones indefinitely?"*

*"Probably not, but that's where the new faculty members come in."*

*"What new faculty members?"*

*"The ones in the new distinguished chairs, of course."*

*"You mean the ones you endowed from the 50 million?"*

*"No, the eight new ones that will come from the 150 million. We're going to be able to pay those puppies a lot more than the chancellor gets and almost as much as the football coach—the Stanford and MIT faculties will be falling all over themselves to get some of that action."*

*"That would make sense, since you'll be getting their*

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*"Right, and with those new professors on board, we can get it down to one. Pretty sweet, eh? Besides, who'll advise the new graduate students if we don't bring in more faculty?"*

*"I forgot about that."*

*"See, that's your problem—you keep missing the big picture. Now, what do you think will happen when we've got all those new faculty members and graduate students on board?"*

*"It will get even harder for you to find a parking place on campus?"*

*"No...well, yes, but never mind that. Think about all the grants we'll pull in and the papers we'll churn out and the research dollars we'll spend—we'll be right up there with Stanford and MIT!"*

*"You should be ahead of them since you'll have most of their faculty and graduate students...anyway, I'm still not sure I see the point."*

*"It's simple. Since* U.S. News & World Report *bases its ratings on grants and papers and research expenditures, we'll move right up into the top ten..."*

*"And then..."*

*"And then our graduate school applications from other top ten schools will go up and we can boost our productivity and cut down our teaching loads even more, and we'll become attractive to faculty at..."*

*"Cal Tech and Minnesota because there's no one left at Stanford and MIT?"*

*"Right! Is that a plan, or what?"*

*"Let me see if I have it straight. You're trying to squeeze 150 million dollars out of companies and alumni so you can build new facilities to house new faculty members and graduate students who will increase your research funding and output, enabling you to recruit even more new faculty and graduate students?"*

*"I couldn't have put it better myself."*

*"But where will you put* those *people?"*

*"Aha—glad you asked! The Dean has put me in charge of the 'Engineering the Dream of a Brighter Tomorrow at the Dawn of the New Global Millennium' campaign we're getting ready to announce."*

*"Catchy title."*

*"Yeah, the Dean thought of it himself. We're thinking that 400 million dollars should cover most of our needs for at least two years."*

*"I like how you think big, Kreplach, but where are you going to find any more companies and alumni willing to kick in after all those other campaigns?"*

*"We thought about that, and we came up with two untapped sources with a strong vested interest in making us* numero uno*. Here, check this out."*

*"Let's see—whoa, a pledge form for the faculty with check-off boxes for salary tithes and a free legal service to help them redraw their wills. Outstanding!"*

*"Yeah, and don't overlook the space for the number of boxes of cookies they commit to sell every year."*

*"Brilliant thinking, Kreplach—I know everyone on your faculty will jump at the chance to help out...but what's your other group of eager donors? I can't believe there's a turnip you haven't already tried to squeeze blood from."*

*"Lots of them, my boy. Think—who is the most important person on campus, the one the faculty and administration are primarily there to serve, the one who gets more benefits from the university than anyone else?"*

*"That would be the football coach."*

*"Don't be absurd—it's the undergraduate student. The value of a college education to every undergraduate over the course of a lifetime is over a million dollars, right?"*

*"Yes, but..."*

*"So if we just ask each of them to kick in a mere $100,000, which is only a tenth of what we're giving them, we're home free."*

*"Fiendishly clever, Kreplach—our fundraising people would be green with envy."*

*"And who could blame them? Oh, before you go, our chocolate macadamia shortbread wafers are particularly fine this year. How many boxes can I put you down for?"*

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/~cee/

# SENSITIVITY ANALYSIS IN ChE EDUCATION

## *Part 1. Introduction and Application to Explicit Models**

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Engineering analysis and design typically proceed by construction of system models, followed by incorporation of required input quantities and the solution of the model equations to obtain values of output quantities of interest. The construction of models is an important aspect of engineering pedagogy, as is familiarity with numerical methods of solution for their more complex forms.[1] In addition to teaching students to construct and solve models for their outputs, we believe it is also important to emphasize consideration of the effects on outputs when input quantities are subject to variability and/or uncertainty. This is accomplished by sensitivity analysis (SA), which can be defined as the study of the uses of, and methodologies for, quantitatively calculating the effects of changes in input quantities on model outputs, especially for a large number of inputs. (Of course, one can directly calculate values of output quantities as functions of input quantities, but this only reveals sensitivities qualitatively and is only satisfactory when the number of inputs is small, say, $\leq 3$). In addition, a broad pedagogical use of SA is to provide a unifying theme for the study and understanding of topics arising in a number of areas in chemical engineering.

The fundamental concepts of SA are accessible to students who have a basic background in multivariable calculus, but full development requires some knowledge of linear algebra, which may not be a requirement in all undergraduate programs. Thus, although some concepts can be introduced in the undergraduate curriculum, the full treatment is more appropriate at the graduate level.

In chemical engineering, SA has a tradition of importance in the field of optimization.[2,3] Our own experience with SA has been principally in equilibrium models for chemically reacting systems,[4-6] which can be considered as optimization problems. In recent chemical engineering literature, SA has been applied to the design of reactive distillation units[7] and to process simulator models.[8] Varma, *et al.*, have considered SA in the context of chemical reactor models and related situations,[9] and a recent general treatment of SA (not specifically oriented to chemical engineering) was given by Saltelli, *et al.*[10]

Questions addressed by SA in a broad sense include

1. *What are appropriate quantitative measures of sensitivity of model outputs to changes in inputs? Particular measures addressing this question involve the marginal rates of change or marginal sensitivities of each output with respect to each input. These particular measures include the following items, which form the basis of this paper:*
   a. *A measure of the relative importance of each input for a given output is the relative value of the output's marginal sensitivity with respect to each input.*
   b. *A measure of the uncertainties in model outputs*

* Part 2 will be published in the Fall issue of CEE.
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*that result from uncertainties in the inputs. In general, this matter is called uncertainty analysis, and international bodies have published documents describing standards for the expression of such uncertainties.[11,12] Uncertainty analysis is also discussed in some undergraduate texts.[13-16]*

c. *A measure of the overall effects on the outputs of changes in combinations of inputs. This measure shows the relative importance of particular combinations of inputs.*

2. *What is the direction of change (sign) of outputs for a specified direction of input changes, given only the model structure (i.e., without obtaining a solution)?*
3. *Is there a large qualitative change in the outputs for small input changes?*
4. *Do the outputs change significantly when the underlying assumptions of the model change?*

Question 1 is usually considered to be the primary scope of SA, but it may include Question 4,[10] and we add Questions 2 and 3 as being in the same spirit and further broadening its scope. Question 2 is important in requiring only a minimal amount of model information (signs of quantities) as, for example, in a form of Le Chatelier's Principle.[17] Question 3 arises, for example, in the context of models described by differential equations and is addressed by stability and bifurcation theory.[18] A chemical engineering example concerns finding circumstances under which a chemical reactor changes its behavior from steady state to periodic.

Question 4 arises in statistics; the term *robustness* refers to the effects on a statistical analysis of changing the assumptions concerning underlying probability distributions.[19] Another chemical engineering example concerns situations when parameters in models are estimated from experimental data, requiring assumptions regarding measurement errors. It is desirable that the resulting parameter values do not depend strongly on departures from such assumptions.

In these two papers (Parts 1 and 2), we focus on only the first question. In this paper (Part 1), we introduce SA, describe two different classes of engineering models, and apply SA to address items 1a, 1b, and 1c for one of these classes. In Part 2, we will apply SA to the same items for the other class of model. Conclusions, including what is appropriate for the undergraduate curriculum and what can be deferred to the graduate curriculum, will be given at the end of Part 2.

In the following sections, we first describe two types of inputs and two types of models. For one type of model, we then consider, in turn, item 1a for both types of inputs, 1b for one type of input, and 1c for the other type of input (although, in principle, all three items could be considered for both types of inputs).

The reasons for applying items 1b and 1c to different input quantities are: we are usually interested in determining the effects on the outputs of uncertainties in the type considered for specified values of the other inputs (item 1b); conversely, we are usually interested in determining the effects on the outputs of changes in inputs over which the designer has control (item 1c). We will conclude with a pressure drop example for numerical illustration.

The treatment we describe and the examples we use in both Parts 1 and 2 relate to models that are amenable to analytical treatment to obtain values of the sensitivity quantities involved. The methodology, however, is not limited to such cases. In very complicated situations involving many variables, it may be possible to use computer algebra software to obtain values, and if necessary, values can be obtained by numerical differentiation, *e.g.,* using a process simulator.

## TYPES OF MODEL INPUTS
### *SYSTEM VARIABLES AND CONSTITUTIVE PARAMETERS*

It is useful to consider two different types of input quantities in models: *system variables* ($x_j$, j = 1,2,...,J) and *constitutive parameters* ($p_k$, k = 1,2,...,K). System variables (such as temperature, T, and pressure, P) are input quantities that can be manipulated by the designer or are imposed by the external environment; their values are usually considered to be specified precisely, but they may be subject to change. Constitutive parameters (such as viscosity and thermal conductivity) are those that must be obtained externally to the model, either by direct measurement or from correlations; their values are usually subject to uncertainties.

## TYPES OF MODELS
### *EXPLICIT AND IMPLICIT*

It is also useful to consider two different types of models that arise in engineering—explicit and implicit models, terms that denote mathematically how the outputs are available from the model in terms of the inputs. In principle, we can also consider further model classifications involving, for example, continuous versus discrete variables, and deterministic versus stochastic models. Here, however, we treat only the simplest situation of a deterministic model involving continuous variables, and we further assume that any functions involved in the models are differentiable. Although SA can be used for more complex situations, the methodology is correspondingly more complex. Furthermore, continuous-variable and differentiable deterministic models constitute a large class of engineering models.

An explicit model with N outputs, $y_i$, is one that can be written

$$y_i = f_i(\mathbf{x};\mathbf{p}); \qquad i = 1,2,...,N \tag{1}$$

where **x** is the vector of J system variables and **p** is the vector of K constitutive parameters. A simple example is a pressure-explicit three-parameter equation of state (EOS), with output quantity P, system variables molar volume ($\nu$) and T, and constitutive parameters critical temperature ($T_c$), critical pressure ($P_c$), and acentric factor ($\omega$)

$$P = P(v, T; T_c, P_c, \omega) \tag{2}$$

A more complex class of models is that of implicit models, which arise when the output quantities are implicit functions of the inputs, expressed formally as

$$f_i(\mathbf{y}, \mathbf{x}; \mathbf{p}) = 0; \qquad i = 1, 2, ..., N \tag{3}$$

where **y** is the vector of outputs. Implicit models can take many forms. Their distinguishing property is that Eq. (3) cannot be "solved analytically" for $y_i$ (although it is usually assumed that the solution of the equations is unique). A simple example of an implicit model arises in the context of a pressure-explicit EOS when $v$ is the output quantity and (P,T) are system variables; then $v$(T,P) is defined implicitly by

$$P - P[v(T,P), T; T_c, P_c, \omega] = 0 \tag{4}$$

More complex examples of implicit models include sets of nonlinear algebraic or transcendental equations, systems of differential equations (ordinary or partial), and optimization models.

The details of SA methodology are different for explicit and implicit models, but the general mathematical tools are similar. In Part 1, we will consider applications of SA to explicit models, while deferring implicit models to Part 2.

