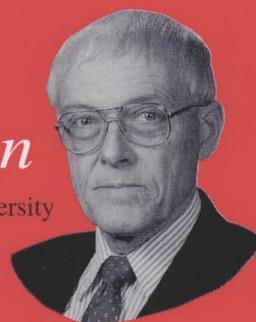




### Maurice A. Larson

of Iowa State University



#### AWARD LECTURE

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*and ChE at . . .*

**Washington State University**



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 Web Page: <http://www.che.ufl.edu/cee/>

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# MAURICE A. LARSON

of  
*Iowa State University*

## “Mr. Crystallization”



*Mauri as a farm boy in 1936,  
as an enlistee in the Armed Forces in 1946,  
and as a distinguished professor in 1998.*

Widely respected and recognized the world over for his research contributions, Maurice Larson is a distinguished and accomplished chemical engineer who has been a influential figure in chemical engineering education and practice for nearly forty years. In the area of crystallization, which he was instrumental in changing from an art to a science and into a thriving field of research, he is looked upon as a father figure. His contributions have been both pioneering and original in the context of their times.

Mauri was born on a farm in the Loess Hills near Missouri Valley, Iowa, the second child in a family of two girls and one boy. He attended a one-room country school that had twenty students in eight grades. (Interestingly, of the six students in his class, three ultimately received PhDs in engineering!) When he was nine, his family moved to another farm, this one near Ayrshire, Iowa, 150 miles away. The school there consisted of all twelve grades and had about 220 students.

Mauri graduated in a class of twenty-one students in 1944. In 1946, he enlisted in the Army and was later discharged just in time to begin study at Iowa State College in the fall of 1947. He initially planned to study chemistry but, influenced by a newspaper article he happened to read, he enrolled in chemical engineering instead. Subsequent to his graduation in 1951, he accepted employment with the Dow Corning Corporation in Midland, Michigan.

Mauri had always had in mind going on to graduate school

and, after marrying Ruth Gugeler, an ISU chemistry graduate and a co-employee at Dow Corning, he decided the time had come to do so. He enrolled in graduate school at Iowa State and secured employment as a teaching assistant. He found he greatly enjoyed working with students and was soon was promoted to instructor. His thesis research was in the area of phosphate fertilizer chemistry and production.

After receiving his PhD in 1958, Mauri was appointed Assistant Professor in the department, and his research broadened from fertilizer technology to process dynamics and control. He organized and taught one of the first undergraduate process control courses in the U.S. and was also one of the first to organize a course around the seminal text *Transport Phenomena* by R. B. Bird, W. E. Stewart, and E. N. Lightfoot. He and his graduate students published in the areas of fertilizer technology and process dynamics, and nationally he was elected Chair of the Division of Fertilizer and Soil Chemistry of the American Chemical Society.

In 1959 a new graduate student, Alan Randolph, arrived at Iowa State with industrial experience in the crystallization of ammonium sulfate. Alan was concerned about the limit cycle in crystal size distribution that occurred in large continuous

crystallizers. Mauri's interest in both process dynamics and fertilizer technology resulted in a perfect interest match with Alan, and a result of their collaboration was the landmark paper "Transient and Steady State Size Distributions in Continuous Mixed Suspension Crystallizers"—an important publication that set the agenda in industrial crystallization research for the next thirty-five years.

"Mauri and I met in 1959 and we immediately realized we had similar research interests," says Alan Randolph, now an Emeritus Professor of Chemical Engineering at the University of Arizona. "I was fortunate to be one of his first PhD students, and he and I have been lifelong colleagues and friends ever since that time. Mauri is clearly responsible for much of the early fundamental work in crystallization. He stimulated the work of many others and the field has benefited greatly from his work," Randolph continues. "A good example of his supportive approach is an occasion when he was visiting our family in Trona, California. Mauri and I went on a trip to see the Panamint Mountains and our old blue Rambler was not able to make it up one of the steep grades. I shouted to Mauri, "Get out and push!" Amazing as it may seem, he actually pushed the car uphill—illustrating that Mauri is not only imperturbable, but he is also a true friend who knows the meaning of support!"

Mauri's subsequent research at Iowa State was concerned with many aspects of solution crystallization. In addition to analyzing continuous crystallizer stability, he developed methods to collect data on and realistically describe nucleation and growth, secondary nucleation effects of additives, and growth dispersion. Alan and Mauri were the first to provide a firm mathematical foundation to the analysis of crystallization by introducing and expanding the use of Alan's population balance models. Their early studies on population balances formed the basis for several entirely new areas of crystallization research and theory. Several of Mauri's twenty-six PhD and twenty-seven MS students have been continuing contributors to crystallization fundamentals and practice.

Many if not all fields of chemical engineering have pioneering names indelibly associated with their growth. By any account, Maurice A. Larson is one such name. No book on crystallization, no review on the subject, indeed no really worthwhile paper in the specific areas of his research, would be complete without reference to his contributions, in particular to the book he coauthored with Alan, *The Theory of Particulate Processes, Analysis and Techniques in Continuous Crystallization* (A. D. Randolph and M. A. Larson, 1st ed. 1972; 2nd ed. 1988; Academic Press). "It has become one of the standard references for the field," says Dr. L. K. Doraiswamy, Anson Marston Distinguished Professor and Herbert L. Stiles Professor of Chemical Engineering.

Mauri's international standing in the area of crystallization is firmly established. His activities have included collaboration with experts from the United Kingdom, Australia, India, China, The Netherlands, Poland, Czechoslovakia, and many other countries. For twenty-five years he has also been active with the European Federation of Chemical Engineering Working Group on Crystallization. To strengthen his research, he spent a year at Stanford on a National Science Foundation Faculty Fellowship, a year at University College London as Shell Visiting Professor, and a year at the University of Manchester Institute of Science and Technology (UMIST).

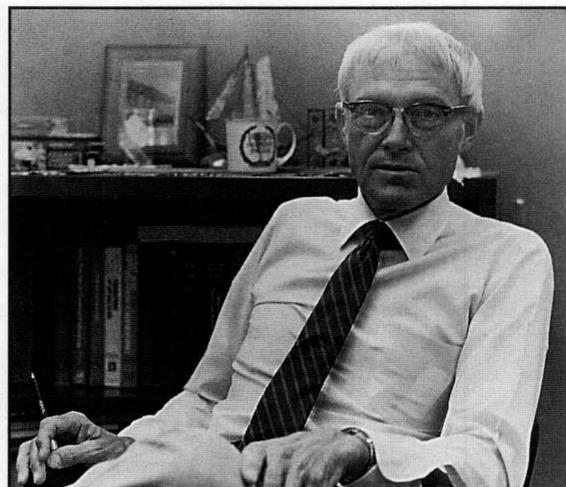
His interest in undergraduate education and opportunities for undergraduate study led him to initiate several chemical engineering student international

***“His vision and example have shaped the culture of the department—a balance of teaching, research, and service. . . . ISU undergraduates, alumni, faculty members across campus, and crystallization researchers around the world hold Mauri in the highest regard.”***



◀ **Gordon Youngquist presents Mauri with a framed copy of the program prepared for a special AIChE session honoring Mauri's 70th birthday and his many contributions to the field of chemical engineering.**

**Mauri's office door has always been open to students and colleagues alike. (1997) ▼**



◀ **Mauri is surrounded by well-wishers on the occasion of his retirement. Each of them has at one time or another served as Chair of the ISU ChE Department: (left to right) Terry S. King, Charles E. Glatz, Maurice A. Larson, R. C. Seagrave, and George Burnet.**



exchange programs, notably with Bradford University, Hamburg University, and University College London. The most successful has been the summer-study program at University College London, which he organized in 1972 during his sabbatical there. The program is still in full force and is now shared by several additional American universities including the University of Wisconsin, Georgia Institute of Technology, Case Western Reserve University, and Virginia Polytechnic Institute and State University.

John Garside, Pro-Vice-Chancellor and Professor of Chemical Engineering UMIST remarks, "I have known Mauri now for well over twenty years. He took a faculty-improvement leave at University College London in 1972 when I was on the faculty there, and I subsequently spent a year working with him at ISU in 1976-77. At UMIST, we use Mauri and Alan's book, *The Theory of Particulate Processes*, for both undergraduate and graduate courses. It is an inspiring book and has had an important impact on teaching in this field throughout the world. Their work has been so influential that use of population-balance modeling is now accepted as a matter of course when dealing with crystallization processes. Before their work, the population balance was almost unheard of."

Crystallization has been a traditional area of chemical engineering education and research, having evolved from its empirical beginnings to the highly sophisticated approaches

practiced today. Maurice Larson has been associated with all stages of recent development of this subject and has been a trendsetter and a pioneer in nurturing and shaping it. Indeed, it is inconceivable that any account of crystallization today would be complete without a reference to Mauri's dominating role.

In 1991, Mauri organized an informal group known as the Association for Crystallization Technology. This organization brings together 70-100 researchers and technologists from industry and academe for three days every year for the sole purpose of discussing the science and technology of crystallization. Mauri's extension programs in the form of workshops in crystallization have always succeeded in bringing together chemical engineers from many parts of the country, indeed the world, and have resulted in reports and valued suggestions for future research.

Mauri has been vigorously involved in many national programs and activities of the American Institute of Chemical Engineers. He was recognized as an AIChE Fellow in 1982 and served as Vice Program Chair for the organization's 1992 Miami Beach meeting. He has also been selected to receive the 1998 AIChE Separation Division's Clarence G. Gerhold Award.

In the American Society for Engineering Education, he

received the Western Electric Fund Award in 1970, served as an officer of the Chemical Engineering Department Heads Group in 1973-74, and was Co-Chair of the 1987 Chemical Engineering Division Summer School. He has served on the editorial boards of the *AICHE Journal* and the *Journal of Separation Process Technology*, and received the U. K. Wilton Park Award in 1978 and the Iowa Governor's Science Medal in 1989.

In addition to his research work, Mauri has always been concerned with the teaching of both graduate and undergraduate courses. Over the years he has taken an active interest in practically all matters pertaining to education and student affairs at ISU. The high national reputation that undergraduate education in chemical engineering at Iowa State enjoys today may be largely credited to his efforts.

Evaluated by his students as one of the best teachers they have encountered, they cite his ability to make his classes rewarding and enjoyable. They are challenged by his dedication and thoroughness. E. L. Cussler, ChE Professor at the University of Minnesota, remembers, "Mauri was a marvelous mentor for young faculty. When I was starting, he found me and encouraged me when I was still surprised to be treated as an adult. I and many like me owe an enormous debt to Mauri for his generosity and time in encouraging and shaping our own careers." Mauri's combined interests of teaching and research resulted in his promotion to Associate Professor in 1961 and to Professor in 1964. In 1977 he was awarded the highest rank in engineering at ISU—that of Anson Marston Distinguished Professor.

Throughout his career, Mauri has also been active in departmental organization and administrative services. He has served on many university, college, and departmental committees and has always contributed to curriculum development, both at the college and the department levels. He served as Department Chair from 1977 to 1983, and many who have visited the department testify to its increased stature as a result of his leadership. As an educator and administrator, Mauri influenced the growth of engineering at ISU through the breadth of his interests and his ability to fashion a common theme from diverse views.

Near the end of his term as Chair, Mauri initiated a campaign to raise funds for a new addition to Sweeney Hall, the chemical engineering department building, to provide expanded research space and an updated teaching laboratory. More than \$1.5 million was raised from friends and alumni and this, with an appropriation of over \$5 million from the State Legislature, resulted in a new wing in 1994. As a result of Mauri's campaign, one of the donors also gave a million dollars to endow the Herbert A. Stiles Professorship in Chemical Engineering.

A special session was programmed at the 1997 AIChE

Annual Meeting in Los Angeles to recognize Mauri's distinguished career and to honor him on the occasion of his 70th birthday. Dr. Terry King, former head of the ISU Chemical Engineering Department and currently Dean of the College of Engineering at Kansas State University, declared

*"Mauri's determination to provide for the building needs of the future for chemical engineering, even when support for such a request was not initially evident, set a pattern for what is now being achieved by the ISU College of Engineering as a whole. He melded a partnership of alumni, industry, and the state to create enthusiasm and funding for a building project from whose laboratories have come many important results being presented today in technical sessions worldwide. That partnership was novel for ISU at the time, and it has been enormously successful, resulting in our new construction. His vision and example have shaped the culture of the department—a balance of teaching, research, and service. As a result, ISU undergraduates, alumni, faculty members across campus, and crystallization researchers around the world hold Mauri in the highest regard."*

Larson has served as a teacher, researcher, ISU supporter, colleague, and an inspiration to his friends for over four decades. He and his wife Ruth are the parents of three children—Richard, who was lost as a teenager in an accident, Janet, who has a horse ranch in New Mexico, and John, who is employed in San Francisco. Mauri and Ruth could not get farming out of their systems and thus have a substantial number of acres of farmland near Ames. Ruth retired in 1996 after working in the ISU Department of Animal Science and the couple has used their free time to travel extensively.

*"Mauri Larson is the quintessential scholar, an outstanding professional, and one of the nicest people I have ever known,"*

states friend and collaborator Ronald W. Rousseau, currently Professor and Chair of the School of Chemical Engineering, Georgia Institute of Technology. Dr. James R. Fair, McKetta Chair Emeritus Professor from the University of Texas-Austin makes things crystal clear when he states,

*"The achievements of Mauri Larson have been notable. One of the foremost has been his rise to a pre-eminent stature as an expert in crystallization. He is considered to be a foremost authority in this field and his many publications bear this out. The record is clear—and well documented—on this issue. He really is Mr. Crystallization." □*

# Washington State University

*Celebrating Fifty Years of Chemical Engineering at the Stroke of the New Millennium*



**Marc VanderSchale and Brian Erickson  
remove CO<sub>2</sub> from air in  
packed-column gas absorber.**

So, what can 50 years of chemical engineering education mean in the context of 2,000 years of calendar time, especially when generated from a relatively small program in the rural town of Pullman, Washington, located in the middle of wheat fields?

Surprisingly, Washington State University's chemical engineering department is a unique example of one of the oldest chemical engineering programs in the country that is still a thriving concern for the university and related industry in today's world. Having evolved from being part of the chemistry department in 1917 into a separate department in 1950, ChemE now focuses on education and research in advanced gas and chemical processing, hazardous material cleanup, and bioengineering.

The department has graduated more than 1,100 students, the majority of whom have taken significant roles in industries such as oil and chemicals, pulp and paper, pharmaceuticals, food, microchip manufacturing, environmental protection, and bioengineering. Alumni can be found in such diverse industries as petroleum refineries, pulp and paper mills, nuclear and synthetic fuel processing facilities, and food processing plants. They are hired by such companies as Dow Chemical, Westinghouse, ARCO, Boeing, Weyerhaeuser, Kaiser Aluminum, Intel, Battelle Pacific Northwest National Labs, as well as other Hanford contractors and smaller companies in the region.

"Graduates from WSU's chemical engineering program are highly marketable," reports Richard Zollars, department chair. "Starting salaries in the mid-\$40,000s are common, as qualified candidates in these fields are highly sought after by industry and agencies."

The small size of the program and connections with industry work in its favor. With about 100 undergraduate, 30 graduate students, and 10 permanent faculty, class sizes of 25-35 afford seminar possibilities

**Washington State University's  
chemical engineering department is a  
unique example of one of the oldest chemical  
engineering programs in the country that is  
still a thriving concern for the university  
and related industry in today's world.**

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and close interaction between faculty and students. Because of its select nature, the program attracts students with above-average scholastic standing, and as many as one-third of all those certified in the chemical engineering program are in WSU Honors Program.

Given the above collegiate atmosphere, the faculty, research, industry partnerships, and educational activities take on a distinctive quality and focus.

### **THE UNDERGRADUATE PROGRAM**

The undergraduate curriculum allows for broad education in the sciences and sound basics in the discipline, but with a flexibility that allows students to individualize studies. In the upper-division, after students certify, the following courses provide the basics in chemical engineering:

#### Sophomore Year

ChemE Process Principles; Process Simulation

#### Junior Year

Transport Phenomena; Fluid Mechanics/Heat Transfer; Thermodynamics; Separations; Kinetics

#### Senior Year

Chemical Engineering Lab I and II; Control; Design I and II; Seminar

Another seven or eight electives allow juniors and seniors to customize their focus in bioengineering, environmental, or other allied fields. They also have opportunities for multidisciplinary study and research.

For example, Becky Russell, a recent graduate who knew she wanted a career that impacted people, explains "I decided to make chemical engineering my preparation for medical school. The skills I learned in technical problem solving and biomedical applications have served me well."

Not all is serious study, however. Students are encouraged to join the College Ambassadors group and to participate in the AIChE student chapter or other engineering societies for networking and leadership growth. WSU's student AIChE chapter recently won first prize at its regional conference for proposing a national competition around student-built chemically controlled cars. The group will put this to the test at the national conference in Miami in mid-November (after the deadline for this article). President Wendy Anna and other officers were able to raise funds from industry to defray the cost of several students' travel to Florida for this purpose.

As the nationwide need to recruit and retain engineering students escalates, WSU's chemical engineering department continues to step up its efforts for scholarships and other incentives. "There's a good chance that students will qualify for a scholarship if they achieve a 3.4 GPA or better and show promise while enrolled," reports Zollars. Because of the generous support of alumni and corporations, about one-third of the

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### **FACULTY**

**Ivory, Cornelius**  
PhD, 1980: Princeton  
*Bioprocessing, separations,  
modeling*

**Lee, James**  
PhD, 1978: Kentucky  
*Bioprocessing, mixing*

**Liddell, KNona**  
PhD, 1979: Iowa State  
*Hazardous wastes,  
electrodeposition*

**Mahalingham, R.**  
PhD, 1968: Newcastle-Upon-  
Tyne, England  
*Hazardous wastes, shock  
reactions*

**Miller, Reid**  
PhD, 1968, California, Berkeley  
*Thermodynamics*

**Petersen, James**  
PhD, 1979: Iowa State  
*Bioremediation*

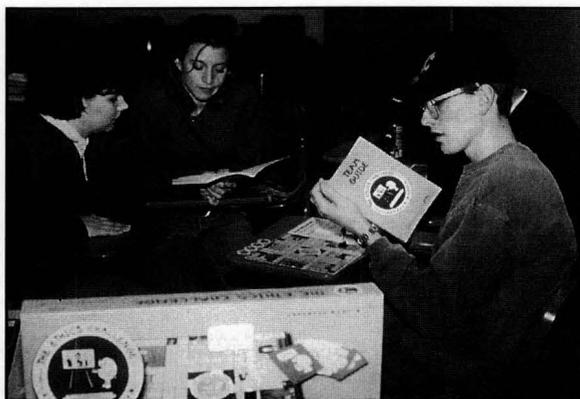
**Peyton, Brent**  
PhD, 1992: Montana State  
*Bioremediation, extremophilic  
bioprocessing*

**Thomson, William**  
PhD, 1969, Idaho  
*Materials, kinetics, catalysis*

**Van Wie, Bernie**  
PhD, 1982, Oklahoma  
*Bioprocessing, biomedical  
engineering*

**Zollars, Richard**  
PhD, 1974, Colorado  
*Colloidal/interfacial phenom-  
ena, reactor engineering*

*Ethics  
are taught in  
one senior class  
by using the  
Dilbert  
Ethics Challenge  
game.  
Teams ponder  
how to handle  
case studies.*



undergraduate students receive some form of financial aid.

With the exception of athletics, chemical engineering's alumni traditionally give the highest per-annum donations of any other unit at WSU.

### **GRADUATE/RESEARCH PROGRAM**

While virtually every undergraduate student who wishes to may get involved in faculty research, the research program is the heart of the graduate program. Currently, more than \$2 million in grant activity is in progress, with healthy prospects for more.

Emphases in bioengineering, environmental restoration, and hydrocarbon processing result in such projects as biotreatment of hazardous contamination, diagnostic medical devices, and converting natural gas to useful products. The current roster of graduate-student research covers such topics as electrodeposition, isoelectric focusing, development of biosensors, protein production in plant cell systems, bioremediation of chlorinated solvents and heavy metals, oxidative coupling of methane, etc.

The Center for Multiphase Environmental Research (CMER), under the direction of Professor James Petersen, conducts interdisciplinary research addressing important environmental problems for industries and government agencies. It seeks opportunities to transfer this technology to industry and, in the process, to educate the next generation of environmental professionals.

CMER faculty are drawn from the civil, environmental, chemical, mechanical, and biological systems engineering departments. The Center and chemical engineering faculty currently play a part in three such projects with large government grants: remediation and recycling of creosote-treated piers at Navy ports and two D.O.E. projects to clean up toxic metals in soils and aquifers.

As a result of her quality work on hazardous waste treatment through CMER, doctoral student Juli Sherwood last year won the university's Harriet Rigas Award from the Association of Faculty Women as WSU's outstanding doctoral woman student, citing her for her research, teaching, and leadership.