## SENSITIVITY COEFFICIENTS

Fundamental quantities used in SA are the marginal rates of change of output quantities in the model in terms of input quantities, *i.e.,* their (partial) derivatives. This addresses item 1a. The first derivatives $\partial y_i/\partial x_j$ and $\partial y_i/\partial p_k$ are called *first-order sensitivity coefficients*. The *normalized* first-order sensitivity coefficients are $\partial \ln y_i/\partial \ln x_j$ and $\partial \ln y_i/\partial \ln p_k$, which have the advantage that their values are independent of the units used. Furthermore a normalized coefficient can be interpreted as the % change in the output $y_i$ for a 1% change in the input $x_i$ or $p_k$. The two types of coefficient are related by

$$\frac{\partial \ln y_i}{\partial \ln x_j} \equiv \frac{x_j}{y_i}\left(\frac{\partial y_i}{\partial x_j}\right) \qquad i = 1,2,...,N \quad j = 1,2,...,J \tag{5}$$

$$\frac{\partial \ln y_i}{\partial \ln p_k} \equiv \frac{p_k}{y_i}\left(\frac{\partial y_i}{\partial p_k}\right) \qquad i = 1,2,...,N \quad k = 1,2,...,K \tag{6}$$

In some situations, it is appropriate to consider second derivatives as *second-order sensitivity coefficients,* $\partial^2 y_i/\partial x_j^2$, $\partial^2 y_i/\partial p_k^2$, and corresponding normalized forms.

## ■ ITEM 1a

***Relative Importance of Changes in Input Quantities***

To address item 1a, a measure of the relative importance of each input (*i.e.,* each system variable and each constitutive parameter) on each output is the absolute value of the relevant sensitivity coefficient, as shown below.

The effects of small changes in the inputs on the outputs can be approximated by a Taylor expansion using the first-order sensitivity coefficients of the outputs with respect to the inputs

$$\delta y_i = \sum_{j=1}^{J}\left(\frac{\partial y_i}{\partial x_j}\right)\delta x_j + \sum_{k=1}^{K}\left(\frac{\partial y_i}{\partial p_k}\right)\delta p_k \qquad i = 1, 2, ..., N \tag{7}$$

In order to consider all outputs and inputs on the same (relative) basis, the logarithmic form of Eq. (7) can be used:

$$\frac{\delta y_i}{y_i} \equiv \delta \ln y_i = \sum_{j=1}^{J}\left(\frac{\partial \ln y_i}{\partial \ln x_j}\right)\delta \ln x_j + \sum_{k=1}^{K}\left(\frac{\partial \ln y_i}{\partial \ln p_k}\right)\delta \ln p_k \qquad i = 1, 2, ..., N \tag{8}$$

For a given value of each input change, the relative importance of each input on the magnitude of each output is the magnitude of the relevant sensitivity coefficient.

## ■ ITEM 1b

***Effects of Constitutive Parameter Changes on Outputs: Uncertainty Analysis***

Here we use the sensitivity coefficients with respect to the constitutive parameters to address item 1b, since uncertainty analysis concerns the effects on outputs of uncertainties in these parameters.

The (standard) uncertainty of measurement of a quantity, $w_i$, is an associated quantity, $u(w_i)$, that characterizes the dispersion of the measured values that could reasonably be ascribed to the quantity.[11] $u(w_i)$ is taken as the square root of the variance, $\sigma_i^2$, if this is available, and approximate 95% uncertainty limits (assuming the uncertainties arise from a normal distribution with zero mean) for $w_i$ are then ($w_i$ - $2u(w_i)$, $w_i + 2u(w_i)$). (If $\sigma_i^2$ is unavailable, an estimate of $u(w_i)$ must be used.[11])

We identify the average value of $\delta y_i^2$ or $(\delta \ln y_i)^2$ obtained from Eq. (7) or (8) with $\sigma^2(y_i)$ or $\sigma^2(\ln y_i)$, respectively, with analogous identifications for the covariances. In terms of uncertainties, this yields

$$u^2(y_i) = \sum_{j=1}^{K}\left(\frac{\partial y_i}{\partial p_j}\right)^2 u^2(p_j) + \sum_{j=1}^{K}\sum_{k \neq j=1}^{K}\left(\frac{\partial y_i}{\partial p_j}\right)\left(\frac{\partial y_i}{\partial p_k}\right)u(p_j, p_k) \qquad i = 1, 2, ..., N \tag{9}$$

where $u(p_j,p_k)$ is the joint uncertainty of $p_j$ and $p_k$. When the constitutive parameters are uncorrelated (the typical case), the last part of Eq. (9) is absent. In this case, the relative importance of each parameter is given by the square of the relevant sensitivity coefficient. An expression analogous to Eq. (9) can be written in terms of relative uncertainties. We note that $u(\ln y_i) \equiv u(y_i)/y_i$, which represents the relative uncertainty in $y_i$ (and correspondingly for $p_j$). Reporting numerical values of uncertainties in such a standard way, in addition to values of the quantities themselves, is an emerging requirement.[11,12]

## ■ ITEM 1c

***Overall Effects of System Variable Changes on Outputs***

To address item 1c, we consider only the system variables, which (unlike the constitutive parameters) are normally under the control of the investigator. The sum of squares of the changes in the model outputs for given changes in the system variables is an appropriate overall measure. In what follows, we give expressions in terms of the sensitivity coefficients themselves; corresponding expressions can be written in terms of the normalized sensitivity coefficients (Eqs. 5 and 6). The change in the overall sum of squares due to small system variable changes is given from Eq. (7) by

$$\delta S = \sum_{i=1}^{N} \delta y_i^2 = \sum_{j=1}^{J} \sum_{k=1}^{J} P_{jk} \delta x_j \delta x_k \tag{10}$$

where $P_{jk}$ are entries in a matrix $\mathbf{P}$:

$$P_{jk} = \sum_{i=1}^{N} \left( \frac{\partial y_i}{\partial x_j} \right) \left( \frac{\partial y_i}{\partial x_k} \right) \qquad j, k = 1, 2, ..., J \tag{11}$$

For a given $\boldsymbol{\delta x}$, $\delta S$ can be calculated from Eq. (10), but further insight can be obtained by expressing $\delta S$ in a simpler form in terms of a new set of system change variables, $\boldsymbol{\delta\theta}$, as follows. The right side of Eq. (10) is a quadratic sum of the system variable changes, and it is a standard exercise in linear algebra to express this as a weighted sum of squares.[20] This is essentially the approach used by Seferlis and Grievink in design and sensitivity analysis for reactive distillation.[7]

An arbitrary change vector $\mathbf{dx}$ can be expressed in terms of a set of normalized (*i.e.,* in the mathematical sense of unit length) linearly independent eigenvectors of $\mathbf{P}$, $\{\mathbf{z}_j, j=1,2,...,J\}$, via

$$\delta \mathbf{x} = \sum_{j=1}^{J} \mathbf{z}_j \delta\theta_j \tag{12}$$

where $\delta\theta_j$ is the coordinate of $\boldsymbol{\delta x}$ with respect to $\mathbf{z}_j$. We then express $\delta S$ in Eq. (10) in the simplified form

$$\delta S = \sum_{i=1}^{J} \sum_{j=1}^{J} \sum_{k=1}^{J} \sum_{\ell=1}^{J} \mathbf{z}_k^T \mathbf{P} \mathbf{z}_\ell \delta\theta_k \delta\theta_\ell = \sum_{j=1}^{J} \lambda_j \delta\theta_j^2 \tag{13}$$

where $\lambda_j$ (which is non-negative[20]) is an eigenvalue of $\mathbf{P}$ corresponding to $\mathbf{z}_j$. Equation (10) represents a J-dimensional ellipsoid involving the variables $\boldsymbol{\delta x}$ for a given value of $\delta S$. Equation (13) expresses this ellipsoid in "standard form" in terms of the new variable $\boldsymbol{\delta\theta}$. Equation (12) resolves $\boldsymbol{\delta x}$ into its coordinates in terms of the new coordinate directions $\mathbf{z}_j$.

Equations (12) and (13) show that if $\boldsymbol{\delta x}$ is proportional to an individual eigenvector $\mathbf{z}_j$, $\delta S$ is given by the product of the square of the proportionality constant $\delta\theta_j$ and the corresponding eigenvalue $\lambda_j$. We can thus assess the relative importance of changes of $\delta S$ from a nominal value in the direction of each eigenvector by ordering the eigenvalues of $\mathbf{P}$.

## EXAMPLE
### *Pressure Drop in a Fixed-Bed Reactor*

A fixed-bed catalytic chemical reactor consists of a bed of catalyst particles through which the reacting system flows. As part (for a simple illustration) of the overall design/analysis of such a reactor, we consider an explicit model that approximates the pressure drop ($-\Delta P$) of a fluid flowing through a cylindrical bed of spherical particles:[21]

$$(-\Delta P) = \frac{64}{\pi^3} \left( \frac{1 - \epsilon_B}{\epsilon_B^3} \right) \frac{\dot{m}^2 V}{\rho_f d_p D^6} \left[ 1.75 + \frac{150(1 - \epsilon_B)\pi\mu_f D^2}{4 \dot{m} d_p} \right]$$
$$= f_1(1.75 + f_2) \tag{14}$$

where

$$f_1 = \frac{64}{\pi^3} \left( \frac{1 - \epsilon_B}{\epsilon_B^3} \right) \frac{\dot{m}^2 V}{\rho_f d_p D^6} \tag{15}$$

$$f_2 = \frac{150(1 - \epsilon_B)\pi\mu_f D^2}{4 \dot{m} d_p} \tag{16}$$

where

| | |
|---|---|
| $V$ | bed volume |
| $D$ | bed volume diameter |
| $u$ | superficial linear fluid velocity |
| $\rho_f$ | fluid density |
| $d_p$ | particle diameter |
| $\epsilon_B$ | bed voidage |
| $\mu_f$ | fluid viscosity |
| $\dot{m}$ | mass flow rate through the bed. |

The values at the reactor inlet are $\rho_f$ and $\mu_f$. The bed depth, L, is given by

$$L = \frac{4V}{\pi D^2} \tag{17}$$

Equations (14) and (17) constitute an explicit model for the output quantities $\{(-\Delta P), L\}$ in terms of the system variables $\{D, V, \dot{m}\}$ and the constitutive parameters $\{\epsilon_B, d_p, \rho_f, \mu_f\}$. For this example, N = 2, J = 3, and K = 4.

Expressions for the first-order sensitivity coefficients, together with the corresponding normalized coefficients are given in Table 1; the numerical values shown are obtained from the following data, relating to the first stage of a particular sulfur dioxide converter.[21]

$$D = 4.31 \text{ m}; \quad V = 12 \text{ m}^3; \quad \dot{m} = 38.0 \text{ kg s}^{-1};$$
$$\rho_f = 0.548 \text{ kg m}^{-3}; \quad \mu_f = 3.8 \times 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1};$$
$$d_p = 0.015 \text{ m}; \quad \epsilon_B = 0.45$$

From these data, $f_1 = 4097$ kg m$^{-1}$ s$^{-2}$ (≡Pa) and $f_2 = 0.08024$.

With regard to item 1a, Column 4 of Table 1 indicates that the most important system variable affecting changes (in an absolute sense) in both (-ΔP) and in L is D; the most important constitutive parameter in this sense affecting (-ΔP) appears to be μ; L is independent of all the constitutive parameters.

For *relative* changes, Column 5 indicates that the most important system variable for both (-ΔP) and L is also D; the most important constitutive parameter for (-ΔP) is $\epsilon_B$. Of these two types of comparison, that involving normalized quantities is more informative, since the coefficients are independent of the units.

To gain further insight concerning the dependence of the outputs on the inputs, we calculate the sensitivity coefficients as functions of the input quantities. For example, since the most important system variable is D, we show in Figure 1 the relative sensitivity coefficients of (-ΔP) as functions of D. They are all weak functions of D, and their relative importance does not change appreciably from that at the conditions of the problem statement, indicated by intersections with the vertical line at 4.31 m.

For item 1b, from the values in Column 5 of Table 1, the uncertainty in ln(-ΔP) in terms of the uncertainties in the constitutive parameters is given by the normalized version of Eq. (9) as

$$u^2\left[\ln(-\Delta P)\right] = u^2\left(\ln \rho_f\right) + (0.0438)^2 u^2\left(\ln \mu_f\right) + (1.044)^2 u^2\left(\ln d_p\right) + (3.854)^2 u^2\left(\ln \epsilon_B\right) \quad (18)$$

where the covariances are assumed to be zero (a typical case). This further indicates the relative importance of the variable $\epsilon_B$. Equation (18) requires values of the uncertainties in the constitutive parameters, $u(p_i)$, as described under item 1b.

**TABLE 1**
**Nonzero* First-Order Sensitivity Coefficients for the Pressure Drop Example****

| *Coefficient* | *Expression for Coefficient (A) (from Eqs 14-17)* | *Expression for Normalized Coefficient (B) (from Eqs. 5-6)* | *Value of (A)* | *Value of (B)* |
|---|---|---|---|---|
| $\frac{\partial(-\Delta P)}{\partial D}$ | $-\frac{f_1}{D}(10.5 + 4f_2)$ | $-2\left(\frac{5.25 + 2f_2}{1.75 + f_2}\right)$ | −10.29 kPa m$^{-1}$ | −5.912 |
| $\frac{\partial(-\Delta P)}{\partial V}$ | $\frac{f_1}{V}(1.75 + f_2)$ | 1 | 0.625 kPa m$^{-3}$ | 1 |
| $\frac{\partial(-\Delta P)}{\partial \dot{m}}$ | $\frac{f_1}{\dot{m}}(3.5 + f_2)$ | $\left(\frac{3.50 + f_2}{1.75 + f_2}\right)$ | 0.386 kPa s kg$^{-1}$ | 1.956 |
| $\frac{\partial(-\Delta P)}{\partial \rho_f}$ | $-\frac{f_1}{\rho_f}(1.75 + f_2)$ | −1 | −13.7 kPa m$^3$ kg$^{-1}$ | −1 |
| $\frac{\partial(-\Delta P)}{\partial \mu_f}$ | $\frac{f_1 f_2}{\mu_f}$ | $\frac{f_2}{1.75 + f_2}$ | 8650 kPa m s kg$^{-1}$ | 0.0438 |
| $\frac{\partial(-\Delta P)}{\partial d_p}$ | $-\frac{f_1}{d_p}(1.75 + 2f_2)$ | $-\left(\frac{1.75 + 2f_2}{1.75 + f_2}\right)$ | −522 kPa m$^{-1}$ | −1.044 |
| $\frac{\partial(-\Delta P)}{\partial \epsilon_B}$ | $-\frac{f_1}{\epsilon_B(1 - \epsilon_B)} \times \left[1.75(3 - 2\epsilon_B) + (3 - \epsilon_B)f_2\right]$ | $-\left[3 + \left(\frac{\epsilon_B}{1 - \epsilon_B}\right)\left(\frac{1.75 + 2f_2}{1.75 + f_2}\right)\right]$ | −64.2 kPa | −3.854 |
| $\frac{\partial L}{\partial D}$ | $-\frac{8V}{\pi D^3}$ | −2 | −0.3817 | −2 |
| $\frac{\partial L}{\partial V}$ | $\frac{4}{\pi D^2}$ | 1 | 0.06854 m$^{-2}$ | 1 |

* $\frac{\partial L}{\partial \dot{m}} = \frac{\partial L}{\partial \rho_f} = \frac{\partial L}{\partial \mu_f} = \frac{\partial L}{\partial d_p} = \frac{\partial L}{\partial \epsilon_B} = 0$

** $f_1$=4.097 Pa; $f_2$=0.08024; $f_1$ and $f_2$ are defined by Eqs. 14 and 15.

For example, a 1% relative uncertainty in each parameter results in a relative uncertainty in (-ΔP) of 4.1%.

For item 1c, to assess the overall effects of relative changes in the system variables on relative changes of the outputs, the equivalent of the matrix **P** defined in Eq. (11) in terms of normalized sensitivity coefficients is calculated from the values in Column 5 of Table 1:

$$\mathbf{P} = \begin{pmatrix} 38.955 & -7.912 & -11.565 \\ -7.912 & 2 & 1.956 \\ -11.565 & 1.956 & 3.827 \end{pmatrix} \qquad (19)$$

The eigenvalues of **P**, $\lambda_i$, and their normalized eigenvectors, $\mathbf{z}_i$, are[22]

$$\left.\begin{aligned} \lambda_1 &= 43.999; \quad & \mathbf{z}_1 &= (0.941, -0.190, -0.280)^T \\ \lambda_2 &= 0.783; \quad & \mathbf{z}_2 &= (0.060, -0.721, 0.691)^T \\ \lambda_3 &= 0; \quad & \mathbf{z}_3 &= (0.333, 0.667, 0.667)^T \end{aligned}\right\} \qquad (20)$$

The normalized equivalent of Eq. (13) gives

$$\delta \ln S \equiv [\delta \ln(-\Delta P)]^2 + [\delta(\Delta \ln L)]^2 = 43.999\,\delta\theta_1^2 + 0.783\,\delta\theta_2^2 + 0\delta\theta_3^2 \qquad (21)$$

This indicates that, when a change vector for the system variables $(\delta \ln D, \delta \ln V, \delta \ln \dot{m})^T$ is proportional to an individual eigenvector $\mathbf{z}_i$ (with proportionality constant $\delta\theta_i$), the relative change in S (δ ln S) is given by $\lambda_i \delta\theta_i^2$. Since $\lambda_1 = 43.999$ is the largest eigenvalue, Eq. (21) indicates that the largest relative change in S occurs in the direction of $\mathbf{z}_1$. For example, a unit change of the system variables $(\delta \ln D, \delta \ln V, \delta \ln \dot{m})^T$ in the direction of $\mathbf{z}_1$ leads to a 44-fold relative change in S. Note also that there is one zero eigenvalue; in general, when N ≤ J, the number of zero eigenvalues is at least J − N. For a system variable change vector proportional to $\mathbf{z}_3$ (corresponding to $\lambda_3 = 0$), the relative change in S is zero.

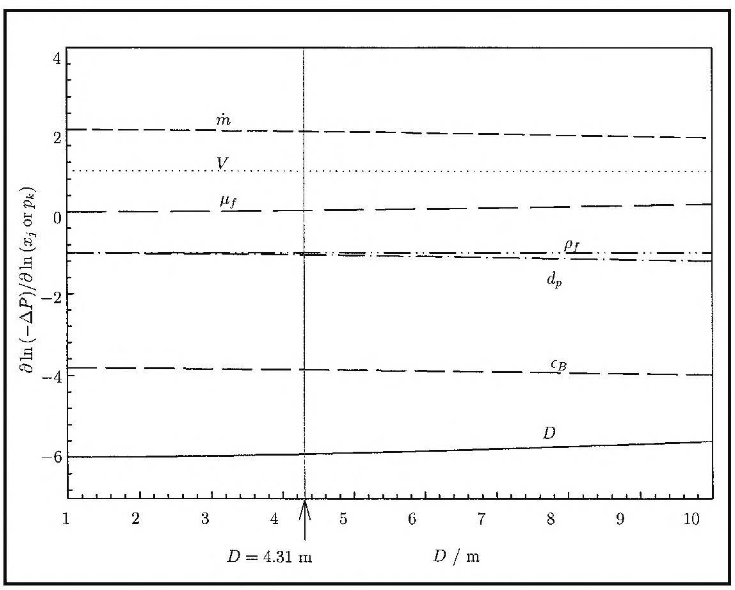


***Figure 1.** Pressure drop example: Normalized sensitivity coefficients for (-ΔP) as functions of bed diameter D; values at D = 4.31 m correspond to those in Table 1.*

## ACKNOWLEDGMENT


Financial assistance has been received from the Natural Sciences and Engineering Research Council of Canada.


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# STOCHASTIC MODELING OF THERMAL DEATH KINETICS OF A CELL POPULATION

## *Revisited*

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Numerous biochemical processes occurring in nature or man-made systems (*e.g.*, biochemical reactors) involve randomly behaving viruses, fungi, bacteria, and plant and animal cells that are discrete and mesoscopic in size. This gives rise to incessant fluctuations in their characteristic properties, including their number concentrations (density), movements, and metabolic activities. Such fluctuations are profoundly magnified when the number concentrations of pores, spores, or cells are very low as found, for instance, in the tail end of thermal disinfection of foodstuffs.

Medical needs and public health concerns often demand that the disinfection process be complete or nearly complete. Hence, it is indeed appropriate that the notion and methodology of stochastic processes have been introduced in most of the major textbooks on biochemical engineering through analysis and modeling of the disinfection process;[1-4] the discourse in these textbooks is based on the original contributions of Fredrickson[5] and Aiba and Toda.[6] According to Ramkrishna,[7] "Fredrickson was the first to point out the importance of stochastic analysis in dealing with sterilization processes." The crux or essence of stochastic analysis and modeling is in their capability to estimate or predict inherent fluctuations of the characteristic property of a random phenomenon or process and the distribution of this fluctuating property. In these textbooks, however, only the mean (the first moment), or at most, the variance (the second moment about the mean) of the fluctuating number concentration of cells during disinfection is given. The evaluation of additional quantities defined in terms of the moments of the number concentration of cells higher than the second moment is useful and often necessary to gain insight into the stochastic, or random, nature of the phenomenon or process of interest.

In fact, mesoscopic entities in the form of bubbles, droplets, and particles are ubiquitous in many phenomena, processes, and operations taught in various courses in chemical engineering besides biochemical engineering. Some of these courses are chemical reaction engineering, transport phenomena, separation, particle technology, material science and engineering, and surface science. The phenomena, processes, and operations involving mesoscopic entities includes heterogeneous reactions,[8] gas absorption,[9] distillation, liquid-liquid extraction, adsorption,[10,11] fluidization,[12,13] filtration,[14] crystallization,[15] solids mixing,[16] and grinding and attrition.[17,18] With slight adaptation, the current contribution can

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surely be made useful for several chemical engineering courses.

The current effort aims at presenting the fluctuations in the microorganism's number concentration in the course of disinfection not only in terms of the variance but also the skewness (the third moment about the mean over the third power of the standard deviation) and the kurtosis (the fourth moment about the mean over the fourth power of the standard deviation). The results would be useful as supplementary materials to what is already available. Following the textbooks mentioned above, the example adopted is the thermal disinfection of a cell population, specifically that of *Staphylococcus aureus,*[19] where the number concentration is considered to decrease according to the first-order rate law.