Another recent graduate student success story is illustrated by Sherman Xu, who within five years gained both his master's and doctoral degree, valuable research expertise, and a job with the Amoco Research Center in Illinois. His research explored a more productive procedure to convert natural gas to ethylene—the feed stock for many of today's plastics.

### **ABOUT THE UNIVERSITY**

WSU is a land-grant research university dedicated to excellence in undergraduate education. Founded in Pullman in 1890, it has 21,000 students at four campuses, several Learning Centers and other sites throughout the state. WSU's nine colleges and approximate 150 undergraduate majors, along with its distance Extended Degree Programs, can almost "Take You Anywhere You Want to Go!" Pullman's residential campus designates special honors and math-science-engineering residence halls. WSU is one of the most "wired" campuses in the west, with good access to computers and learning labs. Semester classes are scheduled from late August through mid-December, January through mid-May, and at varying summer sessions.

### **ABOUT THE COLLEGE**

The Chemical Engineering Department is part of WSU's College of Engineering and Architecture, which is committed to quality curricula and innovation in learning. Through industry-partnered programs and practical approaches, students prepare for technology-based professions and life-long learning.

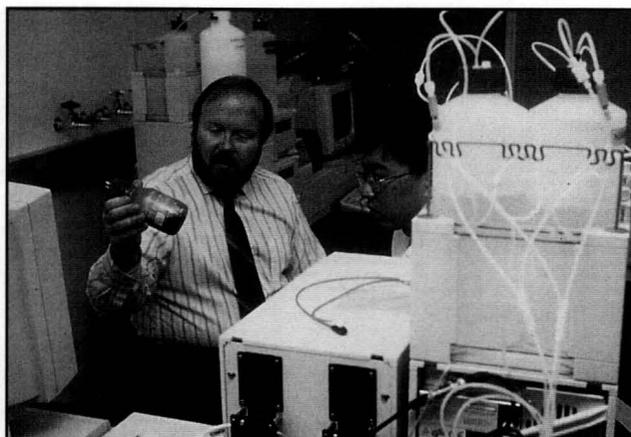
Distinguished faculty and alumni network with industries that offer students scholarships, mentoring, internships, and project opportunities. Approximately 120 permanent faculty serve an average of 2,000 undergraduates, who may join more than 20 student clubs or professional societies for fun and extra challenge. Facilities include numerous labs, classrooms, and other learning spaces in seven buildings on the Pullman campus. A modern 100,000 square foot Engineering Teaching and Research Laboratory recently opened and holds state-of-the-art testing and analysis facilities.

The College assists with tutoring, skills workshops, scholarship applications, orientations, and other special student needs. It also helps recruit and retain individuals from underrepresented groups through the Minority and Women's Engineering Programs.



◀ *O.H. Reaugh Lab dedication: Student Carrie O'Rourke, Chair Dick Zollars, lab director Bill Thomson, WSU President Sam Smith, and alumnus O.H. Reaugh.*

*Reaugh, Thomson, and student Matt Fountain tweak the new equipment. ▼*



▲ *Jim Petersen and graduate student Lin Sha look at grimy creosote being eaten by bacteria and turned into CO<sub>2</sub> in the lab.*



"With my WSU credentials, I found myself very competitive in the job market," says Xu. "I'm grateful to my superior graduate professor who gave me the 'big picture,' and allowed me to find my own answers. His close rapport with industry provided me opportunities to see practical uses of our research."

## FACILITIES

The department's premier research lab—the O.H. Reaugh Oil and Gas Processing Laboratory—was dedicated by its namesake this fall in a ceremony (attended by his family, university leaders, students, industry partners, and friends) that epitomized the momentum that the department's history brings to its future.

Orland Harry Reaugh, a 1933 graduate of the program, became a petroleum engineer and a leader in independent oil production in Oklahoma, Kansas, New Mexico, and Illinois. He has since become a major benefactor of WSU's chemical engineering department, which now has the only such alumni-endowed and -named laboratory within the university. Reaugh provided \$250,000, ARCO another \$50,000, and matching donations are being sought to complete the lab's \$500,000 endowment. The income will ensure a lab that is equipped with state-of-the-art instrumentation.

Lab director William Thomson says the facility "allows us to conduct research that is fast disappearing from the university scene—innovative studies to find less expensive and ecologically friendly ways to add octane to gas, bring natural gas to remote locations, and to create compact, economical hydrogen fuel cells.

More than 9,500 square feet of lab space are located in the

new Engineering Teaching and Research facility containing analytical equipment such as spectrometers, chromatographs fitted with auto-samplers and various detectors, anaerobic incubators, dynamic x-ray diffractometer, laser light scattering, and electrophoresis devices. The George T. Austin endowment for undergraduate lab equipment, augmented by funds from alumnus Gene Voiland, help keep learning technologies current.

Computing equipment and workstations with parallel processing features are provided for all graduate students and researchers. Keeping such quality computing current is always a concern of technical educators, however. Typically, alumni donations help replace one-third of the undergraduate machines every year in the 15-station computing lab. Full-scale commercial versions of Pro Vision, MatLab, Mathematica, MathCAD, spreadsheets, word processors, and other programs are used on these machines.

## INDUSTRY CONNECTIONS

A hallmark of WSU's engineering college is its continuing strong connection to industry. Companies and agencies provide internships, scholarships, collaborative research, and even job exchanges. WSU in turn provides on-site or webbed distance learning, qualified potential hires, and R&D.

One collaborative project is Prof. Bernie Van Wie's work with the Spokane Interdisciplinary Research & Technology Institute and DevTec, an independent industrial partner, to develop and commercialize an automated blood chemistry analyzer. Another collaborative project is Prof. Bill Thomson's work with the Washington Technology Center

and Washington Water Power to refine an efficient fuel cell.

West Coast companies such as ARCO, Boise Cascade, Hanford contractors, SEH America, Kimberly Clarke, and Reynolds Aluminum offer summer jobs and internships (summer plus one semester) to students—and often end up offering them jobs at graduation. They say they are impressed with WSU's students' practical knowledge and leadership experiences outside the classroom.

"Chemical engineers need foundations in science and math, but also in other disciplines that will prepare them to adapt new products into the culture," says Glenn Butler, CEO of the ARCO Refinery at Cherry Point. He and other department advisers urge development of students' skills in communication, presentation, and human relations, in addition to developing a code of ethics and a knowledge of overall business and economic concepts.

John Wolfe, a 1997 chemical engineering graduate now at ARCO in Anaheim, recently returned to the College's Career Fair—this time as a recruiter! "Basically, my ChemE degree helped to more than double my salary as a science lab technician," says Wolfe. "My internship with ARCO during the summers gave me a foot in the door. And now I have a good job with them solving technically complex problems in oil refining." He's now on the lookout for other potential hires who work well in teams of engineers, scientists, customers, plant operators, managers, lawyers, government regulators, and construction workers.

## OUTREACH

WSU Pullman's program remains fairly stable in size. Many families continue sending new generations as legacies. The department also reaches out to the adult, sometimes mid-career, learner through a companion program at the WSU branch campus in Tri-Cities, with access to Hanford and the Environmental Molecular Science Lab. It generally serves full-time employed engineers, offering after-hour courses so that engineers can upgrade their education or work toward the MSChE. It is one of few evening-based MSChE programs in the country. Many of the courses are taught by PhD chemical engineers who are also employed at the Pacific Northwest National Laboratory.

Tri-Cities student projects or theses usually are done with a committee composed of both WSU regular faculty and

"adjunct" faculty from local industry. Three to five students usually earn the MSChE degree through this program each year. This year's graduates will be Penny Colton (Dissolution Kinetics at the Calcite-Water Interface), Dan Schmitt (10 W Proton Exchange Membrane Fuel Cell Design), Chris Johnson (Microbial Growth Kinetics Using Colloidal Polymer as Substrate), Scott Estey (Thin Film Polydimethylsiloxane Oil Evaporation), and Brad Knutson (Evaluation of Ion Exchange Performance Predictive Tools).



***"Team think" in action. Graduate students, professors, researchers, medical professionals, and commercialization experts work on the automated blood analyzer project.***

To develop interest in engineering at earlier ages, for the past five years chemical engineering faculty has conducted a NSF-funded summer program for secondary school teachers. The goal is to familiarize them with engineering and help them develop modules to teach when they return to their classrooms. All together, more than 65 teachers attended—half from Northwest schools, and others from as far away as Korea, Florida, and Connecticut. Feedback from the participants noted that the experience succeeded

in bringing engineering into their science curriculum. One science teacher developed an engineering-related module that contributed to a portfolio that won her state and national teaching awards.

## FUTURE TRENDS

Academic destinies will depend a great deal on the economic and technological trends transforming higher education today. For instance, the Tri-Cities program will be influenced by down-sizing at Hanford. And, as noted earlier, keeping computer equipment and software current is a major and constant challenge. By the same token, developing distance-learning technologies may allow webbing courses beyond campus sites, which will again revolutionize what we do at universities.

While state appropriations can no longer meet the entire departmental needs, outside grants and private funding is on the rise. The department plans to pursue more endowments similar to the O.H. Reaugh Lab, to stabilize funding bases.

Faculty and student numbers are not expected to change dramatically over the next five years. Expansion of multidisciplinary experiences is anticipated, however, particularly in the wake of the Center for Multiphase Environmental Research's path-finding activities. □

## Numerical Computation in Science and Engineering

by C. Pozrikidis

Published by Oxford University Press, Inc., 198 Madison Avenue,  
New York, NY 10016; 627 pages including index, \$75.00 (1998)

Reviewed by

**James N. Petersen**

Washington State University

The necessity of obtaining numerical solutions to physical problems crosses virtually all the discipline boundaries in engineering and science. Only a limited number of books are available, however, that provide the fundamentals of scientific numerical computational techniques, together with application of those techniques. In general, Pozrikidis has been able to achieve this result in his book, which is intended to be used in upper-level undergraduate and beginning graduate courses and may be suitable for individual study. In so doing, he has produced a book that strikes a balance between rigor and practicality.

While not providing lengthy computer codes in the text, he has communicated the essential aspects of various numerical methods by relying on code fragments and pseudoCode that can be translated into any suitable computer language. In so doing, he has covered most of the topics required in an introductory course within a manageable number of pages. To compliment the text, he has also provided access, via the Internet, to a public domain software library of Fortran 77 programs, organized by book chapter.

The book is organized into eleven chapters. Each of them is further divided into sections and subsections. Because the subsections are the intended functional learning entities, the author provides both theoretical and computational problems at the end of each. These problems are designed to complement the theory presented and to provide the student with an immediate opportunity to practice its implementation.

The chapters are organized in a fashion similar to many other numerical methods books. In Chapter 1, the author provides a background of computer hardware, computer arithmetic including both integer and floating-point representations, and errors. In the next three chapters, he first lays a foundation on which to build the solution of linear and nonlinear sets of simultaneous equations. Thus, in Chapter 2 he covers matrix algebra and matrix calculus, and Chapter 3 is devoted to the solution of sets of linear algebraic equations. The solutions of sets of simultaneous nonlinear algebraic equations is discussed in Chapter 4, and he goes on to discuss eigenvalues of matrices in Chapter 5.

*Continued on page 65.***The next generation analysis software for:**

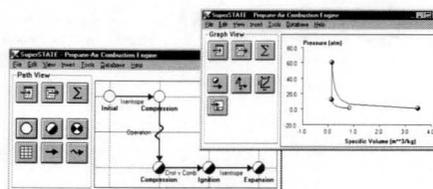
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# DO CHANGES IN THE CHEMICAL INDUSTRY IMPLY CHANGES IN CURRICULUM?

Edward L. Cussler, Institute Professor at the University of Minnesota, received his BE degree from Yale University in 1961, his MS from the University of Wisconsin in 1963, and his PhD from the University of Wisconsin in 1965. He rose from Assistant Professor to Professor of Chemical Engineering at Carnegie-Mellon University during the years from 1967 to 1980, at which time he joined the faculty at the University of Minnesota as Professor of Chemical Engineering. In 1996 he became Institute of Technology Professor at the University of Minnesota, and is currently at Cambridge University in the United Kingdom as Professor of Chemical Engineering.



Ed has won numerous awards during his professional career, some of which are the AIChE Alan P. Colburn Award in 1975, seven Minnesota Institute of Technology Teaching Awards through the years, the George Taylor Distinguished Teaching Award from the University of Minnesota in 1987, the Donald Katz Lecture Award from the University of Michigan in 1996, and the Danckwerts Lecture from the Institution of Chemical Engineers in London in 1997.

Ed serves as Associate Editor of the *AIChE Journal* and is on the Editorial Board of the *Journal of Membrane Science*. He also has served as a Director, Vice President, and President of AIChE, and was Chair of the American Association of Engineering Societies.

He has also been author or co-author of over 160 publications. He is co-author with Belter and Hu of *Bioseparations* (John Wiley and Sons, New York, 1988) and with Baker, Eykamp, Koros, Riley, and Strathmann, of *Membrane Separation Systems*, (Noyes Data Corporation, New Jersey 1991). He is author of the books *Diffusion* (Cambridge University Press, London, 1984; second edition, 1997) and *Multicomponent Diffusion* (Elsevier Publishing Company, Amsterdam, 1976).

E.L. CUSSLER

*University of Minnesota • Minneapolis, MN 55455*

This paper is a synopsis of my Union Carbide Lectureship, an award given at the 1998 meeting of the American Society of Engineering Education. I am flattered to have my research and teaching on diffusion acknowledged. I know that this lecture can often be a review of the past research, centering on a scattering of old slides, like a photograph album of half-remembered vacations.

But the lecture and this paper are too good a forum to waste on my past. Instead of the past, I want to consider the future. In doing so, I remember a conversation I had thirty years ago with the historian, L. Pearce Williams. I was visiting him to gush about his biography of Michael Faraday,<sup>[1]</sup> which I had enjoyed enormously. I suspect that he found my naive enthusiasm both flattering and embarrassing. To make conversation, Williams asked if I knew the real difference between science and the arts. I did not. He responded that in the sciences, we wrote papers and books when we felt we knew everything about our topic. In the arts, he asserted, authors wrote when they knew little initially and used the writing as a way to focus new questions and to explore possible answers.

Whether this arts-science contrast is true or not, I want to use this paper as a way to learn about possible changes in chemical engineering curricula. I am not yet sure if these ideas are correct, but I want to see if they make sense. In the next few years, I'll try them out. For now, though, they're best described under three headings: the changes in the chemical industry, the status in academia, and possible curricular changes.

## CHANGES IN THE CHEMICAL INDUSTRY

Last spring, I taught our introductory chemical engineering course—the one that covers stoichiometry. Early in the course, I

showed pictures of chemical plants to the students. I told them that the tall towers were for distillation and the short, fat ones were often for gas absorption. I pointed out the reactors, with their preheaters and recycles. I spoke of the excitement of running a chemical plant and the satisfaction of using chemical technology to improve our well being.

I did so with hidden reservations that I did not have ten years ago. I know that the chemical industry has changed and that many of the students will not work in the commodity chemical plants I was describing. To see why, we need to review the history of our industry, using as an example the development of synthetic textile fibers.

From 1950 to 1970, the chemical industry produced ever-increasing amounts of synthetic textile fibers, as shown in Table 1. Over the decades, while the production of natural fibers was about constant, the production of synthetics grew 20% per year. This growth was comparable to that of the software industry today; indeed, Du Pont in the 1950s was like Microsoft in the 1990s. It was a golden age for chemicals.

But from 1970 to 1990, synthetic textile fibers grew only four percent a year—at about the same rate as the growth of world population. That’s not surprising; after all, any logarithmic growth can’t continue indefinitely. From 1970 to 1990 the industry stayed profitable by using larger and larger facilities. Bigger profits came from consolidating production into bigger plants, designed for greater efficiency in making one particular product. The interest in computer-optimized design is a vestige of this consolidation. Such optimization meant small producers were forced out. For example, the number of companies making vinyl chloride shrank from twelve in 1964 to only six in 1972.<sup>[2]</sup>

In the last ten years, the industry has used other strategies to stay profitable. These strategies often centered on restructuring, which was three times more likely to affect engineers than the general population. Whether called “restructuring,” “downsizing,” “right-sizing,” or “rationalization,” the strategy meant many mid-career engineers were suddenly looking for a job. The Engineering Workforce Commission now feels that engineers will average seven different jobs per career, a dramatic change from two per career when I graduated in 1961.<sup>[3]</sup> Middle management, that traditional goal of our B-students, is no longer a safe haven. Starting salaries remain high, the envy of other technical professions, but they have not increased faster than inflation in thirty years. In this environment, I applaud the decision of the American Institute of Chemical Engineers (AIChE) to be a “lifetime home” for members of our profession, providing more help in job transitions and financial planning. The AIChE can no longer be only a nineteenth century-style learned society.

Most recently, the chemical industry has become enchanted with the life sciences, often called “biotechnology.” Biotechnology in the industrial sense is most successfully represented by applied agronomy, *i.e.*, by genetically modified seeds. It is usually different from the biotechnology represented in academic chemical engineering that often centers on separations and reactions involving specialty pharmaceuticals. The model for corporate enchantment is Monsanto, which has spun off its commodity chemical operations to compete largely in this new biotechnology. Other companies are imitators. In recent five-year projections, Du Pont has relabeled its chemicals as “materials,” is spinning off Conoco, and plans to double its life-science efforts to one-third of the company’s sales. Hoechst, by some measures the world’s largest chemical company, plans to leave chemicals for the life sciences. It’s a different world beyond our ivory towers.

	<u>1948</u>	<u>1969</u>	<u>1989</u>
Cotton, Wool	4353	4285	4794
Synthetics	92	3480	8612

***I want to use this paper as a way to learn about possible changes in chemical engineering curricula. I am not yet sure if these ideas are correct, but I want to see if they make sense. In the next few years, I'll try them out.***

## THE STATUS IN ACADEMIA

While these industrial changes occur, academic chemical engineering continues along well-established paths. I think that this is good. Universities are both stable and resilient; Clark Kerr, the long-time provost of the University of California, is said to have asserted that universities make up more than 90% of the social institutions that have lasted over 500 years. Moreover, courses in any field evolve slowly. Woodrow Wilson, at the time President of Princeton, said that "changing curricula is like moving graveyards."

Chemical engineering curricula in the USA are no exception. To a large extent, they reflect the scheme first suggested in 1917 by a commission chaired by Arthur D. Little, founder of the firm that bears his name. Building on British precedents, the commission suggested an organization around "unit operations." This was based on the assertion that distillation was based on the same principles for any chemical system, be it rum or crude oil. This organization was codified by the book *Principles of Chemical Engineering*.<sup>[4]</sup>

L. E. Scriven tells the possibly apocryphal story that the book was written only because the authors isolated themselves at a camp in the Adirondacks, where they could not be interrupted.

*Principles of Chemical Engineering* outlines much of what would be a reasonable, accreditable major today. It begins with a chapter on stoichiometry and then covers fluid flow and heat transfer in three chapters. Four chapters on combustion seem the intellectual ancestors of today's reaction engineering. Four chapters on separations center on distillation, humidification, and drying. Only the two chapters on mechanical separations (crushing and grinding) have material missing from modern chemical engineering curricula. I don't mean to overemphasize these parallels, because the contents of these chapters are often qualitative and dated. Still, I find the parallels vivid.

The curriculum implied by *Principles of Chemical Engineering* was challenged most successfully by *Transport Phenomena*, the book by Bird, Stewart, and Lightfoot.<sup>[5]</sup> This book, circulated in 1957 and formally published in 1960, injected more needed science and mathematics into our field. For a while, our profession was divided into those who

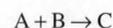
believed in the older *Principles* testament and those who converted to the newer *Transport* gospel. In one recent stimulating article, Astarita and Ottino<sup>[6]</sup> argued that these two books have supplied the only two organizing ideas that our profession has had.

In hindsight, I believe that there are two main reasons why *Transport Phenomena* was so successful. First, by stressing parallels between different transport processes, the book

supplies a pedagogical template that helps all to learn and think about these processes. This template is a mixed blessing. For example, the fact that there is no parallel to chemical reactions in heat transfer means that chemical reactions are superficially treated. This may contribute to our continuing tendency to teach mass transfer without chemical reactions, even though much industrial mass transfer, e.g., acid gas treating, takes place with reaction.

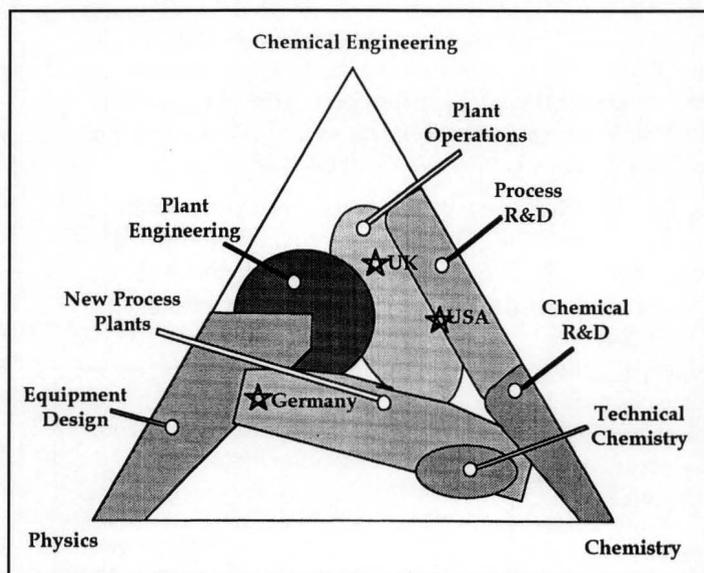
The second reason that *Transport Phenomena* was so successful is a reflection of the boom taking place in the chemical industry when the book was published. As

outlined above, this boom centered on petrochemicals, which of course included the monomers used to make synthetic fibers. When you make petrochemicals, you often deal with a plethora of compounds characterized by a near continuum of boiling points. In such a case, continuum mathematics is appropriate; one can basically ignore the discrete jumps of the periodic table. Indeed, one can ignore most of chemistry, with



i.e., argon plus boron goes to carbon. Moreover, as the petrochemical industry became more competitive, minor improvements in existing processes were important to profitability. These minor improvements could often be found using the mathematical approach in *Transport Phenomena*.

While Astarita and Ottino argue powerfully that these two books provide the only two paradigms in our profession, I feel that Levenspiel's *Chemical Reaction Engineering*,<sup>[7]</sup> first published in 1963, is also important, but for a different reason. The first two books provided a definition of a profession, which implied a curriculum. Levenspiel, on the other hand, reorganized what was already acknowledged into a



**Figure 1.** Skills in Chemical Engineering. These skills are ideas from chemistry, physics, and engineering. Different jobs use different proportions of these ideas.

*The changes in the chemical industry are clear—a movement away from commodities, a romance with biotechnology, and a long-term interest in specialties. . . . These changes in the industry do mean that our students will work much more on chemical products than on chemical processes. As a result, we will want them to think more about product design in addition to process design.*

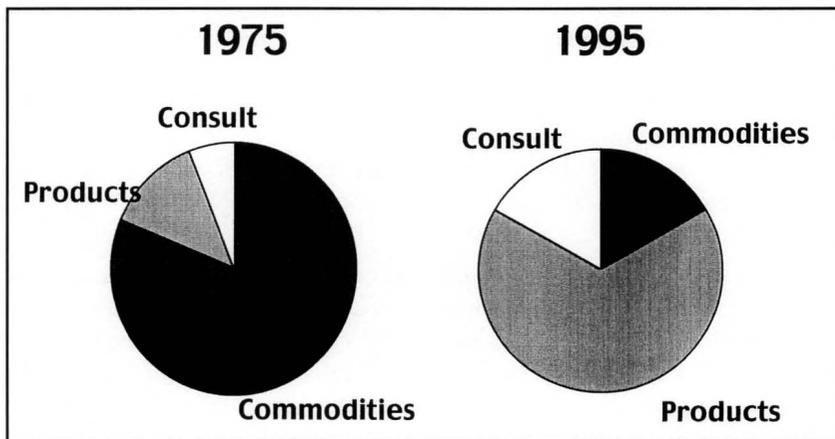
way that made it easier to learn. This can be hard for the founder of a discipline to do. For example, I view T.K. Sherwood as a founder of mass transfer. I find his 1937 book *Absorption and Extraction*,<sup>[8]</sup> more understandable than its 1952 successor *Absorption and Extraction*,<sup>[9]</sup> co-written with Pigford. This second edition is in turn easier for me to understand than the 1975 revision, *Mass Transfer*,<sup>[10]</sup> co-written with Pigford and Wilkie. Levenspiel built on earlier reaction engineering books such as Hougen and Watson's *Chemical Kinetics*,<sup>[11]</sup> but he achieved a new presentation that was much easier to understand.

These various subjects in the chemical engineering curriculum can be represented on the triangular diagram redrawn from Gerhard Froelich, the 1999 AIChE president, and shown in Figure 1. The three corners of this plot represent training in the physical sciences, in the chemical sciences, and in the chemical engineering subjects. Different jobs use these three elements in different proportions, as shown in the figure. There is no surprise in this; plant engineering will demand a greater knowledge of mechanics and a smaller background in chemistry than research and development. Figure 1 also suggests national averages. British chemical engineers seem to have somewhat more chemical engineering and less chemistry than their US counterparts. Please don't take this diagram too literally; use it instead as a catalyst for thought, perhaps for deciding how your department's curriculum should evolve.

## DO INDUSTRY CHANGES IMPLY ACADEMIC RESPONSES?

So far, I have summarized the revolution in the chemical industry and the evolution of academic chemical engineering. I now want to compare the two to see what, if any, changes are needed in what we teach.

Basically, I don't think many changes are indicated. The skills we currently teach seem to prepare our students well. Starting salaries remain high, the envy of most other engineering disciplines. The number of jobs is again high, after almost a decade of bad years caused by restructuring.<sup>[12]</sup> In fact, the job market right now is better than I thought it would be three years ago. Industrial complaints about our teaching seem scattered, with about the same number urging more, say, kinetics as those who urge less kinetics. Most



**Figure 2.** Employment in 1975 versus 1995. Current graduates are much less likely to work for commodity chemical producers and more likely to be involved with products.

industrial complainers who urge us to teach more of a particular topic are hard pressed to suggest which current topics they would omit to make room for their favorite.

Thus, I believe our current curriculum is basically in good shape. One frequent omission does concern me, however. I want to explore this omission next.

My concern centers on the jobs our graduates now hold compared with those they held perhaps twenty years ago. My data for this are fragmentary, so I would be interested in any other data that are available. My data are probably biased toward large corporations, about whom our placement office has better records. My data also have a regional bias towards 3M and food companies such as General Mills that are based here in Minnesota. Still, the data suggest major changes in the last twenty years.

The focus of my analysis is the employment in 1975 versus that in 1995. I chose 1995 because the students often need several years to settle down, to decide which sort of job they really want to do. As shown in Figure 2, there are enormous differences between 1975 and 1995. In 1975, three-quarters of our graduates were working in the commodity chemicals business. The small number who were not were split between work on products, either product design or product development, and work in other areas, which for convenience I have labeled "consulting." That would include those working directly for consulting firms as well as those carrying out specific tasks such as environmental impact statements.

In 1995, the distribution of jobs is different. The majority

of students (in Minnesota's case, about two-thirds) now work primarily on products. This includes not only students who work on materials, but also those who work on pharmaceuticals, on specialty coatings, on adhesives, and on specialty chemicals. The number who work in commodity chemicals has dropped so that it now is less than a quarter of our graduates. The number who work in consulting has risen dramatically, as commodity chemical businesses outsource many of the in-house functions they used to do. For example, in one case, a commodity chemical company took its process engineering group from 1500 to fewer than 50 people. This is not a business cycle; this is a change in the way they expect to do business. This is why the number of people involved in consulting has gone up.

Thus, the nature of the jobs that our students are doing has changed dramatically. The next question concerns where the changes are reflected in our curriculum. To explore this, I have shown a basic generic curriculum in Table 2. It contains the usual stoichiometry, the thermodynamics, and the transport classes. The three classes in kinetics, process control, etc., are the place where departments will have unique offerings. For example, this is the location of courses in polymers or biochemical engineering or environmental engineering. Such uniqueness is a strength of our departments, a way in which we add special skills to a common core.

There are a few places in these classes that contain material on products, that subject on which our students are most likely to work. The most logical place to add this type of material is in the capstone design class. This class usually focuses on process design, the tradition of our discipline. The hierarchy suggested by Jim Douglas<sup>[13]</sup> for this process

design seems to me especially strong and appropriate. It is summarized on the left side of Table 3. After deciding whether a process is batch or continuous, one then moves on to flow sheets, which are almost always continuous. The initial flow sheets center on the stoichiometry. The next level in the hierarchy, which adds the recycles, often involves a discussion of the chemical reactions. Once these are established, one moves on to the separation trains and finally to the heat integration. All of this makes for a good course.

If we want to emphasize product design, we need to go beyond this hierarchy. We cannot simply substitute a product for drug delivery for the existing process and carry out the same kind of hierarchy. Instead, the hierarchy suggested by books on product design (e.g., Ulrich and Eppinger<sup>[14]</sup>) is exemplified by that on the right side of Table 3. After first identifying a corporate need, one generates ideas to fill this need. One then decides between these alternatives and finally decides how to manufacture the chosen product. The manufacturing step essentially includes all of Jim Douglas' hierarchy.

Thus the important steps in product design anticipate those in process design. Product design implies a focus on the initial decisions around the form of the product and implicitly de-emphasizes its manufacture. Such an emphasis shifts the curriculum away from the common engineering calculations that have been our bread and butter. Such an emphasis includes subjects that are normally left to those directly concerned with the business. I am concerned that if I make this shift in a design class, I will wind up teaching my students watered-down business school principles rather than "real" engineering. I undertake this change because

**TABLE 2**  
**Generic Chemical Engineering Curriculum**

*Most universities teach a similar sequence.*

- Stoichiometry (1 course)
- Thermodynamics (3 courses)
- Transport Phenomena and Unit Operations (3 courses)
- Reactors, Process Control, etc. (3 courses)
- Process Design (2 courses)

**TABLE 3**  
**Process Design versus Product Design**

*All of process design is contained in the last step of product design.*

**Process Design**

1. Batch vs. Continuous Process
2. Inputs and Outputs
3. Reactors and Recycles
4. Separations and Heat Integration

**Product Design**

1. Identify Customer Needs
2. Generate Ideas to Meet Needs
3. Select among Ideas
4. Process Design for Manufacturing

**TABLE 4**  
**"Sick House" Ventilation**

1. Customer need; ventilate for under \$800
2. Ideas:
  - Open window
  - Controlled vent
  - Heat exchanger
  - Heat and humidity exchanger
3. Select heat and humidity exchanger
4. Manufacture follows kidney dialysis

so many more of my students are encountering this shift in their professional lives. I want them to see how product design works.

When I've discussed these ideas with other faculty, I often get the indignant reaction that the faculty are already doing this. Some have mailed me syllabi and reports that include aspects of product design. Without exception, what I have received represents good education, but almost without exception, the material seems to skip all steps except the last in the product design hierarchy in Table 3. These earlier steps seem to me too important to leave to the MBAs.

As an example of these ideas, consider the so-called "sick house syndrome" that has developed as houses were built to be energy efficient. Such houses exchange their air as infrequently as twice a day. In contrast, a house built fifty years ago exchanges its air almost every forty minutes. Thus, while the modern house does not cost much to heat, it can concentrate radon from the basement, formaldehyde released from carpeting and drapery, and carbon dioxide from the people who live in the house. The modern house needs more fresh air. Thus the product needed is a device that allows a house to remain energy-efficient, but which provides fresh air at the ASHRE standard of 19 cubic feet/minute/person in the house.

The way in which the product development might proceed is shown in Table 4. The need is for a device costing less than about \$800 that can provide this degree of ventilation. Ideas include opening a window, providing automatic control for opening a window, providing a heat exchanger, and providing an exchanger for both energy and mass. Opening a window sacrifices the energy benefits of insulating the house in the first place. Opening the window with an automatic controller that might anticipate weather cycles makes sense. For example, one could open the window only on sunny winter days and keep the house closed on cold winter nights. Using a heat exchanger can provide the necessary ventilation at an order of magnitude less heat loss. As anyone who has bought a house with such a heat exchanger knows, however, the heat exchanger also exhausts the water vapor in the house. The heat of evaporation of the water is about a third of the heating value in the humidified air. If the heat exchanger runs, the house dries out and becomes very uncomfortable.

The final alternative is the most complicated, but the most satisfying. In this case, one uses a heat exchanger in which the walls are membranes selectively permeable to water vapor. As a result, one captures 90% of the energy and 90% of the water vapor, but exhausts the carbon dioxide, formaldehyde, and radon in the house. The question is cost. The students need a more complete design, perhaps using the manufacturing technology developed for kidney dialysis, to make the membranes. This is an area of active commercial development by several heat-exchanger companies.

## CONCLUSIONS

We are now ready to answer the question posed in the title of this paper: "Do changes in the chemical industry imply changes in the chemical engineering curriculum?" The changes in the chemical industry are clear—a movement away from commodities, a romance with biotechnology, and a long-term interest in specialties. Major changes in the curriculum are probably not needed; our students still have the basic skills necessary not only for the changed chemical industry but also for the other jobs they now hold.

These changes in the industry do mean that our students will work much more on chemical products than on chemical processes. As a result, we will want them to think more about product design in addition to process design. The work on product design will follow a different hierarchy than that which effectively organizes process design.

But I'm not sure of this. You may remember that I began this article by saying that I was going to follow the lead of Pearce Williams to write a paper on what I thought might be done rather than what I had already found effective. With Geoff Moggridge, I am going to teach product design as a Zeneca fellow at Cambridge University in the academic year 1998-1999. If we are successful, I will try to move some of these ideas back into our design courses here at Minnesota. I am not yet sure they will work. I look forward to discussing with you what parts do work and what parts do not.

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# DISCONTINUITIES IN ChE EDUCATION

STEPHEN WHITAKER

University of California • Davis, CA 95616

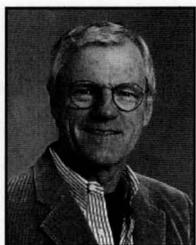
From the perspective of the first-year student, the entire four-year chemical engineering program represents an overwhelming array of courses and subject matter. One must learn about ionic strength and indefinite integrals, acoustics and hydrostatics, turbulence and chemical kinetics, organic chemistry and process dynamics, optics and quantum mechanics, stoichiometry and process synthesis, radiant energy heat transfer and partial differential equations, etc., etc. Viewed in its entirety, the typical chemical engineering program is enough to make a student change majors; but if taken *one step at a time*, the overall objective becomes quite feasible.

In the ideal chemical engineering program, one would like to develop a seamless passage from ionic strength to process synthesis. Given the size of the task, it should not be surprising that the route from A to Z contains a few "leaps of faith." The failed leap of faith within the confines of the university leads only to a lurking sense of insecurity and no real physical damage. Outside the university, however, a failed leap of faith may be a financial disaster, a physical disaster, or both. For this reason, we should avoid or minimize the leaps of faith in our educational programs or we should clearly identify them as such. A discussion of the so-called principle of lost work represents an interesting example of the latter.<sup>(1)</sup>

## THE MECHANICAL DISCONTINUITY

In the first physics course, students encounter Newton's second law for a particle written in the form

$$\frac{d}{dt}(mv) = F \quad (1)$$



**Stephen Whitaker** received his undergraduate degree in chemical engineering from the University of California, Berkeley, and his PhD from the University of Delaware. He is the author of two undergraduate texts, *Introduction to Fluid Mechanics* and *Fundamental Principles of Heat Transfer*, and a monograph, *The Method of Volume Averaging*. He has received a number of awards for his contributions to both undergraduate and graduate teaching.

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Here,  $m$  is the mass of the particle,  $\mathbf{v}$  is the velocity of the particle relative to an inertial frame, and  $\mathbf{F}$  is the force acting on the particle. Given the success of Eq. (1) in predicting the motion of the planets around the sun and in predicting the motion of projectiles in a physics lecture hall, students acquire a certain degree of confidence in Newton's second law. This confidence may begin to weaken when they move on to a chemical engineering study of fluid flow where they are often confronted with a dictum of the form

$$\begin{array}{ccccccc} \text{sum of forces} & & \text{rate of} & & \text{rate of} & & \text{rate of} \\ \text{acting on} & = & \text{momentum out} & - & \text{momentum into} & + & \text{accumulation of} \\ \text{the control} & & \text{of the control} & & \text{the control} & & \text{momentum in the} \\ \text{volume} & & \text{volume} & & \text{volume} & & \text{control volume} \end{array} \quad (2)$$

It is true that the concept of a *control volume* has already been presented in a course on material balances; but the distance between Eq. (1) and Eq. (2) is so great that most students view the latter with some distrust. The student's skepticism is quite justified, but the repeated use of Eq. (2) to solve real problems eventually leads to its acceptance. Such a leap of faith in the design of an oil pipeline passing underneath the city of Los Angeles would never be considered, but Eq. (2) is something that *everyone knows is true*, and many students move successfully through their programs of study with it securely locked in their tool boxes.

## THE THERMODYNAMIC DISCONTINUITY

When students have made sufficient progress in their studies of fluid mechanics, they will often solve a variety of incompressible flow problems (it is important to keep in mind that there are no incompressible fluids, but there are *flows* that can be approximated as incompressible) using the Navier-Stokes equations and the continuity equation. These equations can be expressed as

$$\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \rho \mathbf{g} + \mu \nabla^2 \mathbf{v} \quad (3)$$

$$\nabla \cdot \mathbf{v} = 0 \quad (4)$$

Equation (3) represents the governing differential equation

for the fluid velocity,  $\mathbf{v}$ , and Eq. (4) is the *constraining equation* for the vector field represented by  $\nabla p$ . That is to say that the *momentum source*,  $\nabla p$ , must be distributed in such a manner that the velocity determined by Eq. (3) will be solenoidal. If the pressure is specified at some point, one can use the vector field,  $\nabla p$ , to calculate the pressure everywhere. The actual determination of the pressure field is discussed in some detail in Reference 2.

At the same time that students are using Eqs. (3) and (4) to determine the pressure in a course on fluid mechanics, they are also calculating the pressure in a course on thermodynamics using an equation of state. The simplest equation of state is the ideal gas law given by

$$p = \frac{n}{V} RT \quad (5)$$

This expression for the pressure would appear to have no connection with the pressure that one would determine from Eqs. (3) and (4), thus suggesting that there is a *mechanical pressure* used in the solution of certain fluid-flow problems and a *thermodynamic pressure* used in the solution of thermodynamics problems. It would be best to think of the pressure, as determined by an equation of state, as *the pressure*, and to think of the pressure determined by Eqs. (3) and (4) as a good approximation of *the pressure*. If it is not a good approximation, Eqs. (3) and (4) should not be used to solve the flow problem under consideration. The resolution of the conflict between Eqs. (3) and (4) and an equation of state, such as Eq. (5), relies on Birkhoff's plausible intuitive hypothesis that *small causes give rise to small effects*.

### THE MULTIPHASE DISCONTINUITY

After having completed courses in fluid mechanics, thermodynamics, heat transfer, and mass transfer, chemical engineering students are often confronted with a course on mass transfer operations or unit operations. Since virtually all chemical engineering processes involve multiphase systems, a study of the gas-liquid contacting device illustrated in Figure 1 is a harbinger of things to come, and students approach this problem with a great deal of interest. Often they are equipped with Eqs. (3) and (4) from a course on fluid mechanics, the thermal energy equation from a course on heat transfer<sup>[4]</sup>

$$\rho c_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = k \nabla^2 T \quad (6)$$

and the species continuity equation from a course on mass transfer<sup>[5]</sup>

$$\frac{\partial c_A}{\partial t} + \nabla \cdot (c_A \mathbf{v}_A) = R_A \quad A = 1, 2, \dots, N \quad (7)$$

Most students are somewhat dismayed when the process illustrated in Figure 1 takes on the form shown in Figure 2, and the rigor represented by Eq. (7) is replaced by the

suggestion that

$$\begin{array}{l} \text{mass of A entering} \\ \text{in the gas phase} \end{array} = \begin{array}{l} \text{mass of A leaving} \\ \text{in the gas phase} \end{array} + \begin{array}{l} \text{mass of A transferred} \\ \text{to the liquid phase} \end{array} \quad (8)$$

After the struggle to reach Eq. (7) via a series of challenging courses, it is disappointing to be asked to return to the concepts encountered in the course on material balances. What is worse is that the analysis of the process illustrated in Figure 1 will be heavily based on the intuition suggested by Figure 2 and most students will have no idea how reliable the final result will be. The resolution of this problem can be achieved using the method of volume averaging.<sup>[6]</sup>

### RESOLUTION OF THE MECHANICAL DISCONTINUITY

Rather than leap from Eq. (1) to Eq. (2), one can follow a sequence of steps that begins in the eighteenth century<sup>[7]</sup> and leads to our current understanding of continuum mechanics. A central idea in continuum mechanics is that the laws of physics can be applied to any body that one imagines as being cut out of a distinct body. Truesdell<sup>[7]</sup> attributes this idea to Euler and Cauchy and refers to it as the *cut principle*. Engineering students encounter this idea in a course on statics where it leads them to the concept of a free-body diagram. If we accept this idea, we can cut an arbitrary body from a moving, deforming fluid and state the axioms for mass and mechanics as follows:

#### Mass

$$\frac{d}{dt} \int_{V_m(t)} \rho dV = 0 \quad (9)$$

#### Linear Momentum: Euler's First Law

$$\frac{d}{dt} \int_{V_m(t)} \rho \mathbf{v} dV = \int_{V_m(t)} \rho \mathbf{b} dV + \int_{A_m(t)} \mathbf{t}_{(n)} dA \quad (10)$$

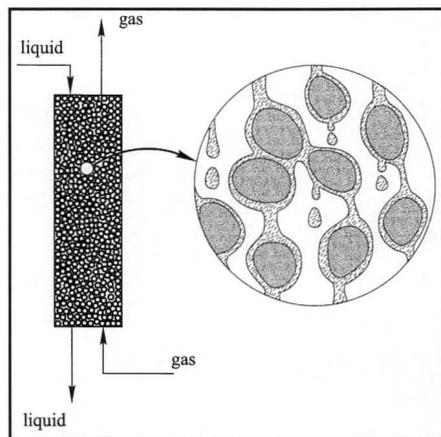


Figure 1. Gas-liquid contacting device.