Interest in stochastically analyzing and modeling bacteria, or cell populations in general, has been steadily growing in recent years in view of their importance in different areas of biochemical engineering and biotechnology. Various researchers have resorted to the master-equation and other closely related algorithms; the majority, if not all, of them have considered linear systems or processes. Tsuchiya, *et al.,*[20] reviewed their works on the growth and replication of cultures of unicellular organisms. Ramkrishna[21] wrote an informative exposition containing a variety of stochastic algorithms for modeling the dynamics of cell populations including the master-equation algorithm. Stephanopoulos and Fredrickson[22] analyzed the extinction process by the prey-predator model involving both deterministic and stochastic components. Nassar, *et al.,*[23] stochastically modeled the dynamics of a unicellular organism population; they[24] also modeled the enzymatic degradation of cellulose. Lauffenburger and Linderman[25] published a monograph based on their earlier works on receptor/ligand trafficking by the master-equation algorithm.

## MODEL FORMULATION

As in any stochastic analysis and modeling, a mathematical model characterized by a random variable or variables is required for the system under consideration. It is formulated according to the procedure outlined below.[26-31]

***Description of the System*** • The system under consideration is the population of microorganisms, or cells, that are thermally deactivated. The status, or state, of the system is specified by the number (or size) of the population, that decreases due to the death of cells that have ceased to grow, one at a time, that do not reproduce throughout the deactivation. It is assumed that each member of the cell population alive at $t = 0$ is independently subjected to the same risk of dying. Moreover, the current size of the cell population depends solely on the size of the immediate past population. In other words, the system possesses the so-called Markovian property, implying that only the current state of the process or system is relevant in determining its future behavior;[26-28] in fact, the system under consideration constitutes a special type of Markov processes (time-continuous Markov chains) called "the pure-death process."[27,28]

***Identification of Random Variable and State Space*** • The number of live microorganisms, simply termed cells hereafter, at time t is taken as the random variable of the process of deactivation, N(t); a realization of N(t) is denoted by n. All the possible numbers of live cells are the states of the process and the collection of these numbers, $\{n_0, n_0-1, \ldots, 2, 1, 0\}$, is the state space, where $n_0$ is the initial number of cells susceptible to thermal disinfection, *i.e.,* n at $t = 0$.

***Construction of Transition Diagram*** • Since no cells will be produced, the size of the population will decrease throughout disinfection. In the transition diagram of the process presented in Figure 1, the circles indicate the possible states of the system and the arrows describe transitions of the system at any moment. The figure is a typical representation of the time-homogeneous pure-death process.

***Definition of Transition-Intensity Functions*** • The rate law adopted here for thermal deactivation (disinfection) is[1-3,5]

$$-\frac{dn}{dt} = kn \tag{1}$$

where n is the number of cells at a specific time t; this expression is known as Chick's law.[32] The intensity of transition (intensity function) is defined as the instantaneous rate of change of the transition probability.[27-28] Hence, the intensity of death, $\mu_n$, for the thermal disinfection under consideration can be assumed to be of the form

$$\mu_n = kn \tag{2}$$

where k is a proportionality constant. This expression implies that the cell-death rate is proportional to the number of

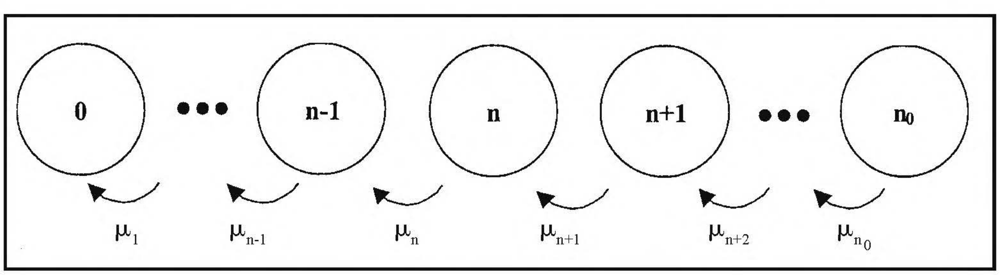


***Figure 1.*** *Transition diagram of the pure-death process: $\mu_n$ is the intensity of death, and $n_0, n_0-1, \ldots, n+1, n, n-1, \ldots, 2, 1, 0$ are the states of the process.*

live cells. Clearly, the intensity of death, $\mu_n$, is only a function of n and independent of time, and thus *time homogeneous.*[27.28]

***Derivation of the Master Equation*** • The governing equation of any Markov process expresses the infinitesimal change of the transition probability, $p_{ij}(s,t)$, between state i at arbitrary time s and state j at time t.[26,27] For convenience, the governing equation is often written in terms of the state (absolute)3õ≤obability rather than the transition probability. The absolute probabilities, $p_j(t)$ and $p_i(t)$, are related through the transition probabilities, $p_{ij}(s,t)$'s, as

$$p_j(t) = \sum_i p_i(s) p_{ij}(s,t)$$

This renders it possible to transform the transition probabilities in the governing equation into the absolute probabilities, thereby yielding the gain-loss or probability-balance equation, or master equation;[28,33] for the pure-death process under consideration, it is derived as follows:

• With N(t) = n given, it is assumed that during time interval (t, t+Δt): (1) the conditional probability that a death will occur, *i.e.*, a live cell will die, is $\mu_n \Delta t + o(\Delta t)$, and (2) the conditional probability that more than one death will occur is $o(\Delta t)$, which is defined such that

$$\lim_{\Delta t \to 0} \frac{o(\Delta t)}{\Delta t} = 0 \qquad (3)$$

Naturally, the conditional probability of no change in the number of live cells during this time interval is $[1 - \mu_n \Delta t - o(\Delta t)]$.

• Let the probability that exactly n cells are alive at time t be denoted as $p_n(t) = \Pr[N(t) = n]$, $n = n_0, n_0 - 1, \ldots, 2, 1, 0$. Then, for the two adjacent time intervals, (0,t) and (t, t+Δt), the occurrence of exactly n cells being alive at time (t+Δt) can be realized in the following mutually exclusive ways:

1) With a probability of $p_{n+1}(t)[\mu_{n+1}\Delta t + o(\Delta t)]$, exactly one cell will die during the time interval (t,t+Δt), provided that exactly (n+1) cells are alive at time t.

2) With a probability of $o(\Delta t)$, exactly j cells will die during the time interval (t, t+Δt), provided that exactly (n+j) cells are alive at time t, where $2 \le j \le (n_0 - n)$.

3) With a probability of $p_n(t)[1 - \mu_n \Delta t - o(\Delta t)]$, no cell will die during the time interval (t, t+Δt), provided that all n cells are alive at time t.

• Summing all these probabilities and consolidating all quantities of $o(\Delta t)$ yield

$$p_n(t+\Delta t) = p_n(t)(1 - \mu_n \Delta t) + p_{n+1}(t)(\mu_{n+1}\Delta t) + o(\Delta t) \qquad (4)$$

• Rearranging this equation and taking the limit as $\Delta t \to 0$ yield the master equation of the pure-death process given below (see Figure 1):

$$\frac{d}{dt} p_n(t) = \mu_{n+1} p_{n+1}(t) - \mu_n p_n(t) \qquad n = n_0, n_0 - 1, \ldots, 2, 1, 0 \qquad (5)$$

For $n = n_0$, we have $\mu_{n_0+1} = 0$; thus

$$\frac{d}{dt} p_{n_0}(t) = -\mu_{n_0} p_{n_0}(t)$$

or, by virtue of Eq. (2),

$$\frac{d}{dt} p_{n_0}(t) = -k n_0 p_{n_0}(t) \qquad (5a)$$

For $n = n_0 - 1, n_0 - 2, \ldots, 2, 1$, Eq. (5) is

$$\frac{d}{dt} p_n(t) = \mu_{n+1} p_{n+1}(t) - \mu_n p_n(t)$$

or

$$\frac{d}{dt} p_n(t) = k(n+1) p_{n+1}(t) - k n p_n(t) \qquad (5b)$$

Finally, for n = 0, we have $\mu_0 = 0$; thus,

$$\frac{d}{dt} p_0(t) = \mu_1 p_1(t)$$

or

$$\frac{d}{dt} p_0(t) = k p_1(t) \qquad (5c)$$

***Solution of the Master Equation*** • As can be discerned from Eq. (2), the intensity of death, $\mu_n$, is of linear form; as

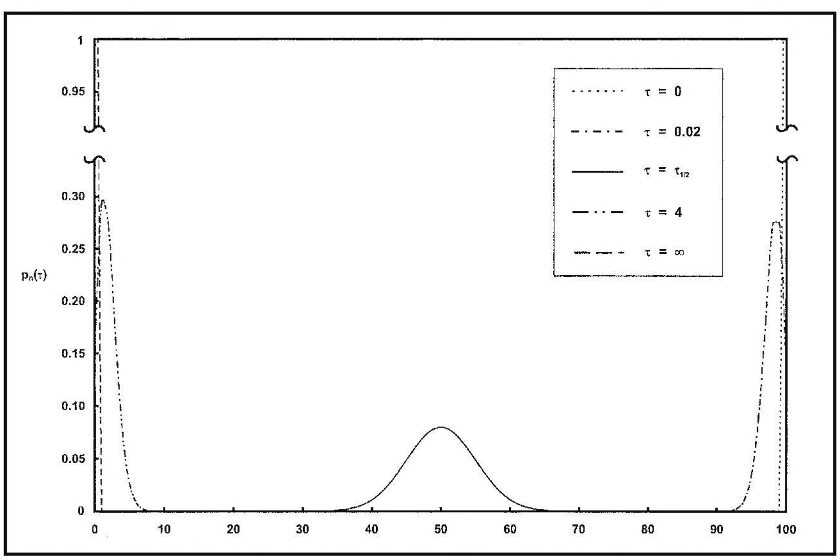


***Figure 2.*** *Temporal evolution of the binomial distribution of the number of live cells, N(t), with $n_0$ = 100.*

a result, the master equation, Eq. (5), can be solved recursively, thereby yielding the probability that n cells will be alive at time t, $p_n(t)$, as[5,34] (see Appendix A, available at <http://www.engg.ksu.edu/CHEDEPT/fan.htm>)

$$p_n(t) = \frac{n_0!}{\left[(n_0 - n)!\, n!\right]}\left(e^{-kt}\right)^n\left(1 - e^{-kt}\right)^{n_0 - n}$$
$$= \binom{n_0}{n}\left(e^{-kt}\right)^n\left(1 - e^{-kt}\right)^{n_0 - n} \tag{6}$$

The above expression indicates that the distribution of random number N(t) is binomial with two parameters. One of the parameters, $n_0$, representing the initial value of N(t), signifies the total number of the events that can possibly occur, and the other parameter, $e^{-kt}$, signifies the probability of occurrence of one event. For the thermal disinfection under consideration, $n_0$ is the number of cells alive at t = 0, which will eventually die, and $e^{-kt}$ is the probability of an individual cell being alive at time t. The temporal evolution of the binomial distribution as given by Eq. (6) is illustrated in Figure 2; for simplicity, $n_0$ is specified to be 100 and kt is lumped as $\tau$.