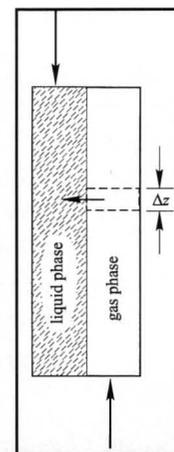


Figure 2. Model of a gas-liquid contacting device.

### Angular Momentum: Euler's Second Law

$$\frac{d}{dt} \int_{\mathcal{V}_m(t)} \mathbf{r} \times \rho \mathbf{v} dV = \int_{\mathcal{V}_m(t)} \mathbf{r} \times \rho \mathbf{b} dV + \int_{\mathcal{A}_m(t)} \mathbf{r} \times \mathbf{t}_{(n)} dA \quad (11)$$

Here,  $\mathcal{V}_m(t)$  represents the time-dependent region occupied by a body,  $\rho$  is the mass density,  $\mathbf{v}$  is the fluid velocity,  $\mathbf{b}$  is the body force per unit mass,  $\mathbf{t}_{(n)}$  is the stress vector, and  $\mathbf{r}$  is the position vector. Both  $\mathbf{v}$  and  $\mathbf{r}$  are measured relative to some inertial frame. The representation of the angular momentum principle given by Eq. (11) assumes that all torques are the moments of forces and this ignores the existence of body torques and couple stresses that have been observed in polar fluids.<sup>[8]</sup> The forms of these three axiomatic statements suggest the need for a study of the kinematics of volume integrals and this leads to the *general transport theorem*<sup>[9]</sup> given by

$$\frac{d}{dt} \int_{\mathcal{V}_a(t)} \psi dV = \int_{\mathcal{V}_a(t)} \frac{\partial \psi}{\partial t} dV + \int_{\mathcal{A}_a(t)} \psi \mathbf{w} \cdot \mathbf{n} dV \quad (12)$$

Here,  $\mathcal{V}_a(t)$  represents the region occupied by an arbitrary moving volume,  $\mathcal{A}_a(t)$  is the bounding surface of this volume, and  $\mathbf{w} \cdot \mathbf{n}$  is the speed of displacement of the bounding surface. When the arbitrary velocity,  $\mathbf{w}$ , is set equal to the fluid velocity,  $\mathbf{v}$ , we obtain the *Reynolds transport theorem* given by

$$\frac{d}{dt} \int_{\mathcal{V}_m(t)} \psi dV = \int_{\mathcal{V}_m(t)} \frac{\partial \psi}{\partial t} dV + \int_{\mathcal{A}_m(t)} \psi \mathbf{v} \cdot \mathbf{n} dV \quad (13)$$

When applied to Eq. (9), this theorem provides

$$\frac{d}{dt} \int_{\mathcal{V}_m(t)} \rho dV = \int_{\mathcal{V}_m(t)} \frac{\partial \rho}{\partial t} dV + \int_{\mathcal{A}_m(t)} \rho \mathbf{v} \cdot \mathbf{n} dV = 0 \quad (14)$$

and use of the divergence theorem leads us to

$$\int_{\mathcal{V}_m(t)} \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] dV = 0 \quad (15)$$

Assuming that the integrand is continuous and noting that the limits of integration are arbitrary leads to the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (16)$$

In order to extract the governing differential equations associated with the linear and angular momentum principles, we first need to follow the work of Cauchy and prove<sup>[7]</sup>

Cauchy's Lemma:

$$\mathbf{t}_{(n)} = -\mathbf{t}_{(-n)} \quad (17)$$

Cauchy's Fundamental Theorem:

$$\mathbf{t}_{(n)} = \mathbf{n} \cdot \mathbf{T} \quad (18)$$

The first of these is introduced as *intuitively obvious* in every statics course where it is applied to the shear stresses

acting on opposing surfaces of a beam that has been subjected to an Eulerian cut. The second result is generally avoided because of its complexity even though most students have completed a course on matrix algebra prior to their study of fluid mechanics.

The use of Eqs. (17) and (18), along with the Reynolds transport theorem, allows us to extract the following differential equations from Eqs. (10) and (11):

Cauchy's First Equation

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \rho \mathbf{g} + \nabla \cdot \mathbf{T} \quad (19)$$

Cauchy's Second Equation

$$\mathbf{T} = \mathbf{T}^T \quad (20)$$

At this point, we are in a position to derive the macroscopic momentum balance that was described in words by Eq. (2). We begin by integrating Eq. (19) over an arbitrary, moving control volume to obtain

$$\int_{\mathcal{V}_a(t)} \frac{\partial}{\partial t} (\rho \mathbf{v}) dV + \int_{\mathcal{V}_a(t)} \nabla \cdot (\rho \mathbf{v} \mathbf{v}) dV = \int_{\mathcal{V}_a(t)} \rho \mathbf{b} dV + \int_{\mathcal{A}_a(t)} \nabla \cdot \mathbf{T} dV \quad (21)$$

We now use the general transport theorem and the divergence theorem to arrange this result in a useful form given by

$$\frac{d}{dt} \int_{\mathcal{V}_a(t)} \rho \mathbf{v} dV + \int_{\mathcal{A}_a(t)} \rho \mathbf{v} (\mathbf{v} - \mathbf{w}) \cdot \mathbf{n} dA = \int_{\mathcal{V}_a(t)} \rho \mathbf{b} dV + \int_{\mathcal{A}_a(t)} \mathbf{t}_{(n)} dA \quad (22)$$

This represents a precise mathematical description of the words contained in Eq. (2), and it clearly indicates that the source of these words is Euler's first law. While the route from the axiom given by Eq. (10) to the proved theorem given by Eq. (22) consists of only a few steps, one must invest a significant amount of time in the study of kinematics and stress in order to derive this result. (At UC Davis we have two ten-week courses in fluid mechanics and time is less of a problem than in most programs.) While kinematics and stress may be confusing, we should heed the words of Pucciani and Hamel,<sup>[10]</sup> who provide the following advice to students:

*There is no learning without confusion. It is by the organization of this confusion that you will progress.*

Said another way, it is better to be confused and frustrated by the concepts of kinematics and stress than to be baffled by the leap of faith from Eq. (1) to Eq. (2).

In order to follow the development from Eq. (10) to Eq. (22) in a successful manner, the faculty must be aware of what students know, what they don't know, and what they are supposed to know. For example, in the typical statics course, students make use of Euler's laws to solve problems, but the laws are never identified in a clear and concise manner. The concept of an Eulerian cut is presented as being *obvious* en route to the development of a free-body diagram,

but no mention is made of the fact that it was not obvious in the eighteenth century. Cauchy's lemma is used in the same way, *i.e.*, the shear is *up* on this side of the cut and *down* on that side of the cut. In order to unravel this mass of intuition, the faculty must be aware of the content of previous courses and must be prepared to extract some order and logic from the student's previous studies. In addition to statics, these previous studies include calculus where the definition of a derivative is presented and the projected area theorem is given.<sup>[11]</sup> These are all that one needs to derive the general transport theorem. Previous studies also include a course on matrix algebra where the students learn that a three-by-three array can be used to transform one set of three numbers to another set of three numbers. This is the essential feature of Cauchy's fundamental theorem.

### RESOLUTION OF THE THERMODYNAMIC DISCONTINUITY

In order to resolve the thermodynamic discontinuity, we begin with a reasonable description of a compressible flow process. This consists of the governing equations for the density, velocity, temperature, and pressure that can be expressed as

Governing equation for  $\rho$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (23)$$

Governing equation for  $\mathbf{v}$

$$\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \rho \mathbf{g} + \mu \nabla^2 \mathbf{v} \quad (24)$$

Governing equation for  $T$

$$\rho c_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = k \nabla^2 T \quad (25)$$

Governing equation for  $p$

$$p = p(\rho, T) \quad (26)$$

The first of these equations represents a completely general form of the continuity equation, while the last represents a completely arbitrary equation of state. Equations (24) and (25) represent special forms of the equations of motions and the thermal energy equation, but they are general enough for our purposes.

The usual concept associated with an incompressible flow is that the variation of the density is *small enough* so that the dependent variable in Eq. (23) can be replaced with a constant,  $\rho_o$ . This means that one of our four dependent variables is determined by some means other than a law of physics and this, in turn, means that we must discard one of our laws of physics. Our new description of the physical process is given by

$$\nabla \cdot \mathbf{v}_m = 0 \quad (27)$$

$$\rho_o \left( \frac{\partial \mathbf{v}_m}{\partial t} + \mathbf{v}_m \cdot \nabla \mathbf{v}_m \right) = -\nabla p_m + \rho_o \mathbf{g} + \mu \nabla^2 \mathbf{v}_m \quad (28)$$

$$\rho_o c_p \left( \frac{\partial T_m}{\partial t} + \mathbf{v}_m \cdot \nabla T_m \right) = k \nabla^2 T_m \quad (29)$$

in which we have used  $\mathbf{v}_m$ ,  $p_m$ , and  $T_m$  to represent the velocity, pressure, and temperature determined by Eqs. (27) through (29). These quantities differ from  $\rho$ ,  $\mathbf{v}$ ,  $p$ , and  $T$  that are determined by Eqs. (23) through (26), and we would like to understand the asymptotic conditions that lead to

$$\rho \rightarrow \rho_o \quad \mathbf{v} \rightarrow \mathbf{v}_m \quad p \rightarrow p_m \quad T \rightarrow T_m \quad (30)$$

When Eqs. (27) through (29) produce velocity, pressure, and temperature fields ( $\mathbf{v}_m$ ,  $p_m$ ,  $T_m$ ) that are good approximations of the fields ( $\mathbf{v}$ ,  $p$ ,  $T$ ) determined by Eqs. (23) through (26), we say that the flow can be approximated as incompressible. Under these circumstances, the pressure can be calculated by purely mechanical means; but it would seem best not to refer to  $p_m$  as a "mechanical pressure," but simply to say that  $p_m$  is a "good approximation" of the pressure determined by an equation of state.

The general asymptotic conditions associated with Eq. (30) are difficult to develop;<sup>[12]</sup> we can, however, explore the first of these conditions for steady flow in the absence of any temperature effects without a great deal of effort. This requires that we consider an isothermal process described by the steady forms of Eqs. (23) through (26), and then search for conditions that lead to

$$\rho \rightarrow \rho_o \quad (31)$$

It will be in the nature of a plausible intuitive hypothesis<sup>[3]</sup> to assume that  $\mathbf{v} \rightarrow \mathbf{v}_m$  and  $p \rightarrow p_m$  when the condition represented by Eq. (31) is satisfied.

For the case in which temperature effects are negligible, we can invert Eq. (26) to obtain

$$\rho = \rho(p) \quad (32)$$

and a Taylor series expansion about  $\rho_o$  leads to

$$\rho = \rho_o + (p - p_o) \left( \frac{\partial \rho}{\partial p} \right)_T + \frac{1}{2} (p - p_o)^2 \left( \frac{\partial^2 \rho}{\partial p^2} \right)_T + \dots \quad (33)$$

Here,  $\rho_o$  is the density determined by Eq. (32) at the reference pressure  $p_o$ . As an *estimate* of the density change that occurs for the process under consideration, we use the first term of the expansion to obtain

$$\rho - \rho_o = \mathbf{O} \left[ \left( \frac{\partial \rho}{\partial p} \right)_T \Delta p \right] \quad (34)$$

in which  $\Delta p$  is representative of the maximum pressure change that occurs in the system. From a thermodynamic analysis, we know that the speed of sound is related to the derivative of the density with respect to the pressure at constant entropy. This relation is given by

$$\left(\frac{\partial p}{\partial p}\right)_s = \frac{1}{c^2} \quad (35)$$

in which  $c$  is the speed of sound. As an approximation, we use

$$\left(\frac{\partial p}{\partial p}\right)_T \sim \frac{1}{c^2} \quad (36)$$

so Eq. (34) takes the form

$$p - p_o = \mathbf{O}\left(\frac{\Delta p}{c^2}\right) \quad (37)$$

In order to obtain an estimate of the pressure change, we first make use of the steady form of Eq. (24) to estimate the gradient of the pressure as

$$\nabla p = \mathbf{O}(\rho g) + \mathbf{O}(\mu \nabla^2 \mathbf{v}) + \mathbf{O}(\rho \mathbf{v} \cdot \nabla \mathbf{v}) \quad (38)$$

The idea associated with this estimate is that  $\nabla p$  may be as large as any of the other terms in Eq. (24) but not significantly larger. In addition, it is possible that  $\nabla p$  may be much smaller than any of those terms, and thus Eq. (38) should be thought of as an overestimate of the pressure gradient. For example, in a laminar boundary layer created by a uniform flow past a flat plate, the pressure gradient is essentially hydrostatic

$$\begin{aligned} &\underline{\text{Laminar boundary layer flow}} \\ &\nabla p \sim \rho g \end{aligned} \quad (39)$$

while the viscous and inertial terms are essentially equal and much larger than  $\nabla p - \rho g$ , *i.e.*,

$$\begin{aligned} &\underline{\text{Laminar boundary layer flow}} \\ &\rho \mathbf{v} \cdot \nabla \mathbf{v} = \mathbf{O}(\mu \nabla^2 \mathbf{v}) \gg \nabla p - \rho g \end{aligned} \quad (40)$$

In this case, only the first estimate given by Eq. (38) is valid and it becomes clear that one must have some idea about the nature of the flow under consideration in order to use Eq. (38) successfully.

If  $u_o$  represents the characteristic velocity for the process, we can use order-of-magnitude analysis<sup>[13]</sup> to obtain the estimates

$$\rho g = \mathbf{O}[(\rho g)\lambda_g] \quad (41a)$$

$$\mu \nabla^2 \mathbf{v} = \mathbf{O}\left[\left(\mu u_o / L_\mu^2\right)\lambda_\mu\right] \quad (41b)$$

$$\rho \mathbf{v} \cdot \nabla \mathbf{v} = \mathbf{O}\left[(\rho u_o^2 / L_\rho)\lambda_\rho\right] \quad (41c)$$

Here,  $L_\mu$  represents the viscous length, and  $L_\rho$  represents the inertial length,<sup>[14]</sup> while  $\lambda_g, \lambda_\mu, \lambda_\rho$  are unit vectors that are parallel to the gravitational term, the viscous term, and the inertial term, respectively. For the laminar boundary layer example discussed above,  $\lambda_\mu$  and  $\lambda_\rho$  are parallel, and  $\lambda_g$  is an arbitrary unit vector.

In order to make use of Eq. (38) to estimate the pressure difference that appears in Eq. (37), we express the pressure gradient as

$$\nabla p = \mathbf{O}(\Delta p / L) \quad (42)$$

Here one must keep in mind that the pressure gradient will be influenced by all three terms represented by Eqs. (41), thus Eq. (42) represents *three separate estimates* and it is left to the reader to keep this fact in mind. Use of Eqs. (41) and (42) in Eq. (38) leads to the following estimate for the pressure change owing to gravitational, viscous, and inertial effects:

$$\Delta p = \mathbf{O}[(\rho g)L] + \mathbf{O}\left[\left(\mu u_o / L_\mu^2\right)L\right] + \mathbf{O}\left[(\rho u_o^2 / L_\rho)L\right] \quad (43)$$

Substitution of this result into Eq. (37) provides the following estimate for the change in density that occurs for the process under consideration:

$$\frac{p - p_o}{\rho} = \mathbf{O}(gL / c^2) + \mathbf{O}(\mu u_o L / \rho L_\mu^2 c^2) + \mathbf{O}(u_o^2 L / L_\rho c^2) \quad (44)$$

If we define a Reynolds number and a Mach number as

$$\text{Re} = \frac{\rho u_o L_\mu}{\mu} \quad \text{M} = \frac{u_o}{c} \quad (45)$$

the estimates given by Eq. (44) take the form

$$\frac{p - p_o}{\rho} = \mathbf{O}(gL / c^2) + \mathbf{O}[\text{Re}^{-1} \text{M}^2 (L / L_\mu)] + \mathbf{O}[\text{M}^2 (L / L_\rho)] \quad (46)$$

From this result we conclude that

$$\frac{p - p_o}{\rho} \ll 1, \quad \text{or} \quad \rho \rightarrow \rho_o \quad (47)$$

when the following constraints are satisfied:

$$gL / c^2 \ll 1 \quad \text{M}^2 \ll \text{Re}(L_\mu / L) \quad \text{M}^2 \ll (L_\rho / L) \quad (48)$$

Here, one must remember that  $L$  has a different meaning in each one of these constraints, which are often replaced by the single condition that the Mach number squared is small compared to one. This has considerable appeal for the last constraint in Eq. (48) since  $L_\rho$  is often large compared to  $L$ ; the simplification given by  $\text{M}^2 \ll 1$  has less appeal as a substitution for the second constraint, however, since  $L_\mu$  is generally small compared to  $L$ . A little thought will indicate that the first constraint given by Eq. (48) is difficult to violate, and thus it is the constraints involving the Mach number that must be considered with care.

It seems plausible that when  $\rho_o$  is a reasonable approximation for  $\rho$ , we can assume that  $\mathbf{v}_m$  and  $p_m$  are reasonable approximations for  $\mathbf{v}$  and  $p$ ; but a rigorous proof would require that we identify the asymptotic conditions that allow us to simplify Eqs. (23) through (26) to the incompressible approximation represented by Eqs. (27) through (29). One should keep in mind that the analysis leading to the constraints given by Eqs. (48) was based on a steady-flow process, and that there are unsteady, low-Mach-number processes for which the flow cannot be treated as incompressible under any circumstances. An example is given in Figure 3, and for that type of process the approximation represented by

$$p - p_o = \mathbf{O}(\nabla p)L \quad (49)$$

is not at all applicable.

The *partial resolution* of the thermodynamic discontinuity required that we clearly identify the general case indicated by Eqs. (23) through (26) and that we discard a law of physics in favor of the approximation given by  $\rho = \rho_0$ . The

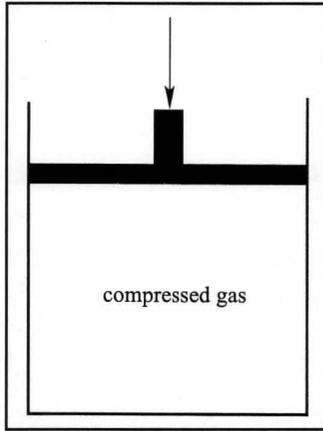


Figure 3. Compression process.

justification of this approximation was based on the equation of state that provided Eq. (37) and the order-of-magnitude analysis given by Eqs. (38) through (46). The use of order-of-magnitude analysis allows students to go beyond the assumptions based on the title of a course, the title of a text, or the title of a chapter in a text. Since these titles are not available to our students when they leave the university, we should encourage them to formulate their own assumptions

and then follow those assumptions with restrictions and constraints.<sup>[13]</sup>

It is important to understand that the thermodynamic discontinuity cannot be resolved only by discussion in fluid mechanics courses. Faculty members who teach thermodynamics must be aware of the problem and speak to the issue. A righteous attitude about the correctness of Eq. (5), or a more general equation of state, provides no help to the student who must deal with the reality of incompressible flows. One must remember that the students take every course in the program and they do not have the luxury to choose their battleground.

## RESOLUTION OF THE MULTIPHASE DISCONTINUITY

Studies of multicomponent mass transport usually include a derivation of the species continuity equation<sup>[5]</sup>, and the molar form of this result is given by

$$\frac{\partial c_A}{\partial t} + \nabla \cdot (c_A \mathbf{v}_A) = R_A \quad A = 1, 2, 3, \dots, N \quad (50)$$

Knowledge of the molar concentration,  $c_A$ , is a central issue in chemical engineering since it forms the basis for all separation and purification processes, for all reactor design calculations, and for all studies of contaminant transport in the land, air, and water. The macroscopic mole balance associated with Eq. (50) can be derived by following the steps that link Eq. (19) to Eq. (22), and the result is given by

$$\frac{d}{dt} \int_{V'_a(t)} c_A dV + \int_{A'_a(t)} c_A (\mathbf{v}_A - \mathbf{w}) \cdot \mathbf{n} dA = \int_{V'_a(t)} R_A dV \quad A = 1, 2, \dots, N \quad (51)$$

Both Eq. (50) and (51) represent powerful problem-solving tools, and most chemical engineering students acquire a certain degree of skill in the application of these results for a variety of single-phase transport problems; their application to multiphase systems, however, is problematic.