***Moments about the Mean*** • With the solution of the master equation in hand, we can proceed to calculate the mean and variance of the process that should constitute the core of any stochastic analysis and modeling. Furthermore, higher moments about the mean, such as skewness and kurtosis, are determined; they provide additional information useful for characterizing the stochastic and statistical properties of the process.[27,34-36] For illustration, the derivation of the skewness is elaborated in Appendix B (available at <http://www.engg.ksu.edu/CHEDEPT/fan.htm>)

*Mean.* The mean, E[N(t)] or m(t), which is the expected value (first moment) of the distribution of random variable N(t), is defined as

$$m(t) = E[N(t)] = \sum_n n p_n(t) \tag{7}$$

The mean or expected value, m(t), is the weighted sum of the realizations of the random variable where the weights are the probabilities corresponding to those realizations.[34]

For the thermal disinfection under consideration, the mean in terms of dimensionless time $\tau$ is

$$m(\tau) = n_0 e^{-\tau} \tag{8}$$

The normalized, *i.e.*, dimensionless form of the mean, $\overline{m}(\tau)$, is

$$\overline{m}(\tau) = \frac{m(\tau)}{n_0} = e^{-\tau} \tag{9}$$

*Variance.* The variance, Var[N(t)] or $\sigma^2(t)$, is the second moment of the distribution of random variable N(t) about the mean, m(t); thus

$$\sigma^2(t) = E\left\{\left[N(t) - E[N(t)]\right]^2\right\} = \sum\left\{n - E[N(t)]\right\}^2 p_n(t) \tag{10}$$

By expanding the above equation, $\sigma^2(t)$ can be related to the mean, m(t), as

$$\sigma^2(t) = E\left[N^2(t)\right] - m^2(t) \tag{11}$$

In the above expression, $E[N^2(t)]$ is the second moment of N(t), *i.e.*

$$E\left[N^2(t)\right] = \sum_n n^2 p_n(t) \tag{12}$$

For the thermal disinfection under consideration, the variance in terms of dimensionless time $\tau$, $\sigma^2(\tau)$, is, from Eqs. (8) and (11)

$$\sigma^2(\tau) = n_0 e^{-\tau}\left(1 - e^{-\tau}\right) \tag{13}$$

*Standard Deviation.* The standard deviation, $\sigma(t)$, of the process is the square root of the variance, $\sigma^2(t)$; thus

$$\sigma(t) = \left[\sigma^2(t)\right]^{1/2} \tag{14}$$

The variance, $\sigma^2(t)$, or more specifically, the standard deviation, $\sigma(t)$, signified the fluctuations, *i.e.*, scatterings, of the values of the random variable about their mean.

For the thermal disinfection under consideration, the standard deviation in terms of dimensionless time $\tau$, $\sigma(\tau)$, is, from Eqs. (13) and (14)

$$\sigma(\tau) = \sqrt{n_0 e^{-\tau}\left(1 - e^{-\tau}\right)} \tag{15}$$

*Coefficient of Variation.* The coefficient of variation, CV(t), is the quotient (or ratio) of the standard deviation, $\sigma(t)$, and the corresponding mean, m(t); thus[35]

$$CV(t) = \frac{\sigma(t)}{m(t)} \tag{16}$$

For the thermal disinfection under consideration, the coefficient of variation in terms of dimensionless time $\tau$, $CV(\tau)$, is, from Eqs. (8) and (15),

$$CV(\tau) = \sqrt{\frac{1 - e^{-\tau}}{n_0 e^{-\tau}}} \tag{17}$$

or

$$CV(\tau) = \sqrt{\frac{1}{n_0 e^{-\tau}} - \frac{1}{n_0}} = \sqrt{\frac{1}{m(\tau)} - \frac{1}{n_0}} \tag{17a}$$

*Skewness.* The skewness, $\gamma(t)$, is the quotient (or ratio) of the third moment of the distribution of random variable N(t) about the mean, m(t), and the third power of the standard deviation, $\sigma(t)$; thus[36]

$$\gamma(t) = \frac{E\left\{\left[N(t) - E[N(t)]\right]^3\right\}}{\left(\sqrt{E\left\{\left[N(t) - E[N(t)]\right]^2\right\}}\right)^3}$$

$$= \frac{1}{\sigma^3(t)} \sum_n \left\{n - E[N(t)]\right\}^3 p_n(t) \tag{18}$$

By expanding the above equation, $\gamma(t)$ can be related to the mean, m(t), and the standard deviation, $\sigma(t)$, as

$$\gamma(t) = \frac{1}{\sigma^3(t)}\left\{E\left[N^3(t)\right] - 3m(t)\sigma^2(t) - m^3(t)\right\} \tag{19}$$

where $E[N^3(t)]$ is the third moment of N(t) defined by

$$E\left[N^3(t)\right] = \sum_n n^3 p_n(t) \tag{20}$$

Skewness characterizes the degree of asymmetry of the distribution of random variable N(t) about the mean, m(t). Positive skewness indicates a distribution with a longer tail to the right of the mean than to the left, and negative skewness indicates a longer tail to the left of the mean than to the right. It vanishes for any symmetric distribution.

For the thermal disinfection under consideration, the skewness in terms of dimensionless time $\tau$, $\gamma(\tau)$, is, from Eqs. (8), (15), and (19)

$$\gamma(\tau) = \frac{\left(1 - e^{-\tau}\right) - e^{-\tau}}{\sqrt{n_0 e^{-\tau}\left(1 - e^{-\tau}\right)}} \tag{21}$$

*Kurtosis (Curtosis).* The kurtosis, k(t), is the quotient (or ratio) of the fourth moment of the distribution of random variable N(t) about the mean, m(t), and the fourth power of the standard deviation, $\sigma(t)$; thus[36]

$$k(t) = \frac{E\left\{\left[N(t) - E[N(t)]\right]^4\right\}}{\left(\sqrt{E\left\{\left[N(t) - E[N(t)]\right]^2\right\}}\right)^4}$$

$$= \frac{1}{\sigma^4(t)} \sum_n \left\{n - E[N(t)]\right\}^4 p_n(t) \tag{22}$$

By expanding the above equation, k(t) can be related to the mean, m(t), the standard deviation, $\sigma(t)$, and the skewness, $\gamma(t)$, as

$$k(t) = \frac{1}{\sigma^4(t)}\left\{E\left[N^4(t)\right] - 4m(t)\gamma(t)\sigma^3(t) - m^2(t)\left[6\sigma^2(t) + m^2(t)\right]\right\} \tag{23}$$

where $E[N^4(t)]$ is the fourth moment of N(t), *i.e.*,

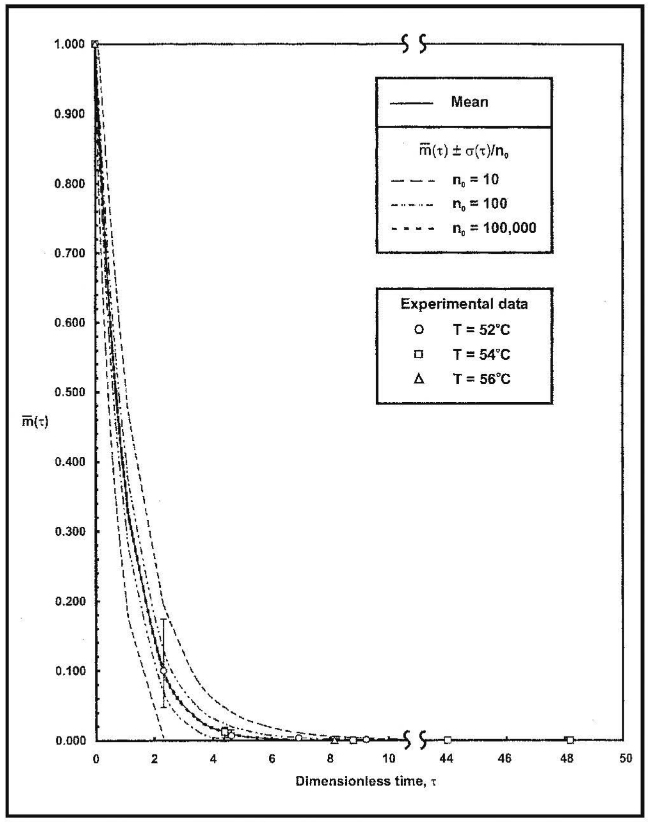


***Figure 3.*** *Normalized mean,* $\overline{m}$*, and standard deviation,* $\sigma$*, as functions of the dimensionless time,* $\tau$*, exhibiting the entire range of the number concentration of live cells.*

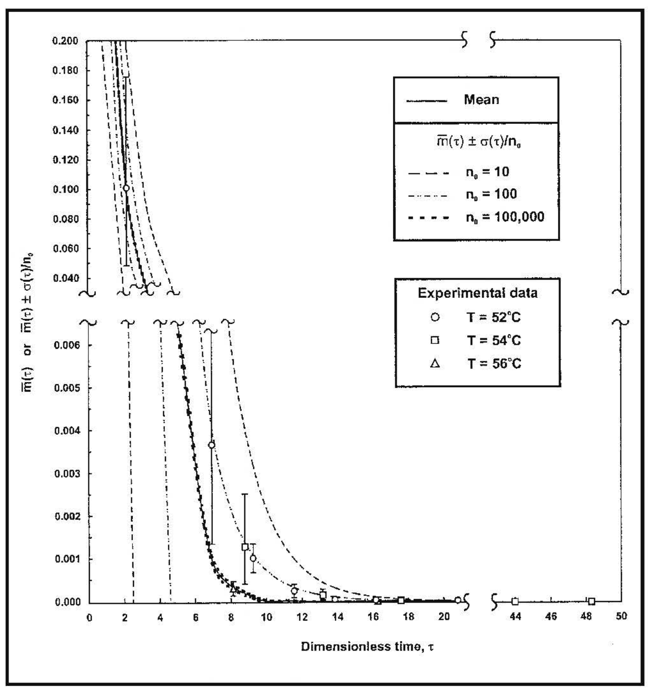


***Figure 4.*** *Normalized mean,* $\overline{m}$*, and standard deviation,* $\sigma$*, as functions of the dimensionless time,* $\tau$*, for the low range of the number concentration of live cells.*

$$E\left[N^4(t)\right]=\sum_n n^4 p_n(t) \tag{24}$$

Kurtosis is a measure of how outlier-prone, or peaked, the distribution of random variable N(t) is. The kurtosis of a distribution that is less outlier-prone than the normal distribution tends to be greater than 3, which is the kurtosis of the normal distribution, and the opposite is the case for a distribution that is more outlier-prone.

For the thermal disinfection under consideration, the kurtosis in terms of dimensionless time $\tau$, is, from Eqs. (8), (15), (21), and (23)

$$k(\tau)=\frac{1-6e^{-\tau}\left(1-e^{-\tau}\right)}{n_0 e^{-\tau}\left(1-e^{-\tau}\right)}+3 \tag{25}$$

## NUMERICAL SOLUTION

The mean, variance, skewness, and kurtosis of N(t) have been computed from their corresponding analytical expressions, Eqs. (8), (13), (21), and (25), respectively. They are functions of both the size of the initial cell population, $n_0$, and the time, t. The value of the proportionality constant, k, in the transition intensity, Eq. (2), can be recovered through the least-square fitting of the expression for the mean, Eq. (8), to the available experimental data of the thermal disinfection by means of a nonlinear minimization method, *e.g.*, the Levenberg-Marquant method.[37]

## RESULTS AND DISCUSSION

The model derived is illustrated with the same set of the available experimental data for the thermal death of *S. aureus* strain S-1 in neutral phosphate buffer[19] as those adopted by the major textbooks in biochemical engineering.[1-4] These data have been obtained at the temperatures of 325.15 K (52°C), 327.15 (54°C), and 329.15 (56°C), thereby yielding the values of k as 0.0192 $s^{-1}$ (1.15 $min^{-1}$), 0.0362 $s^{-1}$ (2.17 $min^{-1}$), and 0.0678 $s^{-1}$ (4.07 $min^{-1}$), respectively. With these values of k, the mean, as well as the variance or standard deviation, skewness, and kurtosis, of the number concentration of live cells have been computed. These quantities are graphically presented and their significance is discussed.

<u>*Mean*</u> • The mean, $m(\tau)$, and the normalized mean, $\overline{m}(\tau)$, have been computed according to Eqs. (8) and (9), respectively. Only the latter, which is the exponential decay function independent of any parameters, is graphically plotted in Figures 3 and 4 as a function of dimensionless time $\tau$. The former exhibits the entire range of $\overline{m}(\tau)$ and the latter, the low range. Naturally, Eq. (8) or (9) as well as $\overline{m}(\tau)$ are in accord with those given in the available textbooks[1-4] as well as in the original contributions.[5,6] The experimental data[19] are also superimposed in both figures for comparison.

<u>*Variance, Standard Deviation and Coefficient of Variation*</u> • The expression for variance, $\sigma^2$, Eq. (13), is given by Blakebrough[1] and Fredrickson.[5] The variance is a measure of the variability, spread, or dispersion of the values of a random variable. Naturally, the larger the value of the variance, the greater the dispersion of the values of the random variable about their mean.

The standard deviation, $\sigma$, is obviously the square root of the variance, $\sigma^2$. The value of $\sigma(\tau)$ as given by Eq. (15) varies from 0 at $\tau$=0, reaches its maximum at $\tau_{1/2}$, or $\tau=\ell n 2$, where $\overline{m}(\tau)=1/2$, and eventually vanishes as $\tau\to\infty$, as expected. This trend of the $\sigma(\tau)$'s variation in terms of $\overline{m}(\tau)\pm\sigma(\tau)/n_0$ for three values of $n_0$ is also illustrated in Figures 3 and 4. Note that in these figures, especially in the latter, the deviations of the majority, if not all, of the available experimental data are substantially more pronounced than those of the deviations predicted by the model in view of the reported $n_0$ between 7.5 x $10^6$ and 19 x $10^6$ in obtaining the experimental data.[19] This is almost always the case: the overall deviations of the experimental data include not only those attributable to the internal or characteristic noises of the process as predicted by the stochastic model, but also to the external noises due to instrumental deficiencies and errors that can never be totally eliminated.

The coefficient of variation, $CV(\tau)$, is defined to provide a meaningful relative measure of the variability, spread, or dispersion of the values of a random variable about their mean. Note that $CV(\tau)$ expresses the random variable's dispersion as a fraction of the mean, or frequently, as a percentage.

For the thermal disinfection under consideration, $CV(\tau)$, specifically, the relative variation of size of the cell population about its mean, at any dimensionless time $\tau$ is inversely proportional to the square root of the initial cell population size, $n_0$, as indicated by Eq. (17) or (17a). By evaluating $CV(\tau)$ for various values of $n_0$, $m(\tau)$, and their combinations, it can be readily shown that

- At any $\tau$, the larger the $n_0$, the smaller the $CV(\tau)$, or the relative extent of the fluctuations
- For any $n_0$, $CV(\tau)$ is initially zero and increases monotonically with $\tau$, and the smaller the $m(\tau)$, the larger the $CV(\tau)$
- For any $m(\tau)$, $CV(\tau)$ increases monotonically with the increase in $n_0$ and asymptotically approaches a constant value, and the smaller the $n_0$, the smaller the $CV(\tau)$.

<u>*Skewness*</u> • Skewness $\gamma(t)$, as defined by Eq. (18), measures the extent of asymmetry of the distribution of random variable N(t) relative to its extent of deviation or dispersion. Thus, it is indeed a meaningful measure of asymmetry; nevertheless, $\gamma(t)$ depends on parameter $n_0$.

For the thermal disinfection under consideration, $\gamma(\tau)$ has been evaluated according to Eq. (21) for $n_0$ of 10, 100, and 100,000; the values of $\gamma(\tau)$ obtained are illustrated in Figure

5. The configurations of the resultant curves can be discerned at least qualitatively from that of the probability distribution of N(t) presented in Figure 2; it is binomial in nature. Note that when $\tau$ is nearly 0, N($\tau$) can assume only those values immediately to the left of $n_0$; thus, its distribution is highly skewed to the left and consequently, gives rise to $\gamma(\tau)$ with an appreciable negative value. The opposite is the case as $\tau \rightarrow \infty$. Naturally, in between these two extremes, $\gamma(\tau)$ approaches from either direction to 0, which is the value of $\gamma(\tau)$ for the normal distribution, at $\tau = \tau_{1/2} = \ell n2$.

<u>Kurtosis</u> • Kurtosis k(t), as defined by Eq. (22), measures the degree of peakedness of the distribution of random variable N(t) relative to its extent of deviation or dispersion. Thus, it is indeed a meaningful measure of peakedness; nevertheless, as for $\gamma(t)$, k(t) depends on parameter $n_0$.

For the thermal disinfection under consideration, the values of $k(\tau)$ have been computed by Eq. (25) for $n_0$ of 10, 100, and 100,000 and plotted in Figure 6. Similar to $\gamma(\tau)$ presented in Figure 5, the configuration of the resultant curves can be readily interpreted in the light of Figure 2. When $\tau$ is nearly 0, N($\tau$) can assume only those values in the immediate vicinity of $n_0$, and thus its distribution is highly peaked, giving rise to $k(\tau)$ with a large positive value; the same is the case at $\tau \rightarrow \infty$ when the values of N($\tau$) are nearly 0. In between these two extremes, $k(\tau)$ approaches from either direction to 3, which is the value of $k(\tau)$ for the normal distribution, at $\tau = \tau_{1/2} = \ell n2$.

## CONCLUSIONS

A stochastic model for the thermal death kinetics of a cell population as a pure-death process has been derived based on the first-order rate law. The solution of the governing differential equation of the model, termed the master equation, yields the probability distribution of the number concentration (density) of live cells during disinfection, which is regarded as the random variable of the process; the resultant distribution is the binomial distribution whose two parameters are the number of cells initially alive, which will eventually die, and the probability of an individual cell being alive, expressed as the exponential decay function. In addition to the mean of live cells, various higher moments about the mean have been derived to characterize this distribution. These higher moments include variance (second moment about the mean), skewness (third moment about the mean over the third power of the standard deviation), and kurtosis (fourth moment about the mean over the fourth power of the standard deviation). Only the expressions for the mean and variance are available in one or more of the existing major textbooks in biochemical engineering. Naturally, augmenting them with the skewness and kurtosis would better characterize the distribution, thereby deepening the understanding of stochastic, *i.e.*, temporally varying probabilistic, nature of thermal death of cells during their disinfection.

Thermal disinfection has long been regarded as a suitable or useful instructional example for illustrating stochastic analysis and modeling of biochemical phenomena or processes, the majority of which deal with discrete mesoscopic entities that are neither microscopic nor macroscopic. To enhance its usefulness, the example has been substantially elaborated in the current exposition. As indicated at the outset of this article, various chemical engineering courses are richly populated with subjects involving mesoscopic entities, such as bubbles, droplets, and particles including nanoparticles. Thus, these subjects would be suitable examples for

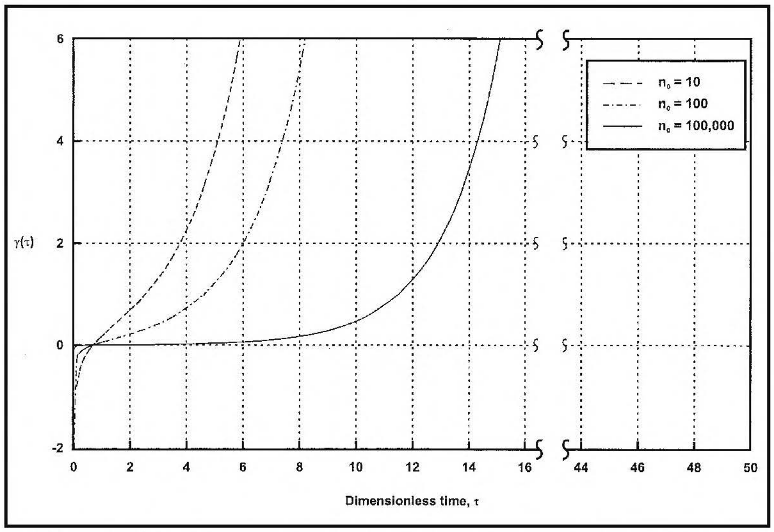


***Figure 5.*** *Skewness as a function of the dimensionless time, $\tau$, and the initial size of cell population, $n_0$, as the parameter.*

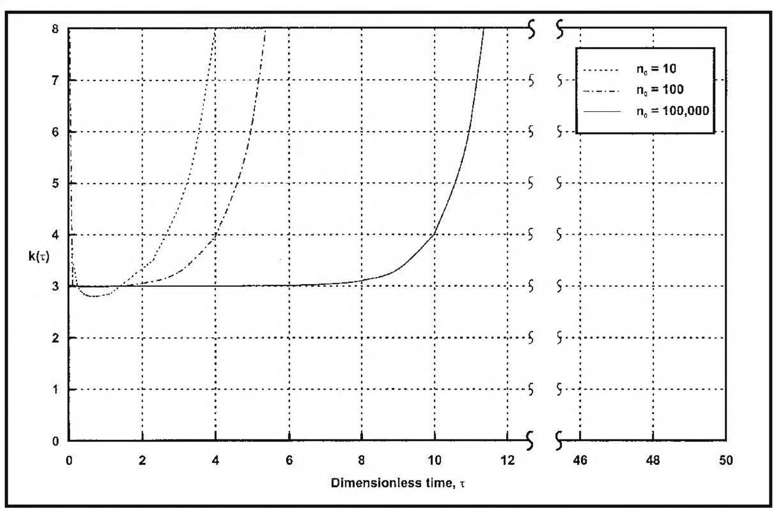


***Figure 6.*** *Kurtosis as a function of the dimensionless time, $\tau$, and the initial size of cell population, $n_0$, as the parameter.*

introducing the application of stochastic processes in these courses, similar to the thermal destruction of microorganisms for biochemical engineering.


## ACKNOWLEDGMENT

The authors are grateful for the constructive criticisms received from the three reviewers, including Professor Ramkrishna of Purdue University.