Most multiphase transport processes cannot be solved directly in terms of either Eq. (50) or Eq. (51), but require instead the local volume-averaged form of Eq. (50).<sup>[15-18]</sup> The development of this form begins by associating an averaging volume with every point in the region under consideration. This allows one to define a volume-averaged concentration everywhere and to generate a spatially smoothed concentration field. In Figure 4 we have illustrated a two-phase system and a spherical averaging volume having the centroid located at the point identified by the position vector  $\mathbf{x}$ . For this system, we identify the point concentration of species A in the  $\gamma$ -phase as  $c_{A\gamma}$  and we define the superficial average concentration by

$$\langle c_{A\gamma} \rangle |_{\mathbf{x}} = \frac{1}{V'_\gamma} \int_{V'_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \quad (52)$$

Here,  $V'_\gamma(\mathbf{x}, t)$  represents the volume of the  $\gamma$ -phase contained within the averaging volume,  $V'_\gamma$ , and we have clearly indicated that the

superficial average concentration is associated with the point located by the position vector  $\mathbf{x}$ . For the particular case illustrated in Figure 4, the position vector  $\mathbf{x}$  locates a point in the  $\sigma$ -phase where the point concentration of species A may be zero.

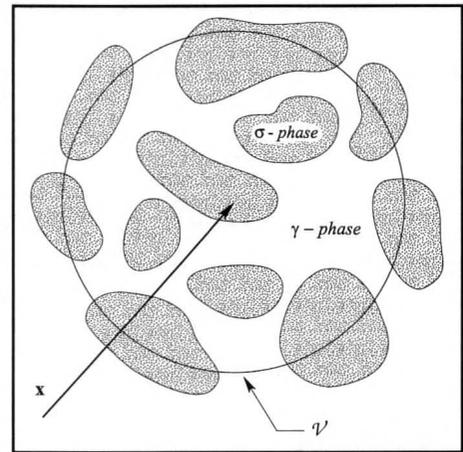


Figure 4. Two-phase system.

In general, the *intrinsic average concentration* is preferred for the analysis of multiphase transport processes, and this is defined by

$$\langle c_{A\gamma} \rangle^Y |_{\mathbf{x}} = \frac{1}{V'_\gamma(\mathbf{x}, t)} \int_{V'_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \quad (53)$$

The superficial and intrinsic average concentrations are related according to

$$\langle c_{A\gamma} \rangle = \epsilon_\gamma \langle c_{A\gamma} \rangle^Y \quad (54)$$

in which  $\epsilon_\gamma$  is the volume fraction of the  $\gamma$ -phase defined explicitly by

$$\varepsilon_\gamma = V_\gamma(\mathbf{x}, t) / \mathcal{V} \quad (55)$$

In many systems, the superficial and intrinsic averages differ by a factor of three or more, and thus it is important to make use of a nomenclature that clearly identifies these two concentrations.

In Figure 5 we have shown a two-phase system for which we would like to develop the design equation for the concentration of species A. We think of the flowing fluid as the  $\gamma$ -phase, while the  $\sigma$ -phase could represent porous catalyst pellets, or droplets of a more dense fluid that is descending through the  $\gamma$ -phase. The governing differential equation for the concentration of species A in the  $\gamma$ -phase is given by

$$\frac{\partial c_{A\gamma}}{\partial t} + \nabla \cdot (c_{A\gamma} \mathbf{v}_{A\gamma}) = R_{A\gamma} \quad (56)$$

and we begin our analysis of this point equation by forming the superficial average to obtain

$$\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \frac{\partial c_{A\gamma}}{\partial t} dV + \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \nabla \cdot (c_{A\gamma} \mathbf{v}_{A\gamma}) dV = \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} R_{A\gamma} dV \quad (57)$$

In order to transform this result to something useful, we make use of two theorems that are essentially extensions of the classic one-dimensional Leibniz rule<sup>[9, Prob. 3-5]</sup> for differentiating an integral. The first of these is the *general transport theorem*, which we used earlier in our treatment of the mechanical discontinuity. This theorem allows us to express the first term in Eq. (57) in the form

$$\frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \frac{\partial c_{A\gamma}}{\partial t} dV = \frac{d}{dt} \left[ \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \right] - \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} \mathbf{w} \cdot \mathbf{n}_{\gamma\sigma} dA \quad (58)$$

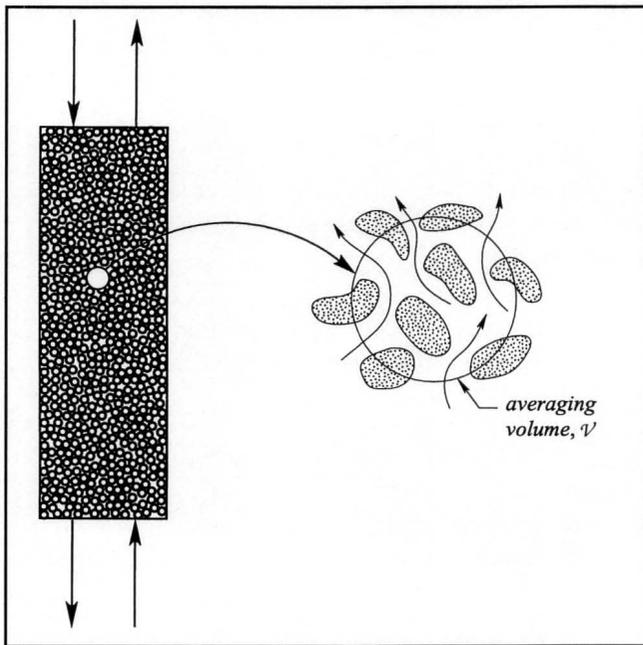


Figure 5. Mass transfer and reaction process in a two-phase system.

Here,  $\mathbf{n}_{\gamma\sigma}$  represents the unit normal vector directed from the  $\gamma$ -phase toward the  $\sigma$ -phase, and  $\mathbf{w} \cdot \mathbf{n}_{\gamma\sigma}$  represents the speed of displacement of the  $\gamma$ - $\sigma$  interface. This is zero if the system under consideration is a packed-bed catalytic reactor, but would be non-zero for a fluidized-bed reactor or any fluid-fluid system. The second theorem needed for the analysis of Eq. (57) is the *spatial averaging theorem*, and the derivation of this theorem<sup>[6,19]</sup> is analogous to the derivation of the general transport theorem. Application of the spatial averaging theorem provides

$$\begin{aligned} & \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} \nabla \cdot (c_{A\gamma} \mathbf{v}_{A\gamma}) dV \\ &= \nabla \cdot \left[ \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} dV \right] + \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} \cdot \mathbf{n}_{\gamma\sigma} dA \end{aligned} \quad (59)$$

and use of this result, along with Eq. (58), in Eq. (57) leads to

$$\begin{aligned} & \frac{d}{dt} \left[ \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} dV \right] + \nabla \cdot \left[ \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} dV \right] \\ &+ \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} (\mathbf{v}_{A\gamma} - \mathbf{w}) \cdot \mathbf{n}_{\gamma\sigma} dA = \frac{1}{\mathcal{V}} \int_{V_\gamma(\mathbf{x}, t)} R_{A\gamma} dV \end{aligned} \quad (60)$$

One should note that this result is a superficial average transport equation, and thus each term has units of moles of species A per unit time per unit volume of the  $\gamma$ - $\sigma$  system. Use of the nomenclature for the superficial average indicated by Eq. 52 allows us to express Eq. (60) in the more compact form given by

$$\underbrace{\frac{\partial}{\partial t} \langle c_{A\gamma} \rangle}_{\text{accumulation}} + \underbrace{\nabla \cdot \langle c_{A\gamma} \mathbf{v}_{A\gamma} \rangle}_{\text{transport}} + \underbrace{\frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} (\mathbf{v}_{A\gamma} - \mathbf{w}) \cdot \mathbf{n}_{\gamma\sigma} dA}_{\text{interfacial transport}} = \underbrace{\langle R_{A\gamma} \rangle}_{\text{homogeneous reaction}} \quad (61)$$

Here it is understood that the averaged quantities are associated with the centroid of the averaging volume identified by the position vector  $\mathbf{x}$  in Figure 4. In addition, we have expressed the accumulation in terms of the partial time derivative since  $\langle c_{A\gamma} \rangle$  is associated with a point that is fixed in space.

The first and last terms in Eq. (61) can be expressed in terms of intrinsic averages by using the relation given by Eq. (54), and this leads to

$$\begin{aligned} & \frac{\partial}{\partial t} \left( \varepsilon_\gamma \langle c_{A\gamma} \rangle^\gamma \right) + \nabla \cdot \langle c_{A\gamma} \mathbf{v}_{A\gamma} \rangle \\ &= - \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} (\mathbf{v}_{A\gamma} - \mathbf{w}) \cdot \mathbf{n}_{\gamma\sigma} dA + \varepsilon_\gamma \langle R_{A\gamma} \rangle^\gamma \end{aligned} \quad (62)$$

In order to simplify the convective transport term, one can use the averaging theorem and the divergence theorem to show that

$$\nabla \cdot \langle c_{A\gamma} \mathbf{v}_{A\gamma} \rangle = - \frac{1}{\mathcal{V}} \int_{A_{\gamma\sigma}(\mathbf{x}, t)} c_{A\gamma} \mathbf{v}_{A\gamma} \cdot \mathbf{n}_{\gamma\sigma} dA \quad (63)$$



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@engin.umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

# NON-ADIABATIC CONTAINER FILLING AND EMPTYING

NOEL DE NEVERS

University of Utah • Salt Lake City, UT 84112

All thermodynamics textbooks present container filling and container emptying (often called bottle filling and bottle emptying) as the simplest examples of unsteady-state, varying-inventory processes. If the process is adiabatic and the contents of the container are well mixed, then the differential mass and energy balances can be combined and integrated, leading to closed-form solutions. The classic problems are of the form:

**Problem 1** • An evacuated, rigid, adiabatic container is connected to a compressed air line at a pressure of 738 kPa and a temperature of 22°C. The connecting valve is opened, and the air flows in until the container pressure is 738 kPa. What is the final temperature in the container?

**Problem 2** • A rigid, adiabatic container contains air at 641 kPa and 29°C. Its valve is opened and it exhausts to the atmosphere at 86 kPa (at Salt Lake City, 1460 m above sea level). When the pressure in the container is the same as atmospheric pressure, what is the temperature in the container?

## GENERAL THEORY FOR ADIABATIC FILLING AND EMPTYING

For a rigid container with flow of matter in or out, the energy balance on the contents, ignoring kinetic, gravitational, electrostatic, and magnetic energies,<sup>[1]</sup> is

$$d(\mu)_{\text{system}} = h_{\text{in}} dm_{\text{in}} - h_{\text{out}} dm_{\text{out}} + dQ \quad (1)$$

and the corresponding mass balance is

$$dm_{\text{system}} = dm_{\text{in}} - dm_{\text{out}} \quad (2)$$

For a container filling from some reservoir (e.g., the atmosphere into an evacuated container, or a large compressed-air or steam line into a container), we may assume perfect internal mixing and that  $h_{\text{in}}$  is a constant, combine Eqs. (1) and (2), and integrate to

$$(\mu)_{\text{system,final}} - (\mu)_{\text{system,initial}} = h_{\text{in}}(m_{\text{final}} - m_{\text{initial}}) + \Delta Q \quad (3)$$

If the mixing is not perfect, then the specific properties shown in Eq. (3) and throughout this paper should be interpreted as mass-average values. For emptying (discharge, blowdown), the simple integration leading to Eq. (3) is not correct because the expansion work done by the fluid during the emptying process causes the temperature, and hence  $h_{\text{out}}$ , to decrease during the process. If one uses an average value of  $h_{\text{out}}$ , one can then use this integration.<sup>[2]</sup> If the material originally present in the system and flowing in or out is a



**Noel de Nevers** is Professor of Chemical Engineering at the University of Utah, where he has been on the faculty since 1963. He has written texts on Fluid Mechanics for Chemical Engineers and Air Pollution Control Engineering. In addition, he works in thermodynamics and accident investigations.

perfect gas, we can substitute and change Eqs. (1) and (3) to

$$d(mC_V T)_{\text{system}} = C_p T_{\text{in}} dm_{\text{in}} - C_p T_{\text{out}} dm_{\text{out}} + dQ \quad (4)$$

For filling, we can integrate Eq. (4) to

$$(mC_V T)_{\text{system, final}} - (mC_V T)_{\text{system, initial}} = C_p T_{\text{in}} (m_{\text{final}} - m_{\text{initial}}) + \Delta Q \quad (5)$$

If  $m_{\text{initial}}$  and  $dQ$  are both zero (initially empty container and adiabatic process), then for filling, Eq. (5) becomes

$$T_{\text{system, final}} = kT_{\text{in}} \quad (6)$$

If the container is not originally empty, but contains a gas with the same value of  $k$  as the gas that enters,  $\Delta Q=0$  and  $T_{\text{initial}} = T_{\text{in}}$ , then the solution is

$$T_{\text{system, final}} = kT_{\text{in}} - T_{\text{initial}} (k-1) \frac{m_{\text{initial}}}{m_{\text{final}}} \quad (7)$$

For adiabatic emptying, the perfect mixing assumption allows us to set the system temperature equal to the outflow temperature and integrate Eq. (4) to

$$\frac{T_{\text{final}}}{T_{\text{initial}}} = \left( \frac{m_{\text{final}}}{m_{\text{initial}}} \right)^{(k-1)} \quad (8)$$

Replacement of the  $m$  terms by their ideal-gas-law values produces

$$\frac{T_{\text{final}}}{T_{\text{initial}}} = \left( \frac{P_{\text{final}}}{P_{\text{initial}}} \right)^{\left( \frac{k-1}{k} \right)} \quad (9)$$

which is the relation for an isentropic expansion of an ideal gas.

### PROBLEM SOLUTION

Using Eqs. (6) and (9), with the adiabatic assumption and the further assumption that air is an ideal gas with  $k = 1.40$ , we can solve Problems 1 and 2, finding

$$T_{\text{system, final}} = kT_{\text{in}} = (1.40)(295 \text{ K}) = 413 \text{ K} = 140^\circ\text{C}$$

and

$$\frac{T_{\text{final}}}{T_{\text{initial}}} = \left( \frac{P_{\text{final}}}{P_{\text{initial}}} \right)^{\left( \frac{k-1}{k} \right)} = \left( \frac{86 \text{ kpa}}{641 \text{ kpa}} \right)^{\left( \frac{0.4}{1.4} \right)} = 0.563$$

$$T_{\text{final}} = 0.563 T_{\text{initial}} = (0.563)(302 \text{ K}) = 170 \text{ K} = -103^\circ\text{C}$$

But experimental results<sup>[3]</sup> do not agree, even approximately, with these simple theories. This disagreement is explained<sup>[3]</sup> as being due to significant heat transfer. This appears startling, because the filling and emptying experiments are normally finished in a few seconds. But, as shown

below, it is correct.

**General Theory for Non-Adiabatic filling** • If we now allow for heat transfer, and replace  $dQ$  by  $hA(T - T_{\text{surroundings}})dt$  and keep the ideal gas assumption, then Eq. (4) becomes

$$d(mC_V T)_{\text{system}} = C_p T_{\text{in}} dm_{\text{in}} - C_p T_{\text{out}} dm_{\text{out}} + hA(T_{\text{system}} - T_{\text{surroundings}})dt \quad (10)$$

For filling, we drop the outflow term and rearrange to

$$\frac{d(mT)_{\text{system}}}{dt} = \dot{m}_{\text{in}} kT_{\text{in}} - \frac{hA}{C_V} (T_{\text{system}} - T_{\text{surroundings}}) \quad (11)$$

To save writing, we define  $\alpha = hA/C_V$  and drop the subscript on  $T_{\text{system}}$ . If we assume a constant filling rate, we can replace the instantaneous system mass with

$$m = m_{\text{initial}} + \dot{m}_{\text{in}} t \quad (12)$$

and rearrange to

$$(m_{\text{initial}} + \dot{m}_{\text{in}} t) \frac{dT}{dt} = \dot{m}_{\text{in}} (kT_{\text{in}} - T) - \alpha (T - T_{\text{surroundings}}) \quad (13)$$

Separating variables, integrating from start to finish, and assuming that the  $T_{\text{surroundings}}$  is constant and equal to the initial temperature of the gas in the container, we find

$$\frac{-T + \left( \frac{\dot{m}_{\text{in}}}{\dot{m}_{\text{in}} + \alpha} \right) kT_{\text{in}} + \left( \frac{\alpha}{\dot{m}_{\text{in}} + \alpha} \right) T_{\text{surroundings}}}{\left( \frac{\dot{m}_{\text{in}}}{\dot{m}_{\text{in}} + \alpha} \right) kT_{\text{in}} + \left( \frac{\alpha}{\dot{m}_{\text{in}} + \alpha} - 1 \right) T_{\text{surroundings}}} = \left( \frac{m_{\text{initial}} + \dot{m}_{\text{in}} t}{m_{\text{initial}}} \right)^{\left( 1 + \frac{\alpha}{\dot{m}_{\text{in}}} \right)} \quad (14)$$

If, instead of assuming a constant inflow rate, we assume an inflow rate that declines linearly with time, we can write

$$m_{\text{system}} = m_{\text{initial}} + \int (a - bt) dt = m_{\text{initial}} + at - 0.5bt^2 \quad (15)$$

where  $a$  and  $b$  are data-fitting constants. Substituting this for  $m_{\text{system}}$  in Eq. (11) and rearranging, we find

$$\frac{dT}{dt} = \frac{(a - bt)(kT_{\text{in}} - T) - \alpha(T - T_{\text{surroundings}})}{m_{\text{initial}} + at - 0.5bt^2} \quad (16)$$

which can be integrated numerically.

**General Theory for Non-Adiabatic Emptying** • For container emptying, Eq. (11) becomes

$$\frac{d(mT)_{\text{system}}}{dt} = -\dot{m}_{\text{out}} kT - \alpha(T - T_{\text{surroundings}}) \quad (17)$$

For an assumed constant flow rate, the equivalent of Eq. (13) is

$$(m_{\text{initial}} - \dot{m}_{\text{out}} t) \frac{dT}{dt} = -\dot{m}_{\text{out}} T(k-1) - \alpha(T - T_{\text{surroundings}}) \quad (18)$$

and the equivalent of Eq. (14) is

$$\frac{[-\dot{m}_{\text{out}}(k-1) - \alpha]T + \alpha T_{\text{surroundings}}}{[-\dot{m}_{\text{out}}(k-1) - \alpha]T_{\text{initial}} + \alpha T_{\text{surroundings}}} = \left( \frac{m_{\text{initial}} - \dot{m}_{\text{out}} t}{m_{\text{initial}}} \right)^{\left[ (k-1) + \frac{\alpha}{\dot{m}_{\text{out}}} \right]} \quad (19)$$

For the assumed linearly decreasing mass flow rate out, the equivalent of Eq. (16) is

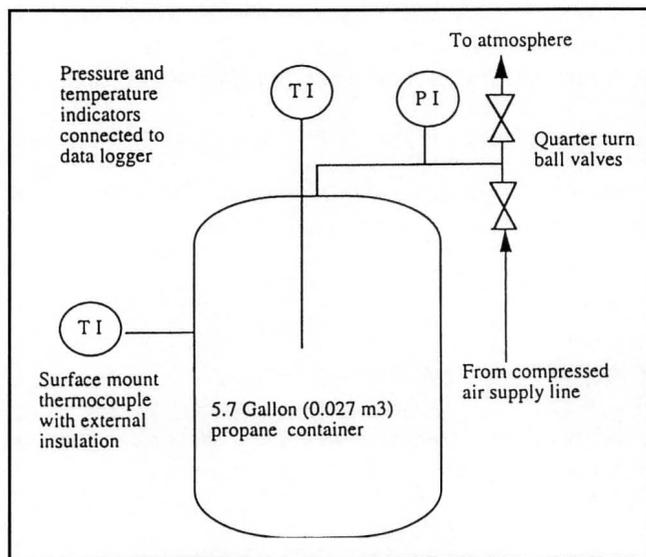
$$\frac{dT}{dt} = \frac{-(a-bt)(k-1)T - \alpha(T - T_{\text{surroundings}})}{m_{\text{initial}} - at + 0.5bt^2} \quad (20)$$

which is also suitable for numerical integration.