## NOMENCLATURE

| | |
|---|---|
| $E[N(t)]$ | mean, expected value, or the first moment of the random variable, $N(t)$ |
| $E[N^2(t)]$ | second moment of the random variable, $N(t)$ |
| $E[N^3(t)]$ | third moment of the random variable, $N(t)$ |
| $E[N^4(t)]$ | fourth moment of the random variable, $N(t)$ |
| $k$ | proportionality constant in the intensity of death, Eq. (2), $min^{-1}$ |
| $k(t)$ | kurtosis of the random variable, $N(t)$ |
| $N(t)$ | random variable |
| $m(t)$ | $E[N(t)]$ |
| $n$ | realization of the random variable, $N(t)$ |
| $n_0$ | number of live cells at $t = 0$ |
| $p_n(t)$ | probability that the process will be in state n at time t |
| $t$ | time |
| $\gamma(t)$ | skewness of the random variable, $N(t)$ |
| $\mu_n$ | intensity of death for the pure-death process in state n |
| $\sigma^2(t)$ | $Var[N(t)]$ |
| $\sigma(t)$ | standard deviation of the random variable, $N(t)$, as defined in Eq. (14) |

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The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested, as well as those that are more traditional in nature and that elucidate difficult concepts. Manuscripts should not exceed ten double-spaced pages if possible and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

# CHOOSING AND EVALUATING EQUATIONS OF STATE FOR THERMOPHYSICAL PROPERTIES

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Two kinds of pressure-volume-temperaure P-$\nu$-T diagrams for real substances are usually introduced in the first undergraduate thermodynamics course (hereafter, "thermo I"): a typical P-$\nu$-T diagram for a substance that contracts on freezing, *e.g.,* carbon dioxide, and a P-$\nu$-T diagram for a substance that expands on freezing, usually water (see, for example, References 1-4). The relevance of the P-$\nu$-T data is usually discussed, and different P-$\nu$-T functions or equations of state are introduced. From this moment until the end of their professional life, chemical engineering students (or chemical engineers) will have to deal with the P-$\nu$-T relations, in one way or another.

Most chemical engineers will never develop a new EOS, but they will often be in the position of having to select an equation that is the most appropriate for a specific situation. De Nevers and Seader[5] pointed out ten years ago that students must learn that "computer answers may depend strongly on which correlations for thermodynamic properties are used. Students need to learn of the many sources of such correlations, along with their limitations and recommended regions of applicability. Also, they need to be aware of experimental sources of data and how to make comparisons between experimental data and empirical correlations."

It is well known that practical engineering applications are deeply affected by fundamentals of thermodynamics. Harvey and Laesecke[6] recently stated, "Engineers should learn the value of thermophysical properties in college." We agree with this statement. Students must be able to choose from among several methods and be aware of how their choice may depend on the nature of the system and state conditions; moreover, they should be exposed to this matter at an early stage of their career.

In traditional chemical engineering curricula, students start to evaluate different models using process simulators such as ASPEN PLUS, ProSIm, or ChemStation in their chemical process courses, typically during the third and/or fourth year

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of their studies. In this work, we give an example of how students can be introduced to this topic from an early stage in their career (thermo I), continuing progressively to their professional life (or graduate studies). We present a thermo project where the student will need to use the Internet, handle some software, and read tables.

## PROJECT STATEMENT

Carbon dioxide ($CO_2$) has been studied since the days of van der Waals, since it exhibits supercritical behavior at moderate conditions. Nowdays, $CO_2$ is used in a variety of fields, *e.g.,* in the oil industry (as a carrier gas for enhanced oil recovery) and in "green chemistry," where research efforts are under way to identify sustainable processes and products using $CO_2$-related technology. Carbon dioxide is extremely attractive in industrial applications because it is the second most abundant and the second least expensive solvent on earth.

In this project, the student is asked to evaluate the P-$\nu$-T prediction capabilities of different models for carbon dioxide. They are asked to obtain P$\nu$ (or P$\rho$, where $\rho = 1/\nu$ = density) diagrams for carbon dioxide showing at least three isotherms, 278.15 K, 198.15 K, and 360 K, for a pressure range from 0.51795 MPa up to 100 MPa, in the gas and liquid phases, as well as the vapor-liquid equilibrium region (from the triple point [$T_t$ = 216.592 K, $P_t$ = 0.51795 MPa] up to the critical point). They are told to compare the volume (or density) predictions in each phase (including the critical region) obtained from

- Two cubic equations of state (*e.g.,* Soave-Redlich-Kwong[7,1] and Peng-Robinson[8,1])
- A three-parameter corresponding states method (*e.g.,* Lee-Kesler[9,1] tables)
- A multiparametric EOS for $CO_2$ (*e.g.,* Span-Wagner[10,11])
- Tables of thermodynamic properties for $CO_2$ (IUPAC[12] tables)

For extra credit, the student can comment on the use of the virial EOS (truncated at the second virial term, in the density expansion) and the Rackett[13,14,1] equation for the determination of volume for the gas and saturated liquid phases, respectively.

The tables mentioned in Section d, below, are from fits of thermodynamic properties to multiparametric equations, *i.e.,* they are smoothed data. But these tables[12] are based on older carbon dioxide data. We believe that the Span-Wagner equation[10] is the best representation of the experimental data for carbon dioxide and should be used as the standard against which to test the other equations of state and the corresponding states method.[15] Span and Wagner made a careful analysis of all the experimental data for carbon dioxide, including recent data, and excluded data that did not satisfy the thermodynamic consistency conditions when fitting their equation of state.

### *Justification*

a. This project would not have been feasible for a thermo I course ten to fifteen years ago, but with the availability of computers, software, and the Internet, it is now rather straightforward. Textbooks come with computer-aided strategies for solving cubic equations of state, such as a) the use of "meta-computing" software involving the use of packages such as Maple, Mathematica, Mathcad, and Matlab[*i.e.,*1, 3]; b) the use of spreadsheets such as EXCEL,[*i.e.,*3] or c) the supply of a "code" that can be used for a specific cubic or multiparametric equation of state.[2,3] Additionally, several sites can be found on the Internet where on-line cubic EOS software is available at no charge.[*i.e.,*16]

b. Corresponding-state correlations are usually introduced in textbooks[1-4] in graphical or tabular form. We believe that students must become familiar with the use of tables and graphs, but we should also keep in mind the pedagogic importance of the implementation of corresponding-state principles by meta-computing software, as was recently discussed by Smith, *et al.*[17]

c. Students should also be exposed to state-of-the-art multiparametric EOS available in up-to-date databases. This can be pursued through the Internet, where leading institutions such as NIST or DECHEMA have friendly web pages. For example, the NIST chemistry webbook[11] contains thermophysical properties for 33 pure substances. Tester and Modell[18] list in Chapter 13 of their book some of the commonly used sources of pure component and mixture data in both published and electronic form. Additionally, they give examples of United States research centers that focus on physical property measurements and data correlation.
Ideally, recent developments in molecular-based EOS should also be included. Unfortunately, to the best of our knowledge, molecular-based EOS (*e.g.,* Statistical Associating Fluid Theory, or SAFT[19]) software is not yet available for use at the undergraduate level. The availability of such software in the near future is likely, however, as these kinds of EOS are already included in graduate-level textbooks[18,20] and in at least one introductory textbook.[3]

d. Students should become familiar with the use of tables for the determination of thermodynamic properties of fluids. Usually, the steam tables are in an appendix in thermodynamic textbooks, and sometimes a few extra tables for different substances are also included. It should be made clear to the students that no published thermodynamics table is a direct transcript of experimental measurements, because such data must be smoothed, correlated, and made internally consistent by means of a mathematical model, *i.e.,* by an equation of state. Thus, thermodynamic tables can become obsolete as new data and improved fundamental EOSs become available. For carbon dioxide, several sources are available.[10,11,21,22]

## SOLUTION

Homogeneous fluids are normally divided into liquids and gases, but this distinction cannot always be sharply drawn because the two phases become indistinguishable at the critical point. Several authors[1-4] define the supercritical region as the region existing at temperatures and pressures above the critical temperature and critical pressure; this region is bounded by the dotted lines in Figure 1. For simplicity, in this project we will use this definition of the supercritical state. The critical conditions for $CO_2$ are $T_c$ = 304.128 K, $P_c$ = 7.3773 MPa, and $\rho_c$ = 467.6 kg/m$^3$. Thus, the isotherm at 360 K will be analyzed as supercritical for pressures above the critical pressure.

In this work, we use the Internet to obtain the predictions of the Span-Wagner EOS through the NIST webbook[11] and to obtain the predictions of the Peng-Robinson equation from Reference 16. We read the tables presented in the Appendix of Reference 1 for the Lee-Kesler model and also the tables presented in Reference 12 for pure carbon dioxide. Finally, we program the Soave-Redlich-Kwong EOS using the VisualBasic macro of Excel and use that program to show the results. This is only one of several possible lines of attack that students can choose to solve their assignment.

***Vapor-Liquid Equilibria Region***

The phase envelope (vapor-liquid equilibria or saturation conditions) for carbon dioxide is shown in Figure 2. Results are shown for the Span-Wagner, Peng-Robinson, and Soave-Redlich-Kwong equations and also from the IUPAC tables. Results from the Lee-Kesler method are not shown because the available tables in Reference 1 (as well as in the original publication[9]) are provided only for the single phase (liquid or vapor). (The reason is that the Lee-Kesler method fails to predict a well-behaved van der Waals loop at near-critical temperatures, thus making it impossible to find two fluid states with the same fugacity; in normal practice, saturation pressures from the Lee-Kessler EOS are obtained from a separate linear correlation proposed by the same authors.[9])

This figure illustrates the predictive capabilities of multiparametric equations of state. The Span-Wagner EOS is the equation most frequently used for carbon dioxide and can be taken as a reference (for a more detailed discussion, see References 10 and 11). On the scale of the graph, results from the IUPAC tables are equivalent. It is worth mentioning that tables,[1] software, and Internet[11] were used in this stage of the project, and they can also be used to show that "old" methods (tables) are not necessarily less accurate than "new" methods (Internet), or vice versa. Deficiencies of cubic equations of state in the critical region as well as in the prediction of liquid densities are shown by the SRK and PR results. For carbon dioxide, in the region under study, the PR equation is more accurate than SRK.