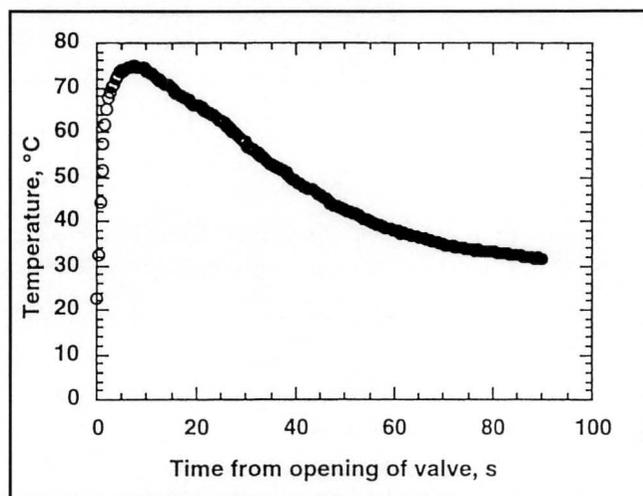
## EXPERIMENTAL TESTS

The experimental apparatus,<sup>[4]</sup> sketched in Figure 1, consisted of an ordinary 0.027 m<sup>3</sup> propane storage container, a pressure transducer, thermocouples, and a data logger. The container was evacuated, filled from a compressed air main, and then emptied to the atmosphere several times, with several sizes of thermocouples (see discussion of thermocouple measuring lag below), and with inlet and outlet flow restrictors, in some cases, to slow the flow. Figures 2 and 3 show the temperature measurements for typical filling and emptying experiments. The measured maximum and minimum temperatures are far from those computed above.

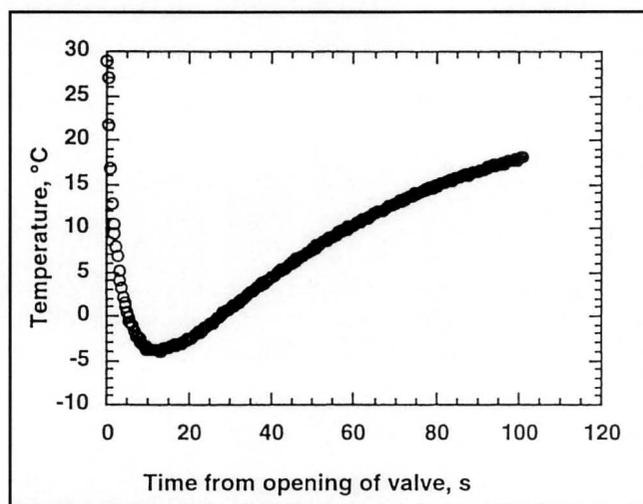
We can estimate the heat transfer coefficient between the



**Figure 1.** Flow and instrumentation diagram of the experimental apparatus. The data logger records temperatures and pressures at 1/3-second intervals.



**Figure 2.** Temperature-time plot for filling the container from the laboratory compressed air main at 738 kPa. The pressure reached that value in  $\approx 5.3$  s. The temperature rose from 22 to 74.5°C, reaching the peak at 6 s. The air inlet valve was closed at 5 s, and the pressure allowed to decrease as the air in the container cooled. The metal walls of the tank rose in temperature from 26 to 29.3°C. After the peak temperature, the gas cooled slowly toward room temperature. For the adiabatic assumption, the peak temperature, calculated in the text, was 140°C.

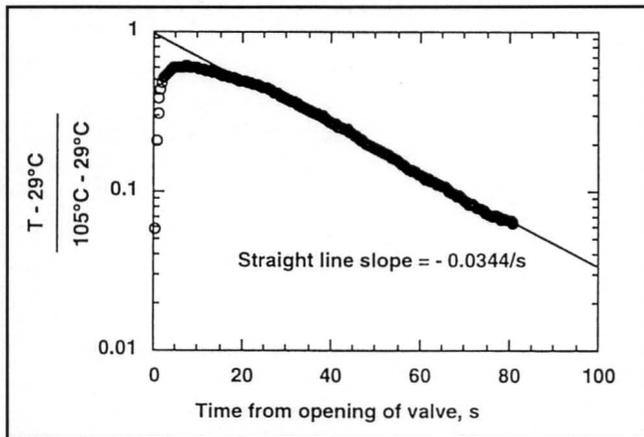


**Figure 3.** Temperature-time plot for emptying the container to the atmosphere (at 86 kPa) from an initial pressure of 641 kPa. The pressure reached atmospheric in  $\approx 1.7$  s. The temperature fell from 29 to -4°C, reaching its minimum at 9.7 s. The metal walls of the tank fell in temperature from 28.8 to 27.5°C. After the minimum temperature, the gas warmed slowly toward room temperature with the exit valve open. For the adiabatic assumption, the minimum temperature, calculated in the text, was -103°C.

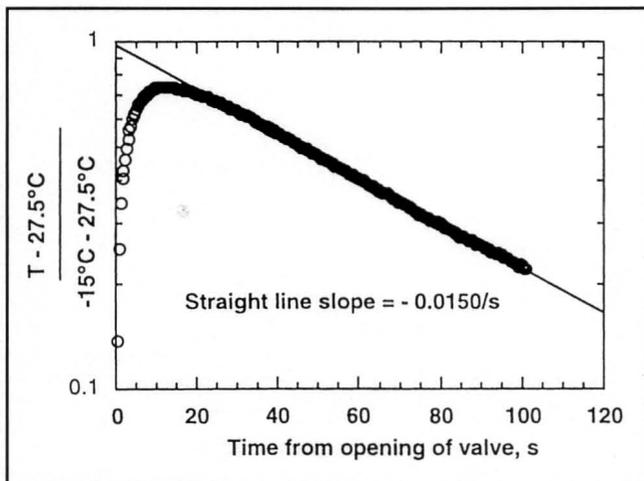
air in the containers and the container walls if we assume that the thermocouple lag was small compared to 100 s and that in each process the gas underwent a step change in temperature and was then cooled or heated by simple convective heat transfer with a constant-temperature container wall. With these assumptions, the gas temperature is given by

$$\frac{T - T_{\text{wall}}}{T_{\text{after step}} - T_{\text{wall}}} = \exp\left(-\frac{hA}{mC} t\right) \quad (21)$$

suggesting that a plot of the ln of the temperature ratio at the left of Eq. (21) vs.  $t$  should form a straight line, from which  $h$  could be estimated. Figures 4 and 5 show such plots; from the slopes, one may infer the values of the heat-transfer coefficients. The choice of  $T_{\text{after step}}$  is arbitrary, made to force the straight lines through 1.0 on the ordinate. Changing these values moves the curves up and down without changing their slopes.



**Figure 4.** Replot of temperature-time data from Figure 2, in the form suggested by Eq. (21).



**Figure 5.** Replot of temperature-time data from Figure 3 in the form suggested by Eq. (21).

From these tests, one can estimate the heat-transfer coefficients. For example, for the filling test (Figures 2 and 4), with  $C = C_v = 2.5R$

$$h = \frac{(166 \text{ g})(2.5)(8.314) \left(\frac{\text{J}}{\text{mol K}}\right) \left(\frac{0.0344}{\text{s}}\right) \frac{\text{mol}}{29 \text{ g}}}{0.390 \text{ m}^2} = 10.49 \frac{\text{W}}{\text{m}^2 \text{K}}$$

and for emptying (Figures 3 and 5), with  $C = C_p = 3.5 R$

$$h = 0.91 \frac{\text{W}}{\text{m}^2 \text{K}}$$

The surprisingly large difference is largely due to the difference in air densities (due to differing pressures) for the two cases. The heat-transfer coefficients, estimated from a flat-wall natural convection correlation<sup>[5]</sup>

$$\text{Nu} = 0.0210(\text{Gr Pr})^{0.4} \quad (22)$$

using average values of the gas density and the temperature differences, are 11.9 and 1.7 W/(m<sup>2</sup>K). The first is close to the value calculated from the cooling curve and the second about twice the value calculated from the warming curve.

If we assume that the processes were practically two-step, with a quick adiabatic process followed by a slow transfer of heat to or from the walls of the container, then by energy balance, we can compute that

$$\Delta T_{\text{container walls}} = \frac{[mC(T_{\text{adiabatic}} - T_{\text{final}})]_{\text{gas in container}}}{(mC)_{\text{container walls}}} \quad (23)$$

For the filling experiment, with  $C = C_v$ , the value are

$$\Delta T_{\text{container walls}} = \frac{\left\{182 \text{ g} \left[ \frac{(2.5)(8.314) \text{ J}}{29 \text{ gK}} \right] (140^\circ\text{C} - 29^\circ\text{C}) \right\}}{\left[ (7.03 \text{ kg})(0.46) \frac{\text{kJ}}{\text{kg K}} \right]} = 4.48^\circ\text{C}$$

and the corresponding value for emptying, with  $C = C_p$ , is  $-0.94^\circ\text{C}$ . The measured values are 3.3 and  $-1.3^\circ\text{C}$ .

## THERMOCOUPLE LAG

A major part of the difference between the steep parts of the temperature curves on Figures 2 and 4 and the values calculated from adiabatic behavior, or those computed by Eqs. (14), (16), (19), and (20), is due to thermocouple lag. This is normally characterized<sup>[6]</sup> in terms of the first-order time constant of the thermocouple. If we assume that the gas in the container undergoes a step increase or decrease in temperature, followed by a first-order decay toward the surrounding temperature, and that the thermocouple responds as described in Reference 6, then the equation for the thermocouple reading will be

$$\frac{dT_{\text{thermocouple}}}{dt} = b \left[ T_{\text{wall}} + (T_{\text{end of step}} - T_{\text{wall}}) \exp(-at) - T \right] \quad (24)$$

where  $a$  and  $b$  are the time constants of the cooling or heating air in the container and of the thermocouple. The integrated form is

$$\frac{T_{\text{thermocouple}} - T_{\text{wall}}}{T_{\text{end of step}} - T_{\text{wall}}} = \frac{a}{b-a} [\exp(-at) - \exp(-bt)] \quad (25)$$

with the peak value of  $T_{\text{thermocouple}}$  occurring at

$$t = \frac{\ln(b/a)}{b-a} \quad (26)$$

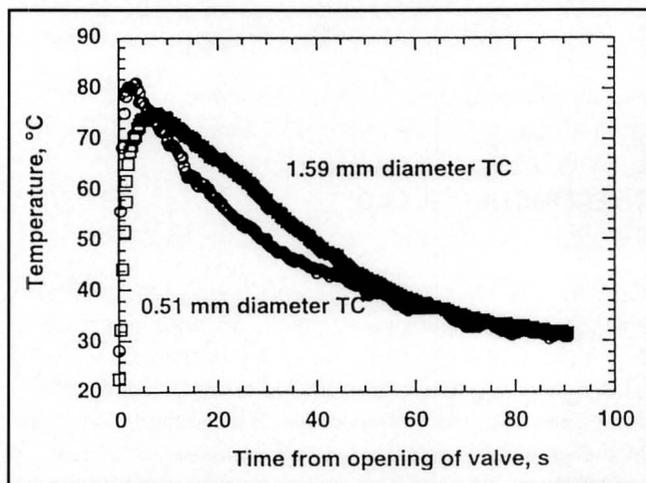
with maximum value

$$\left( \frac{T_{\text{thermocouple}} - T_{\text{wall}}}{T_{\text{end of step}} - T_{\text{wall}}} \right)_{\text{maximum}} = \left( \frac{a}{b} \right) \left( \frac{b}{b-a} \right) \quad (27)$$

Figure 6 shows a comparison of the reported temperatures for two sizes of thermocouple for identical filling experiments. As expected, the smaller thermocouple reports a higher peak temperature and reaches it sooner. Table 1 shows the comparison of the time-to-peak reported  $T$  and the estimated value of  $T_{\text{end of step}}$  calculated from Eqs. (26) and (27). The computed and observed times-to-peak reported temperature are in good agreement, but the computed maximum temperatures are far too high, indicating that after a few seconds, the two-first-order-processes-in-series model works well, but its extrapolation to  $t=0$  does not. If the contained gas temperatures were not changing rapidly due to heat transfer, this thermocouple lag would pose no problem.

### ESTIMATING MAXIMUM TEMPERATURES

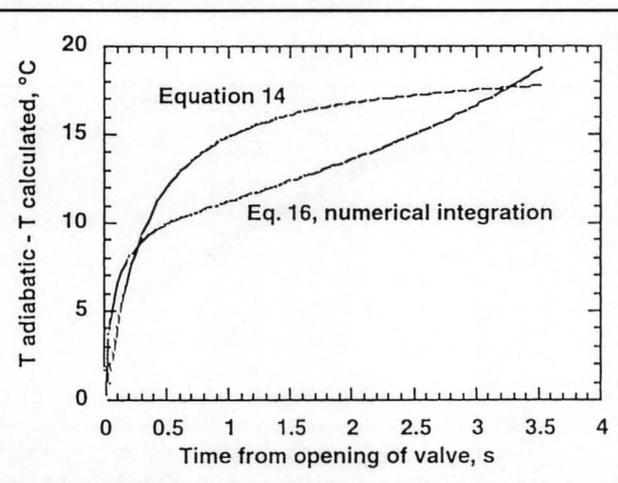
To estimate the maximum temperatures from Eqs. (14), (16), (19), and (20), the mass flow rates were computed by



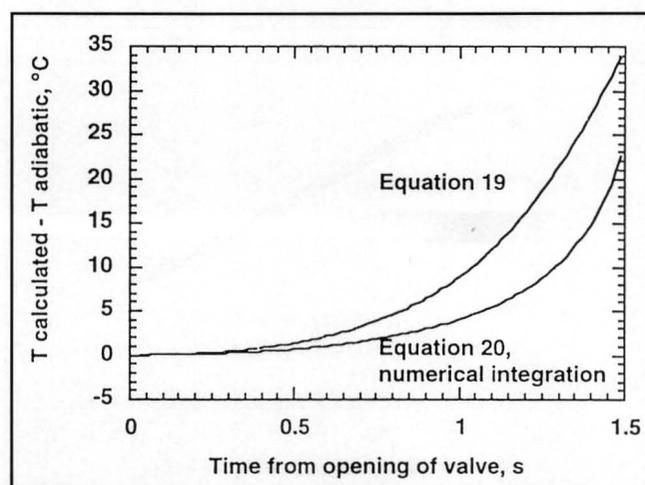
**Figure 6.** Reported temperatures for two identical filling experiments with different size thermocouples. The 0.51-mm diameter thermocouple reached its peak reading at 3.3 s; the 1.59-mm diameter thermocouple reached its at 7.67 s.

**TABLE 1**  
Applications of Eqs. (26) and (27) with the Time Constant of Cooling the Container Assumed = 0.034/s (See Figure 4)

	0.51-mm diameter Thermocouple	1.59-mm diameter Thermocouple
Reported time constant, <sup>[6]</sup> s	1/4 = 0.25	1/9 = 1.11
Observed time to peak reported T, s	3.3	7.67
Calculated time to peak T, by Eq. (26), s	3.2	9.3
Right-hand side of Eq. (27)	0.027	0.099
Calculated $T_{\text{end of step}}$ from Eq. (27), °C	2000	500



**Figure 7.** Computed departure of the tank temperature for tank filling from the calculated adiabatic temperature for the same conditions. Here,  $m_{\text{initial}}=3.5$  g.



**Figure 8.** Computed departure of the tank temperature for tank emptying from the calculated adiabatic temperature for the same conditions.

differencing the calculated mass in the container at each 1/3-second measuring interval. This has the drawback that it relies on the thermocouple reading, which is known to lag the true temperature. With this caveat, the flow rates corresponding to Figures 2 and 3 were estimated as

$$\dot{m} = 100 \frac{\text{g}}{\text{s}} - 28.6 \frac{\text{g}}{\text{s}^2} t; \quad 0 \leq t \leq 3.5\text{s}$$

and

$$\dot{m} = 239 \frac{\text{g}}{\text{s}} - 171 \frac{\text{g}}{\text{s}^2} t; \quad 0 \leq t \leq 1.5\text{s}$$

For both filling and emptying, the heat-transfer coefficient was estimated from Eq. (22) and assumed constant. At the average density and temperature difference between wall and gas, the estimated values were 8.9 and 9.0 W/(m<sup>2</sup>K) for filling and emptying. Figures 7 and 8 show the calculated departures from the corresponding adiabatic solutions (Eqs. 7 and 8). From them we see that in both cases the major departure occurs at the boundary of the process at which the mass of air in the container is least (the start for filling, the finish for emptying); this is the natural consequence of dividing a calculated heat flow that is assumed independent of the mass by a small mass rather than a large one. Because of the strength of the assumptions and the thermocouple lag problem, these figures should be seen as order-of-magnitude. Nonetheless, they make clear that even for these fast processes, with plausible heat-transfer coefficients, the calculated temperatures are substantially different from the computed adiabatic temperatures.

### APPLICATION TO LARGER TANKS

Equations (14) and (19) show that for the constant mass-flow-rate in or out simplification, and for  $T_{\text{in}} = T_{\text{initial}} = T_{\text{surroundings}}$ , the T-t behavior depends only on the two dimensionless groups  $m/m_0$  and  $\alpha/\dot{m}$ . Thus the experimental results shown here should also be observed in any container for which these parameters have the same values. The first can take on any value, but the second is a function of container geometry. If the initial conditions in the container and the reservoir conditions for filling and emptying are the same for two tanks, then  $\dot{m}$  should be proportional to the cross-sectional area of the inlet pipe. If the heat-transfer coefficient does not change, then  $\alpha$  is proportional to the surface area of the container. If the ratio of the inlet pipe cross-sectional area to the surface area of the container does not change, then the second of these dimensionless groups should also not change (or change much with changes in the heat-transfer coefficient). Thus, while the experiments reported here were all performed in a 0.027 m<sup>3</sup> container, they should be directly applicable to larger tanks with the same dimension ratios.

### CONCLUSIONS

The adiabatic, ideal-gas container filling and emptying solutions have a traditional place in thermodynamics text-

books because they are the simplest unsteady-state, varying-inventory problems that can be solved in closed form. In practice, it is impossible to conduct these processes without heat-transfer-producing gas temperatures far different from the adiabatic flow solutions, mostly because while the amount of heat transferred is small, the mass of gas into which it is transferred is also small. The effects of such heat transfer on the temperature-time behavior of such processes can be estimated with at least order-of-magnitude accuracy.

Thermocouple lag adds to the effect of the heat transfer, further increasing the difference between the observed temperature extremes and the values calculated for adiabatic filling and emptying.

A different version of this problem and experiment appeared while this paper was in press.<sup>[7]</sup>

### NOMENCLATURE

A	area
a	time constant of cooling or heating air in the container
a,b	constants in data-fitting equations
b	time constant of thermocouple
C	heat capacity
C <sub>p</sub>	heat capacity at constant pressure
C <sub>v</sub>	heat capacity at constant volume
Gr	Grashof Number
h	heat-transfer coefficient
h	specific enthalpy
k	C <sub>p</sub> /C <sub>v</sub>
m	mass
$\dot{m}$	mass flow rate
Nu	Nusselt number
P	pressure
Pr	Prandtl number
Q	heat quantity
R	universal gas constant
T	temperature
t	time
u	specific internal energy
$\alpha$	hA/C <sub>v</sub>

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# Random Thoughts . . .

## FAQS

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

At the teaching workshops we give, we propose a variety of instructional methods that deviate from traditional teaching practice. We recommend, for example, that instructors break up their lectures at frequent intervals with brief individual or small group exercises. We suggest using formal cooperative learning, in which students work on assignments in instructor-formed teams under conditions structured to assure individual accountability for all of the assigned material. We caution against giving tests that only the best students in the class have time to finish, and we argue strongly against curving grades.

Predictably, critical questions are raised about these recommendations and others we offer. In a series of columns beginning with this one, we want to review some of the most frequently asked questions (FAQs) and our responses. We have two reasons for doing this. First, the suggestions we offer at the workshops are far from unique with us: they are being made with increasing frequency by educational researchers, national study commissions, employers of engineering graduates, and accrediting bodies like ABET. If you have not already been exposed to them, you almost certainly

will be before long, and some of our responses may be helpful as you consider the ideas being advanced. Our second objective is to offer those of you who are already using the new methods some answers to give your colleagues, administrators, and students, who are certain to raise the same questions with you.

Here, then, is our top ten list of questions frequently asked at teaching workshops.

1. *Is there any real evidence that these methods work?*
2. I have a lot of material to get through in a semester.  
*Can I use these methods and still have time to cover my syllabus?*
3. I teach a class of 175 students in a fixed-seat auditorium.  
*Will these methods work in large classes?*
4. I'm teaching a course by distance education.  
*How can I get students active when I'm not in the same room with them?*
5. I tried putting students to work in groups, but some of them hated it and one complained to my department head.  
*Why are some students so hostile to cooperative learning and what am I supposed to do about the hostility?*
6. Many of my students are (a) unmotivated, (b) self-centered, (c) apathetic, (d) lazy, (e) materialistic, (f) unprepared, (g) unable to do high school math, (h) unable to write, (i) unable to read, (j) spoiled rotten. (Pick any subset.)  
*How can you teach people who don't have the right background or the willingness to work or even the*

**Richard M. Felder** is Hoechst Celanese Professor of Chemical Engineering at North Carolina State University. He received his BChE from City College of CUNY and his PhD from Princeton. He has presented courses on chemical engineering principles, reactor design, process optimization, and effective teaching to various American and foreign industries and institutions. He is coauthor of the text *Elementary Principles of Chemical Processes* (Wiley, 1986).



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

*desire to learn?*

7. Engineers constantly have to face deadlines.  
*What's wrong with giving tests that only the best students have time to finish?*
8. *What difference does it make if my test averages are in the 50's, since I'm going to curve in the end?*
9. My department head says that we can't count teaching too much in promotion and tenure decisions because we don't know how to evaluate teaching.  
*Is there a meaningful way to evaluate teaching?*
10. The people who go to teaching workshops are mostly excellent teachers—the ones who most need to change wouldn't go to a teaching workshop at gunpoint.  
*How can I persuade my traditional colleagues to do some of the nontraditional things you're recommending?*

The workshop participants who ask these questions are doing what they have been trained to do as scientists and engineers and educated people, which is to ask for hard evidence before changing the way they've always done things. We applaud them for asking. In this column we'll offer an answer to the first question, and subsequent columns will deal with the others.

**Q:** *Is there any REAL evidence that these nontraditional methods work?*

**A:** *Tons of it.*

Cognitive and educational scientists have learned a great deal about learning in recent years. The near-unanimous consensus is that we learn mainly by doing things and reflecting on the outcomes, taking in relatively little of what we just see and hear (e.g., in lectures) and retaining even less. Countless studies have compared the academic performance and attitudes of students taught using active and cooperative methods with the performance and attitudes of students taught more traditionally. The evidence for the effectiveness of the nontraditional methods is overwhelming. (Specific references will be cited shortly.)

Unfortunately, most professors have never seen a monograph, paper, or seminar on research into teaching and learning and would be hard pressed to name a journal or conference where such research might show up. When the "Prove it!" card is played at our workshops (and even if it isn't), we

therefore urge our questioners not to take our word for anything we say but to approach the matter scientifically and check the literature. We point them to a series of three papers in *Chemical Engineering Education* written by Jim Haile,<sup>[1]</sup> which collectively provide the best summary we've ever seen of what cognitive science has discovered about the learning process and the implications of this knowledge for teaching. We introduce them to the classic *Teaching Tips*,<sup>[2]</sup> in which Wilbert McKeachie offers an abundance of practical suggestions about every aspect of college teaching along with citations of the research that backs up the suggestions. We tell them about *What Matters in College*,<sup>[3,4]</sup> Alexander Astin's monumental study of nearly 25,000 students at over 300 institutions that powerfully demonstrates the deficiencies of the traditional instructional model. We cite references on cooperative learning (e.g., Johnson, Johnson, and Smith<sup>[5]</sup>) that in turn cite hundreds of research studies attesting to the effectiveness of this approach, and we discuss the results of a longitudinal study one of us carried out of the effectiveness of cooperative learning in chemical engineering education.<sup>[6,7]</sup> "Browse these references," we urge. "Then decide whether the research and the methods we're advocating are worthy of serious consideration."

More to come.

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# EVALUATION OF COMPUTER-SIMULATION EXPERIMENTS IN A SENIOR-LEVEL CAPSTONE ChE COURSE

SCOTT R. WHITE, GEORGE M. BODNER  
Purdue University • West Lafayette, IN 47907-1393

In 1986, the School of Chemical Engineering at Purdue University began a revision of its senior-level capstone laboratory courses, including the development of a series of computer-simulation experiments described elsewhere.<sup>[1-7]</sup> For each computer simulation, the students are given a budget (*i.e.*, \$35,000) that is the amount they can spend on experimental runs, wages, and consultation fees. The computer also keeps track of the “virtual” time the students use for each run and charges extra for work that has to be done on weekends.

This paper describes the results of an evaluation of the effect of using these simulations. It is based on three assumptions:

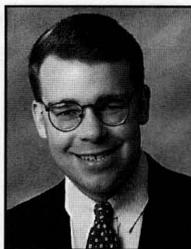
- *When we change what we teach, or how we teach, we change what the students learn.*
- *A systematic evaluation should be done whenever major changes are made in an established curriculum.*
- *Systematic evaluations should look behind the facade of answers to the questions, “Do the students like it?” toward deeper questions such as “What will students learn that they were not learning before?” and “If we could provide students with a voice to express their opinions and concerns, what changes would they recommend?”*

The basic research question behind this study was: “How do the students’ experiences with computer simulations compare with their experiences with traditional laboratory experiments?” Corollary research questions included: “What did the students perceive as a valuable experience in both laboratory formats?”; “How did the students’ decision-making processes and other group-related interactions differ between the two formats?”; “What do the students believe makes the computer-simulation experiment a legitimate ex-

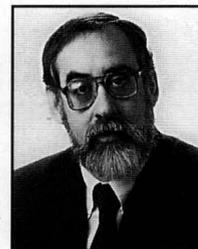
ercise to include in the chemical engineering curriculum?”

## DEVELOPING EVALUATION METHODS

The study was based on a collaboration between members of a chemical education research group<sup>[8]</sup> and faculty and staff from the School of Chemical Engineering who had developed and implemented the computer simulations. We began by scrutinizing a list of questions generated by Professor R. G. Squires and Dr. S. Jayakumar for use in a quantitative study of student attitudes toward the simulations. Some of the questions were retained and others were modified to make them either less complex or less “leading.” The result of this review was a 15-item five-point Likert-scale questionnaire that included space for students to write additional comments and/or suggestions. The questionnaire was given to the students after they had completed both a traditional



**Scott R. White** is a PhD graduate student in Science Education at Purdue University. He received his BS in Chemistry and Secondary Education Certification in 1992 from Harding University. He received his MS in Chemistry from Purdue University in 1996 with G.M. Bodner. His research interests are in teaching and learning in science and curriculum reform.



**George M. Bodner** is Professor of Chemistry and Education at Purdue. He received his BS in Chemistry from the State University at New York, Buffalo (1969) and his PhD in inorganic and organic chemistry from Indiana University (1972). His research interests are learning theory, overcoming barriers to curriculum reform, and understanding the conditions for appropriate use of technology in teaching and learning chemistry.

**TABLE 1**  
Survey Percentage Responses\*

Item	Statement	Agree	Neutral	Disagree	Avg.
1.	I like using computer simulations.	91	3	6	4.2
2.	When using the computer simulation, I worried that my data would be lost, or that the program would fail.	22	16	62	2.4
3.	Time and budget constraints made the computer experiments more realistic.	86	3	11	4.2
4.	The conventional lab experiments worked better than the computer experiments.	5	11	84	1.9
5.	The video tour of the plant added little to the value of the computer experiment.	30	30	40	3.0
6.	It was easy to learn and operate the computer simulation.	95	0	5	4.3
7.	Computer-simulation experiments intimidate me.	6	8	86	1.8
8.	The speed of data acquisition in the computer experiments makes me uneasy.	6	5	89	1.7
9.	Computer experiments allowed me to focus on the principles to be learned rather than on the details of operating a particular piece of equipment.	82	10	8	4.2
10.	Computer experiments are more interesting than conventional experiments.	40	38	22	3.3
11.	One disadvantage of computer experiments is that I do not gain experience with the real plant equipment.	60	24	16	3.6
12.	I would like to see more computer-simulated experiments in the chemical engineering curriculum.	73	14	13	3.8
13.	I would rather work on a computer simulation because it is less hazardous than a conventional experiment.	27	27	46	2.8
14.	Conventional experiments give me a better sense of the kinds of problems likely to be encountered in industry.	54	22	24	3.6
15.	My group cooperated better during the conventional lab experiments.	13	43	44	2.6
16.	The design problem imposed by the computer simulation is not as challenging as those encountered during conventional experiments.	30	22	49	2.8
17.	A higher percentage of our time was spent planning the design of computer experiments.	86	3	11	4.1
18.	The computer simulation allowed me to study problems that are more complex and realistic than the conventional experiments.	78	19	3	4.0
19.	Computer simulations allow me to make more effective use of time by reducing the amount of time needed to run experiments.	95	5	0	4.4
20.	The conventional lab experiments were easier to learn and operate than the computer experiment.	6	8	86	1.9
21.	Computer simulations are a good way to learn new processes and concepts.	79	22	0	4.1
22.	Computer simulations work better than the conventional experiments.	60	35	5	3.8
23.	Computer simulations are more likely to "work" than conventional experiments.	81	14	5	4.1
24.	Overall, I think the present combination of computer simulations and conventional experiments is appropriate.	57	14	29	3.4

\*This table summarizes the results of two semesters. We combined the "Strongly Agree" and "Agree" responses into one category—"Agree." "Strongly Disagree" and "Disagree" have been combined into the "Disagree" category. The "Undecided" responses are indicated as "Neutral (N)."

experiment and a computer-simulation experiment. Results of this survey for students from two semesters are summarized in Table 1.

The authors developed a qualitative component of the evaluation<sup>[9]</sup> based on structured interviews with individual students or with groups of students; observations and field notes collected in the laboratories, written comments from the surveys described above, and interactions with the students in the labs. As those familiar with qualitative techniques might expect, the qualitative component provided the "richest" source of data for this study.

Collection of qualitative data began with the researcher sitting in a corner of the traditional lab, taking field notes as he observed what was happening. The students would frequently start conversations with the researcher, asking what he was doing there and relating what they thought about the experiment they were doing or what they thought or had heard about the computer-simulation experiments. Frequently the students would physically point out things that were working or not working with their traditional experiments, which helped the researcher gain an understanding of the experiments the students were performing.

As these interactions continued, the researcher found it useful to switch from the role of an objective observer sitting in a corner of the room taking notes to that of a participant-observer, listening to and talking with students while they worked. The students also seemed more comfortable with this approach. The result was an environment in which a good rapport was developed between the researcher and the students prior to the structured interviews. This approach also provided the researcher with a set of experiences that allowed him to prod the students' memories during the subsequent interviews when they were asked to compare the two different laboratory formats.

Observations collected while students were working in the computer lab did not prove useful because most of the decision-making process had already been accomplished during group meetings before the students came to the lab and the students

were less likely to involve the researcher in their activities while they worked with the computer. Insight into these group meetings and the interactions between members of the group was provided by the structured interviews, however.

The structured interviews were the core of the qualitative evaluation methods. The researcher developed a list of questions that he wished to cover during the interviews, covering many of the same topics as the Likert-scale surveys so that the researcher could triangulate his conclusions from different data sources.<sup>[10]</sup> Using the structured topic list produced interviews that followed a similar pattern, but the students had ample opportunity to bring up any subject they felt appropriate.

The interviews were recorded, transcribed, and then analyzed using the method of inductive analysis.<sup>[11]</sup> The analysis consisted of reading the transcripts multiple times and condensing the students' comments to common and uncommon categories by literally cutting and pasting together similar comments obtained in different interviews.

## QUANTITATIVE RESULTS AND DISCUSSION

The results of the Likert-scale survey indicated that the students liked using the simulations (91%; Q1); found the simulations easy to learn and operate (95%; Q6); reported that the computer simulations did not intimidate them (86%; Q7); would like to see more of them (73%; Q12); believed that the computer simulations allowed them to study more complex and realistic problems (78%; Q18); valued the budgetary constraints included with the simulations, which made the simulations more realistic (86%; Q3); and believed that they spent a higher percentage of their time planning the design of the computer simulation (86%; Q17), which suggests that the simulations provide the students with an experience that is different from the traditional lab. The students liked the simulations for a variety of reasons, including the fact that they were more likely to work than the traditional experiments (81%; Q23), thus giving the students reasonable and workable data.

The computer simulations were very different from traditional labs because of the speed with which data could be acquired. This did not bother the students or make them feel uneasy about the computer experiment (89%; Q8). In fact, they felt that this made more efficient use of their time (95%; Q19). The students felt the simulations allowed them to focus on the principles involved in an experiment (82%; Q9) and therefore were a good way to learn new processes and concepts (79%; Q21). But a majority (54%; Q14) of the students felt that the traditional experiments gave them a better sense of the problems likely to be encountered in industry. Thus it is not surprising that a majority (57%; Q24) felt that the present combination of computer and simulation experiments was appropriate.

The quantitative results produced a sense of conflict, or

dualism, in the students' opinions. They simultaneously believed the computer simulations are a good instructional technique that helped them better focus on the principles they were expected to apply, and at the same time that the traditional experiments gave them a better sense of the problems they might encounter in industry. The source of this dualism cannot be extracted from the results of a Likert-scale survey, but they can be obtained by triangulating this data source with the results of qualitative research techniques.

As we will see, the students simultaneously regarded the computer simulations as both "good" and "bad." They are good because they allowed students to tackle more complex problems in which they were compelled to proceed with realistic budgetary and time constraints, and because these experiments were more likely to "work," providing the students with data that allowed them to complete a realistic scale-up. The simulations are "bad" because they are not real; they cannot fail in the same way a traditional experiment would fail. Even though the students tended to value the ability to focus on important conceptual engineering issues in the simulation experiments, they recognized that this "ability" has little to do with the world in which they actually live.

## QUALITATIVE RESULTS AND DISCUSSION

Twelve students were interviewed after they had completed one experiment of each type. The theoretical framework for this portion of the study falls within the domain of hermeneutics<sup>[12]</sup> in the sense that we are trying to give students the opportunity to be heard, to have a "voice," through interpretations of the meanings of their statements and actions. The interviews were used to probe more deeply into the students' experiences, opinions, and beliefs about traditional versus computer-simulation experiments; to probe how students constructed the knowledge they gained from doing the lab experiments; to examine how they perceived computer-simulation experiments (*e.g.*, as just one long equation to be worked out with data generated by the computer or as a chance to do meaningful engineering work similar to that done in industry); to explore their opinions on whether the computer simulations were more (or less) realistic than traditional experiments; to discern whether the simulations require a particular teaching style from the instructor; and to determine the aspects of the computer simulation that make it more (or less) difficult than the traditional experiments.

In some ways, the students felt the computer simulation was more realistic, and perhaps more difficult, than their other experiments. (In the following vignettes, "I" stands for the interviewer and the names are nicknames given to protect the students' identities.)

*I: You were talking about the computer simulation being more "in-depth." What did you mean by that?*

**Andy:** *Instead of dealing with the unit, you dealt with more of what you'd deal with in the real plant...the computer interfaced you to multiple types of equipment and more "real" equipment than you would use in industry rather than just the small glass tube that we used for the cation exchange. And I thought that was better because you get more of a full view of the operation rather than just one small aspect of it.*

**Jody:** *In addition to that, too, we had a budget that we had to follow. Which is gonna be true in real life once we graduate and do what we need to do to get data and stuff like that.*

The time and budgetary constraints imposed on the computer-simulation experiments had the tendency to change the students' decision-making process by forcing them to reflect on their decisions before taking actions, as illustrated by comments made by Adam and Don, who were in separate groups.

**Adam:** *It made it more "real-world" I guess. Before, on the other experiments, if you wanted to ask the professor a question, we'd just go up and ask; even if it was just a stupid question. Now if we wanted to talk to the professor it would cost us \$500 for a consulting fee. It made you stop and think about it instead of just running up and asking the professor when you could have figured it out yourself if you'd just have thought about it.*

**Don:** *It was good to have a budget. If there was no actual planning involved, with no budget, we would just have run it for hours and hours and had stacks of paper for results. We wouldn't have thought about what we were doing.*

These comments are echoed by the results of the survey, which showed that the majority of the students felt that use of budget and time constraints made the simulation more realistic than the traditional laboratory experiments. Darrin and Laura found the realism introduced by the budget/time constraints intimidating.

**I:** *Let me ask you about the computer simulation. What did you think of it when you first saw it?*

**Darrin:** *Heh! Intimidating.*

**I:** *How?*

**Darrin:** *Well, even though we sat through a whole lecture, I felt that I really didn't know where to begin, and really I was ready to get another apparatus - experimental problem. With this [comp. simulation] I had no idea how to start. I was afraid that I was going to make a mistake. . . . And plus there's this thing that if you ask a question it would cost you like \$500 or something. [consultation fee] So you're kinda tentative.*

Laura provided insight into why her group felt intimidated by the computer experiment when she responded to a question that asked for her impression of the computer simulation.

**Laura:** *I was scared because it wasn't like any of our other labs were, even if you, like, totally get bad data . . . you don't have anything to lose. You can still write up your report and say that your results are no good. But on this lab [computer simulation] you have to find your constants.*

The problem was simple—there was no place for the students to "hide." They could not gloss over or "fudge" poor data collected during the computer experiment the way they said they could when discussing traditional experiments.

Darrin and Laura's comments are not representative of the perceptions of the group of students who completed the computer experiment during the evaluation, but their comments raise an important issue in evaluation. Historically, evaluations of curriculum-reform projects have been based on what we have called a "sports-mentality" approach.<sup>[13]</sup> Statistical techniques, such as a t-test on the mean scores of some measure of performance of students in experimental versus control sections of the course, are used to answer the questions "Is the new curriculum better or worse than the old curriculum?"

Darrin and Laura's comments remind us that any substantive change in curriculum will have both positive and negative effects. Some students will benefit, but others will be hurt. Evaluative studies, such as this one, allow one to search for both effects and then probe what additional changes could be made to maximize the positive effect and minimize the negative effect.

Darrin and Laura's interviews identified another source of differences in students' perceptions of the computer simulations—the amount of success the students felt they had enjoyed. In general, the students who were interviewed felt that they had enjoyed success with the computer simulation. Darrin and Laura's group did not share this perspective, however, as illustrated by the following comments:

**I:** *What was the computer simulation supposed to do and what did it really do as you look back on it now? What was it supposed to represent?*

**Darrin:** *I think that it was supposed to represent a better way . . . of solving a large problem that we could never have solved on a laboratory scale. With the amount of trials we ran. . . it was supposed to demonstrate how much work you could get done, . . . how many trials you could get done on the computer. But what it turned out to be was just trial and error.*

**Laura:** *I think that what the . . . simulation was doing was to show us how we can use a computer to simulate something and then to optimize conditions. And then apply them to an actual plant or whatever. And, . . . I guess it did it, . . . I don't know! I don't really know because I still don't really understand how our values correlated to the actual running of the simulation and the running of pilot plant. . . . I don't really think that I learned anything from it. I just learned to manipulate what we were trying to do . . . I'm still a little unclear on some things.*

The interviews provided useful information about the students' perception of the role of the computer in their response to the question "Which experiment gave you the best experience?"

**Dallas:** *[The computer experiment] was the best. Granted,*

that they wanted to try to give us some sort of real-life simulation . . . what it's like in real industry. . . . We were actually able to get our numbers and do our scale-ups, and do our actual engineering work without trying to mess around trying to get something to work. Or trying to get some data or making up data . . . we were actually able to do engineering.

**Don:** [In the computer experiment] you could kind of estimate sort of where . . . what would happen under certain circumstances. Whereas in the experimental part of the regular lab, you would get such confusing results. It was so difficult to try to extrapolate that onto any large scale. We basically said, "We'll just have to throw this out and we'll see what somebody else did or make up something."

These comments reflect the common perception among students that the simulations were more likely to work than the traditional experiments; that they could acquire feasible data from the computer simulation. But other students questioned whether the computer simulation gave them the best experience.

**Adam:** The best experience was probably with the water cation exchange, just because we did a lot more research with that to learn how to get the right data and stuff like that. The computer simulation was interesting but pretty much all the data was right there in front of you. . . . The computer simulation was pretty neat. But it was a lot of wasted time for three people to sit there and do it, because only one person could get on the computer and run it.

Ruth and Tina provided further insight into the computer experiment.

**Ruth:** With the computer experiment all we did was calculations, . . . with the spreadsheet and stuff. That's all we did. The whole lab was one big long calculation.

**Tina:** The whole lab was just finding numbers you had to put in the simulation. You had to work through a bunch of equations.

## EFFECT OF THE PROFESSOR'S TEACHING STYLE

Unlike surveys, which can only provide answers to questions that are explicitly stated, interviews often provide data on topics or questions one might not have anticipated. Consider the role of the professor's teaching style, for example. This topic was not covered in the survey, but the interviews showed that it had a significant impact on the students' experiences. It was clear from the interview data that the professor's "hands-on" teaching style during the planning sessions had a direct impact on the students' perception of the computer simulations and the success of these simulations.

## CONCLUSIONS

The results of this study suggest that it would be a mistake to ask which laboratory format is "better" for students. They indicate that computer simulations and traditional experiments have different roles in the curriculum because they emphasize different aspects of engineering and require both

different levels and types of expertise.

Students who were frustrated with traditional lab equipment seemed to enjoy "actually doing" the engineering required to tackle the complex problems provided by the computer simulation. They did not have to worry about "making up data . . . or seeing what someone else did" when the traditional lab failed. For these students, the computer simulations were more "realistic" than the traditional lab that gave results students described as ". . . I'd turn it in for a grade but I certainly wouldn't buy it!" For other students, the simulations were less "realistic" because they cannot fail, the way a traditional lab fails.