The phase envelope for carbon dioxide is also shown in Figure 3, but in a P-ρ diagram, which can be used to show the practical convenience of

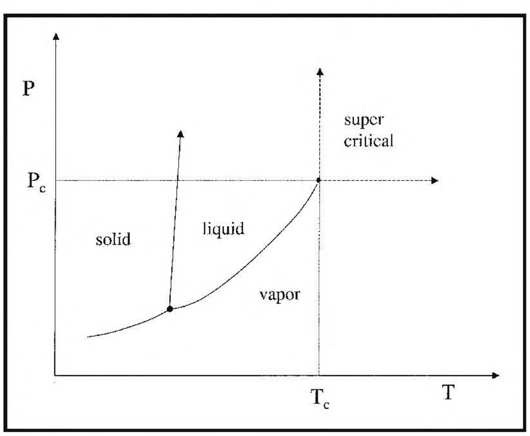


***Figure 1.*** *PT diagram for a pure substance that contracts on freezing.*

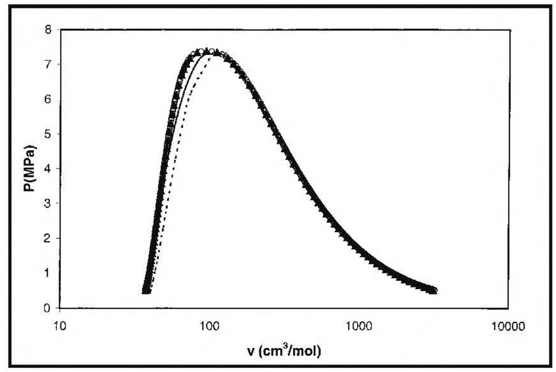


***Figure 2.*** *Vapor-liquid phase envelope for carbon dioxide shown as a P-v diagram. Continuous line predicted by the Peng-Robinson EOS,[8] dashed line predicted by the Soave-Redlich-Kwong EOS,[7] (○) predicted by the Span-Wagner EOS,[10] and (▲) predicted from the IUPAC tables.*

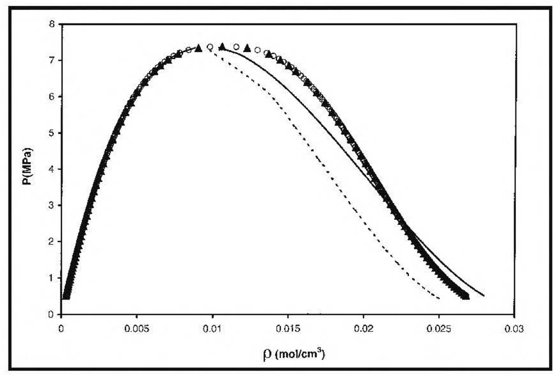


***Figure 3.*** *Vapor-liquid phase envelope for carbon dioxide shown as a P-ρ diagram. Continuous line predicted by the Peng-Robinson EOS,[8] dashed line predicted by the Soave-Redlich-Kwong EOS,[7] (○) predicted by the Span-Wagner EOS,[10] and (▲) predicted from the IUPAC tables.*

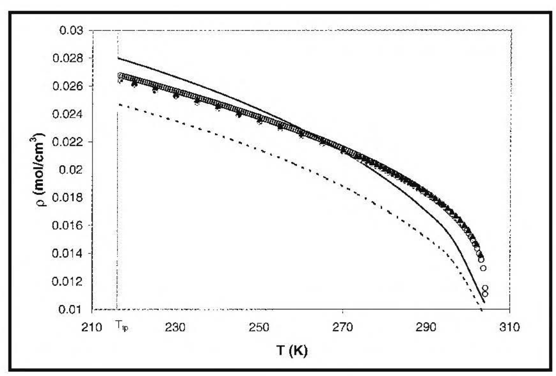


***Figure 4.*** *Saturated liquid density versus temperature diagram for carbon dioxide. Continuous line predicted by the Peng-Robinson EOS[8], dashed line predicted by the Soave-Redlich-Kwong EOS,[7] (○) predicted by the Span-Wagner EOS,[10] (●) from the Rackett equation,[13] and (▲) from the modified Racket equation due to Spencer and Adler.[14]*

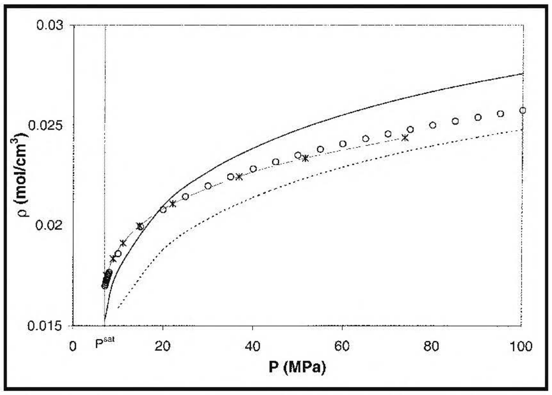


***Figure 5.** Density versus pressure diagram for carbon dioxide at 298.15 K, liquid phase. Continuous line predicted by the Peng-Robinson EOS,[8] dashed line predicted by the Soave-Redlich-Kwong EOS,[7] (○) predicted by the Span-Wagner EOS,[10] and (*) from the corresponding states method (Lee-Kesler tables in [1]).*

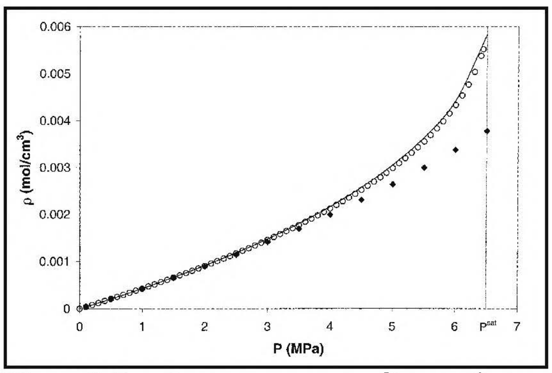


***Figure 6.** Density versus pressure diagram for carbon dioxide at 298.15 K, vapor phase. Continuous lines predicted by Peng-Robinson EOS,[8] (○) predicted by Span-Wagner EOS,[10] and (◆) predicted by virial equation (expanded in the density series and truncated at its second term).*

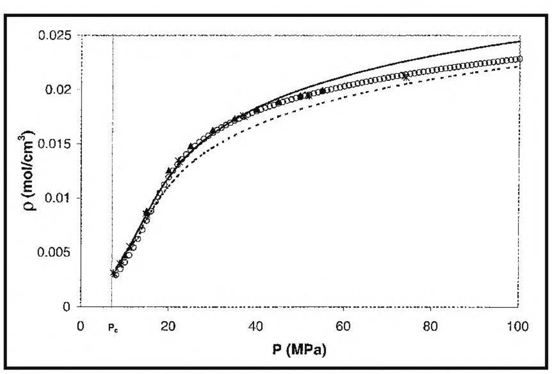


***Figure 7.** Density versus pressure diagram for carbon dioxide at 360 K, a supercritical state. The continuous line is the Peng-Robinson EOS,[8] (○) is predicted by Span-Wagner EOS,[10] and (◆) is predicted by the virial equation (expanded in the density series and truncated at its second term).*

working in terms of density. (Density is convenient to use because it always stays finite as P –> 0, whereas V diverges.[3])

The Rackett equation[13] is a simple empirical equation for determination of saturated liquid volumes and relates them to the reduced temperature and the critical compressibility factor. Molar densities obtained from the original Rackett equation are shown in Figure 4 (closed gray circles); closed triangles represent the prediction from the modified Rackett equation due to Spencer and Adler.[14] Among the methods studied here, the modified Rackett equation gives the best prediction of saturated liquid densities.

### *Liquid Phase*

The density versus pressure diagram for carbon dioxide at 298.15 K is shown in Figure 5, from the saturation pressure (6.43 MPa) up to 100 MPa. Results are shown for the Span-Wagner, Peng-Robinson, and Soave-Redlich-Kwong equations and also from the corresponding states method (Lee-Kesler tables). Results from the IUPAC tables are not shown for clarity of the graph, but the results are equivalent to the Span-Wagner equation up to 60 MPa (range of validity of the IUPAC tables). This figure corroborated deficiencies of cubic equations of state in the prediction of liquid densities, as shown by the SRK and PR results. Prediction from the Lee-Kesler method are also shown in this figure, and good agreement with the Span-Wagner equation is obtained up to the range of validity of the tables (73.7 MPa or $P_r = P/P_c = 10$).

### *Vapor Phase*

Except for the virial equation, all EOSs represent the saturated vapor region very well, as seen from Figures 2 and 3. In Table 1 we present the relative errors with respect to the Span-Wagner prediction for the two isotherms under study (278.15 and 298.15), from 0.51795 MPa (triple point) up to the vapor pressure at each temperature. Table 1 shows that all equations behave very well in the vapor phase, with an average error less than 2%, except the virial equation.

The virial equation (expanded in the density series and truncated at its second term) is often recommended[1-4] for use at low pressures (under 1 MPa). The results in Figure 6 show that for carbon dioxide at 298.15 K the virial equation can be used up to 2.5 MPa, with an error less than 2%. The PR EOS predictions are shown for comparison. The second virial coefficient was taken from the correlation due to Pitzer and Curl and presented in Reference 1.

### *Supercritical State*

The density versus pressure diagram for carbon dioxide at 360 K is shown

**TABLE 1**
**Relative Errors* for the Vapor Phase with Respect to the Span-Wagner EOS Predictions**

| EOS/Temperature (K) | Virial | SRK[7] | PR[8] | LK[9] | IUPAC[12] |
|---|---|---|---|---|---|
| 278.15 ($P^{sat}$ = 3.9695 MPa) | 5 | 2.7 | 1.3 | 0.82 | 1.76 |
| 298.15 ($P^{sat}$ = 6.4342 MPa) | 4.6 | 1.9 | 0.76 | 0.64 | 1.17 |

$$* \quad \sum_{n=1}^{Np}\left(\frac{\rho_{Span-Wagner} - \rho_{EOS}}{\rho_{Span-Wagner}}\right)100$$

in Figure 7, from the critical pressure up to 100 MPa. Results are shown for the same equations and methods presented for the liquid phase (Figure 5) corroborating the validity of the corresponding states method (Lee-Kesler tables) for carbon dioxide in the homogeneous phase up to the range of validity of the tables (73.7 MPa or $P_r = P/P_c = 10$). Deficiencies of cubic equations of state in the prediction of liquid-like densities (high pressures) are shown by the SRK and PR results.

***The "Complete" P-ν Diagram***

The P-*ν* diagram for carbon dioxide predicted from the Span-Wagner equation is shown in Figure 8. The construction of this diagram is straightforward for the student from the NIST webpage.[11]

## FINAL COMMENTS

The results in Figures 2-7 can be used to discuss the advantages and deficiencies of the various methods. For example, Figure 3 can be used to discuss the deficiencies of cubic equations of state in the critical region as well as in the prediction of liquid densities, and Figure 5 can serve to show the importance of using a model within its range of validity; *e.g.*, if the IUPAC tables are extrapolated to 100 MPa (results not shown), errors up to 200% can be found.

Care must be taken to emphasize that although it is possible to draw conclusions about the best EOS for $CO_2$ (or any other substance) for a given property and range of state conditions, such conclusions cannot be extended to other fluids, properties, or state conditions without further calculations. Thus, although the PR equation is found to be superior to the SRK equation for $CO_2$ properties studied here, quite different conclusions may be drawn for another fluid. For this purpose,

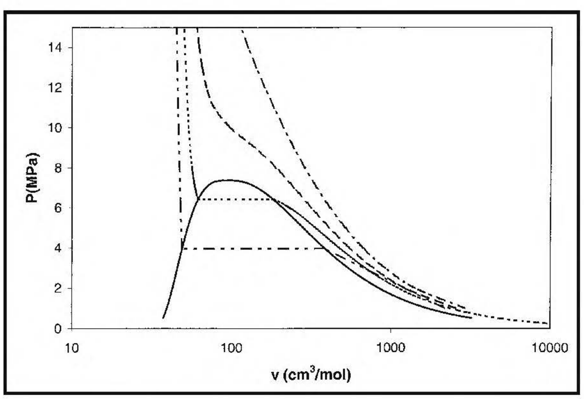


***Figure 8.*** *Carbon dioxide P-ν diagram predicted by Span-Wagner EOS.[10] The continuous line represents the vapor-liquid phase envelope. The dotted-dashed line is the 360 K isotherm, the dashed line is the 320 K isotherm, the dotted line is the 298.15 K isotherm, and the double-dotted dashed line is the 278.15 K isotherm.*

different substances can be assigned to each student, or results for other substances/regions can be shown in class.


## ACKNOWLEDGMENTS

We would like to thank our students at both Simón Bolívar and North Carolina State Universities for their support, feedback, and motivation on the implementation of this project. This material is based on work supported in part by the STC Program of the National Science Foundation under Agreement No. CHE 9876674.


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