This study provided insight into the role of the environment in which computer simulations are implemented. Our results clearly indicated that budgetary and time constraints played an important role in making the computer simulations seem "realistic"—so realistic that a few students felt intimidated by this aspect of the simulations.

This study also suggests that computer simulations, by themselves, are not magic bullets that provide instructional and pedagogical benefits for the students in the absence of a human interaction between the students and the instructor. They are best thought of in terms of being a tool for instruction rather than a replacement for the instructor.

The authors hope that this study leads others to recognize the importance of asking the correct questions when evaluating curriculum reform projects, as required by ABET and NSF, and the importance of collecting qualitative interview data to both reinforce quantitative data collected in anonymous surveys and to provide a deeper understanding of the effect of curriculum changes on students' attitudes and opinions.

## ACKNOWLEDGMENTS

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## ChE book review

### *Alternative Fuels*

by S. Lee

Taylor & Francis, Bristol, PA; 485 pages, \$83.95 (1996)

Reviewed by

Thomas R. Marrero

University of Missouri-Columbia

Knowledge of chemical processes is important in the development of more environmentally friendly fuels because of the implementation of stricter constraints on energy utilization by almost all nations. The main objective of *Alternative Fuels* is to comprehensively describe the science and technology of various process treatments for the clean use of coal and coal products, synthesis gas, alcohols, shale oil crude, biomass, and solid wastes. This ambitious objective is presented in eleven topical chapters that include current references to the state-of-the-art for each type of fuel processing. Dr. Lee has successfully compiled a comprehensive collection of pertinent data and information that were scattered throughout the literature. *Alternative Fuels* is necessarily lengthy, but neat, clear, and consistent. It can well serve as a chemical engineering text and as a reference book for practicing engineers and researchers.

*Alternative Fuels*, a book in the Applied Energy Technology Series, has 485 pages, 172 one-line process diagrams, graphs, and sketches, and 96 tables of data. The index lists 470 subject terms, excluding numerous sub-terms. All these features succinctly provide a wealth of informative data that is easily accessed by the reader. In addition, each chapter has a set of problems (useful for students), and a solution manual is available. It has 586 references, with 250 of them published since 1990. References to relatively inactive clean-coal technologies, such as oil shale, shale oil, and tar sands, are primarily taken from studies published prior to 1980.

The first chapter presents a global overview of energy production, consumption, and reserves for coal, gas, and oil. Additional data are presented for electric power generation

from renewable energy sources: biomass, geothermal, hydroelectric, solar, and wind. This chapter summarizes the global energy situation with 18 graphs and 13 tables.

Chapter 2, in 60 pages, focuses on three major topics that could produce environmentally clean solid and liquid fuels from processed coal. First, the basic properties of coal are presented along with safety issues related to coal mining and environmental issues related to coal combustion. In the second part, many developments in coal technology are described for use as a means to clean fuel. The third part of Chapter 2 presents environmental issues and regulations, particularly related to coal mining.

Chapter 3 deals with coal gasification, which includes a series of processes that convert coal containing C, H, and O as well as impurities such as S and N into fuel and/or synthesis gas. A total of 10 gasification processes are summarized in about 30 pages. Then the equations are presented for stoichiometry, thermodynamics, and reaction kinetics relative to coal gasification.

Chapter 4 presents more than two dozen processes to develop alternative liquid fuels from coal by pyrolysis, direct and indirect liquefaction, and several other known established chemical-process techniques. This material does not include process economics.

The next topic, Chapter 5, is the development of gas fuels from coal. This material summarizes pertinent advances in the DOE (multibillion dollar) Clean Coal Technology Programs and an extensive discussion of Integrated Gasification Combined Cycle (IGCC) systems. The IGCC technology economics are discussed. Advantages and disadvantages of combined-cycle systems are delineated as potential sources of fuel.

Chapters 6, 7, and 8 are presentations of more established technologies (coal slurry, oil shale, and tar sands) as potential sources of fuel. The coal slurry focuses on transportation and handleability, but no economics. Descriptions of oil shale and tar sand are focused around process diagrams and pertinent chemical reactions.

Continued on page 83.

# PROCESS ANALYSIS

## *An Electronic Version*

GEORGE B. DELANCEY

*Stevens Institute of Technology • Hoboken, NJ 07030*

Here at Stevens we adhere to the widespread proposition that using the Internet and the Intranet can be substantially beneficial to undergraduate chemical engineering education, both administratively and pedagogically.<sup>[1,2]</sup> There is also evidence that using software such as spreadsheets and equation solvers<sup>[3-5]</sup> not only develops the skills and flexibility necessary for ready adoption of different software packages<sup>[6]</sup> for professional activities in industry, but also substantially supports learning. We believe that effective use of these tools requires a “cultural” change, or enhancement, on the part of both faculty and students. Full course integration is desirable<sup>[6]</sup> and requires broad faculty participation, which comes slowly in many cases.<sup>[7]</sup> The skill level and motivation of the students, however, can significantly stimulate the faculty culture.

At Stevens, our initial focus has been on the students. We have attempted to forge a paradigm for a departmental electronic culture in our first chemical engineering course, Process Analysis, that comes in the second term of the sophomore year. Our efforts to do this are summarized in this article.

### COURSE SUMMARY

The objectives of the course are to introduce students to chemical engineering, to chemical processing equipment and chemical processes, and to apply material balances and basic phase equilibria to processing systems and the design of equipment from the equilibrium-stage point of view. At the same time, the course is being developed in an electronic environment in order to prepare students for this emerging characteristic of the workplace, to enhance their learning, and to establish a basis for distance learning and asynchronous delivery. By “electronic environment” we mean the ubiquitous use of software for problem solving and transmission, communication between constituencies, presentations, introduction to process simulators, graphics, and computer-aided instruction and learning.

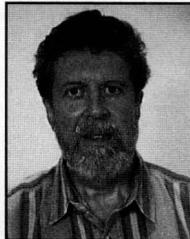
The course, which uses the Luyben and Wenzel text,<sup>[8]</sup> is

summarized in Table 1. Throughout the course the physical and chemical bases of the process or equipment being discussed are emphasized and class discussions are often based on the problem assignments and examples in the text. The students are required to complete a project involving construction or enhancement of a website devoted to a chemical process or to a class of chemical processing equipment, and each group presents its project later in the semester. Throughout the semester, students are encouraged to use the computer-aided instruction modules developed at the University of Michigan and distributed by CACHE (Computer Aids in Chemical Engineering).

It should be noted that the integrity of individual and group work is subject to the Stevens Honor System. This system is managed by the students through an Honor Board. Individual cases are investigated and tried on the basis of well-defined procedures approved by both faculty and students. Penalties range from warnings through grade loss to expulsion from the Institute. All homework and examinations in the course are signed by the students and attest to the fact that they have adhered to the Honor Code.

### SOFTWARE

Students are required to purchase computers when entering Stevens. The software suite that comes with the computers includes MS Office Pro 97, Mathcad, Scientific Notebook, X-win32, WinQVT, Netscape, Java, and Matlab. Software used in the course that is not included in this package is available for purchase on campus. An exten-



*George B. DeLancey is Professor of Chemical Engineering at Stevens Institute of Technology. He received his BS, MS, and PhD degrees in chemical engineering from the University of Pittsburgh. He has presented undergraduate courses in process analysis, transport phenomena, reactor design, process control, separation processes, and thermodynamics. His current research interests are in biotechnology.*

*... the course is being developed in an electronic environment in order to prepare students for this emerging characteristic of the workplace, to enhance their learning, and to establish a basis for distance learning and asynchronous delivery.*

sive application of Ethernet supports communications from the academic buildings, computational facilities, and residence halls, and a gateway from the Ethernet is provided for access to the Internet.

WebCT, described at (<http://homebrew.cs.ubc.ca/webct>) is used to organize the sites summarized in Figure 1, to make grades, examples, and solutions available to the students, to provide E-mail and Bulletin Board communication tools as well as a Calendar. The underlying html files

were created with Microsoft Word, except possibly for the student project pages.

The Calendar is used on a class basis to post important events such as examination and assignment due-dates, class activities, vacations, etc. The Calendar can also be used on a personal basis by individual students or the instructor without others being able to view their entries.

Examinations are posted on the Bulletin Board and the students can download/view the examination file. All questions concerning the examination contents are posted on the Bulletin Board along with the responses of the instructor. Postings from both parties may take place at any convenient time and from any convenient location and may be viewed by the entire class. This function is very useful, especially when the exams are not due for several days or over a weekend. Questions involving problem assignments are handled in a similar fashion except that viewing may be limited to the group in question, and the grader for the class may respond as well. The Bulletin Board is also used on a group basis to manage group discussions on project and problem assignments and to transfer files associated with these activities within the group.

E-mail serves the common communication needs as well as being the vehicle for transferring homework, examinations, and project files between two parties. The subject entry on the e-mail message is important for quick overviews of previous messages and for the search function supplied by WebCT.

Scientific Notebook (SNB), found at

<http://scinotebook.tcisoft.com>

is used primarily for solving systems of nonlinear equations arising from material balances and in phase-equilibrium calculations. SNB has a user-friendly front end with a Maple kernel and supports a word processing format. No special code is required, and SNB can interface with the web and serve as a browser for Tex files. Users can quickly perform symbolic computations, integration, differentiation, matrix and vector operations, and many other more complex computations involved in calculus, linear algebra, differential equations, and statistics. For these reasons, we chose to adopt SNB rather than Mathcad<sup>[5,7]</sup> or Mathematica.<sup>[3]</sup> The solution to simultaneous nonlinear equations associated with material balances is illustrated in Example 1, while Example 2 illustrates how SNB is used to solve equilibrium flash calculations.

Microsoft Excel is used for graphical (McCabe-Thiele) solutions of equilibrium-stage problems: stripper with a

**TABLE 1**  
**Course Summary**

Subject	Weeks
Overview of Chemical Industry and Processes	} 3
Process Equipment: Construction and Operation	
Process Analyses: Flow Sheets and Process Conditions	
Mass Balances, Degrees of Freedom, and Chemical Reaction	4
Equilibrium Separations: McCabe-Thiele Analyses	4
Multi-Component Phase Equilibrium: Isothermal Flash	2
Class Presentations	1

**Process Analysis**

**Welcome to Chemical Engineering 210**

[Bulletin Board](#)    [Online Chat](#)    [Change Password](#)  
[Private Mail](#)    [Calendar](#)    [My Record](#)  
[Course Information](#)    [Schedule, Examples and Assignments](#)    [Project](#)  
[Chemical Processes](#)    [Process Equipment](#)    [Solutions](#)

Click on one of the icons above

[References](#) | [Group Memberships](#) | [Grading Policy](#) | [Schedule and Assignments](#) |  
[Preparation and Submission of Solutions](#) | [Process Equipment](#) | [Chemical Processes](#) |  
[Project](#) | [Micromentor](#) | [Scientific Notebook](#) | [User Notes for Software](#) | [Scanning](#) |  
[Mailing Files](#) | [Zipping Files](#) | [Downloading/Viewing Solutions and Examples](#) | [McLean Computer Room](#) | [Virtual Library](#) | [Chemical Engineering News Group](#) | [American Institute of Chemical Engineers](#) | [Course Homepage](#)

**Figure 1.** Course homepage and information hyperlinks.

reboiler, gas absorption and stripping, distillation, and liquid-liquid extraction. We have elected to preserve the graphical construction modality available in Excel for this introductory course rather than the spreadsheet solutions to the material balance equations used at some other institutions.<sup>[4]</sup> The stage steps are constructed with the drawing tool in Excel.

Distillation is illustrated in Example 3 and extraction in Example 4. Calculations can be done on the spreadsheet or SNB may be used, saved with a screen capturing software (e.g., Snagit) and pasted into Excel. Equilibrium data may be generated from a function (Example 3) or plotted directly as an input data series (Example 4). Stream points are entered as a new data series for convenience when zooming in for stage stepping (Example 3) or zooming out for the operating point in extraction (Example 4).

The course also makes use of the MicroMENTOR system for delivery of the educational software modules developed

at the University of Michigan and distributed by CACHE. The modules suggested for use during the class are: UM-Units, UM-Ber, MATBAL, UM-Hawaii, UM-POP, and UM-McCabe. The modules have been required in some cases and left to the discretion of the students in others.

Distill is a program, available from CACHE, that does multicomponent flash and distillation calculations. It considers both the liquid and gas to be nonideal and it includes a database of 98 compounds. The vapor-phase fugacity is calculated with the Redlich-Kwong equation of state. The liquid-phase activity coefficients are based on the Hildebrand solubility parameter. This program is used in several assignments to illustrate the effect of assuming ideal conditions in flash and bubble/dew point calculations for hydrocarbons.

ChemWindows is made available to the students for drawing schematics, flow sheets (see the figure in Example 1, for example) and chemical formulae. They have not yet been required to use this software and may use others if they wish.

### EXAMPLE 1

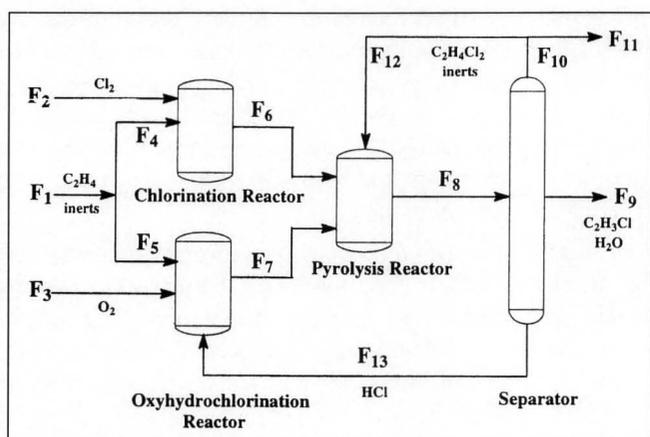
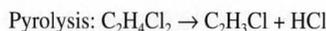
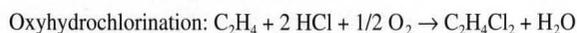
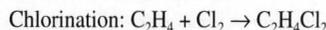


Figure 1

The flow diagram in Figure 1 illustrates a simplified version of the main steps in the production of vinyl chloride ( $C_2H_3Cl$ ) from ethylene ( $C_2H_4$ ). The reactions, which occur separately in the different reactors, are:



The ethylene feed,  $F_1$ , is 90 mole % ethylene and the remainder is inerts. The chlorine and oxygen feeds,  $F_2$  and  $F_3$ , respectively, are pure. All of the ethylene, oxygen, and chlorine react and all of the hydrochloric acid (HCl) fed to the oxyhydrochlorination unit reacts.

Only 50% of the total dichloroethane ( $C_2H_4Cl_2$ ) fed to the pyrolysis reactor is converted, with the remainder being separated and recycled with inerts in stream  $F_{12}$ . The inert concentration in the recycle stream is 50 mole %. Pure hydrochloric acid (HCl) is recycled in stream  $F_{13}$ . The final product stream,  $F_9$ , consists only of vinyl chloride and water.

Determine all of the unknown flow rates,  $F_j$ , and mole fractions,  $x_{i,j}$  (mole fraction  $i$  in stream  $j$ ). Set  $F_1=1$  mole/hr as a basis. The species are labeled as shown in the following Table 1.

Species	Index	Species	Index
$C_2H_4$	1	$C_2H_4Cl_2$	5
$Cl_2$	2	$C_2H_3Cl$	6
HCl	3	$H_2O$	7
$O_2$	4	Inerts	8

SNB solves the material balance equations given in Figure 2 in SNB format (single column) in less than one minute. The solution is shown in Figure 3 after some reordering for convenience.

$$\begin{array}{ll}
 F_2=0.90F_4 & 0.50(x_{5,6}F_6+x_{5,7}F_7+0.50F_{12})=x_{6,8}F_8 \\
 F_3=(0.90/2)F_5 & 0.50(x_{5,6}F_6+x_{5,7}F_7+0.50F_{12})=x_{3,8}F_8 \\
 F_4+F_5=F_1 & x_{7,7}F_7=x_{7,8}F_8 \\
 x_{5,6}F_6=0.90F_4 & x_{8,6}F_6+x_{8,7}F_7+0.50F_{12}=x_{8,8}F_8 \\
 x_{8,6}F_6=0.10F_4 & x_{3,8}+x_{5,8}+x_{6,8}+x_{7,8}+x_{8,8}=1 \\
 x_{5,6}+x_{8,6}=1 & x_{3,8}F_8=F_{13} \\
 x_{7,7}F_7=0.90F_5 & x_{5,8}F_8=0.50F_{10} \\
 x_{5,7}F_7=0.90F_5 & x_{6,8}F_8=x_{6,9}F_9 \\
 F_{13}=2(0.90F_5) & x_{7,8}F_8=x_{7,9}F_9 \\
 x_{8,7}F_7=0.10F_5 & x_{8,8}F_8=0.50F_{10} \\
 x_{5,7}+x_{7,7}+x_{8,7}=1 & x_{6,9}+x_{7,9}=1 \\
 0.50(x_{5,6}F_6+x_{5,7}F_7+0.50F_{12})=x_{5,8}F_8 & F_{10}=F_{11}+F_{12}
 \end{array}$$

Figure 2. Material Balances

$$\begin{array}{l}
 F_2 = .5, F_3 = .2, F_4 = .55556, F_5 = .44444, \\
 F_6 = .55556, F_7 = .84444, F_8 = 3.6, F_9 = 1.2, \\
 F_{10} = 1.6, F_{11} = .2, F_{12} = 1.4, F_{13} = .8, \\
 x_{3,8} = .22222, x_{5,8} = .22222, x_{6,8} = .22222, x_{7,8} = .11111, x_{8,8} = .22222, \\
 x_{5,6} = .9, x_{8,6} = .1, \\
 x_{5,7} = .47368, x_{7,7} = .47368, x_{8,7} = 5.2632 \times 10^{-2} \\
 x_{6,9} = .66667, x_{7,9} = .33333, F_1 = 1.0
 \end{array}$$

Figure 3. Solutions

## EXAMPLE 2

A petrochemical stream consisting of 30 mole % propane, 10 mole % n-butane, 15 mole % n-pentane, and 45 mole % n-hexane is to be flashed to 200 kPa. (a) Determine strict bounds on the operating temperature. (b) Find the vapor flow rate per unit of feed and the product compositions for a temperature mid-way between these limits. The equilibrium data are given in Table 1.

**TABLE 1**  
Phase Equilibrium Data

Equilibrium data:  $y = Kx$ ,  $T = ^\circ R$ , and  $p = \text{psia}$ :

$$\ln K(T,p) = (a_1/T^2) + a_3 + b_1 \ln p + (b_2/p)$$

Species	$a_1$	$a_3$	$b_1$	$b_2$
$C_3H_8$	-970,688.5625	7.15059	-0.76984	6.90224
n- $C_4H_{10}$	-1,280,557	7.94986	-0.96455	0
n- $C_5H_{12}$	-1,524,891	7.33129	-0.89143	0
n- $C_6H_{14}$	-1,778,901	6.96783	-0.84634	0

The solution procedure in SNB is as follows:

The functions in Figure 1 are defined in SNB format. Bounds for the bubble and dew points of the feed are at unity K values for propane ( $j=1$ ) and n-hexane ( $j=4$ ). These values are obtained from the roots of the K function at the prevailing values of  $p$  (200 kPa) and  $j$ . The solutions are shown in SNB format in Figure 2. The bubble and dew points of the feed are roots of the associated functions at the prevailing  $p$ . The results in SNB format are shown in Figure 3. The vapor flow at the midpoint temperature,  $561.4^\circ R$ , is obtained similarly and is shown in Figure 4.

$$\text{Equilibrium: } K(i,T,p) = \exp\left(\frac{a_{i,1}}{T^2} + a_{i,3} + b_{i,1} \ln p + \frac{b_{i,2}}{p}\right)$$

$$\text{Bubble point: } f(T,p) = 1 - \sum_{i=1}^4 K(i,T,p)z_{i,1}$$

$$\text{Dew point: } g(T,p) = 1 - \sum_{i=1}^4 \frac{z_{i,1}}{K(i,T,p)}$$

$$\text{Isothermal flash: } h(\vartheta,T,p) = \sum_{i=1}^4 \frac{z_{i,1}[K(i,T,p)-1]}{1+\vartheta[K(i,T,p)-1]}$$

**Figure 1**

$$\frac{a_{j,1}}{T^2} + a_{j,3} + b_{j,1} \ln p + \frac{b_{j,2}}{p} = 0$$

Solution is  $\{T=657.27\}, \{T=449.88\}$   
 $T \in (0, \infty)$

**Figure 2**

$$\frac{f(T,p)=0}{T \in (449,658)} \text{ Solution is } \{T=509.27\} \quad \frac{g(T,p)=0}{T \in (449,658)} \text{ Solution is } \{T=613.54\}$$

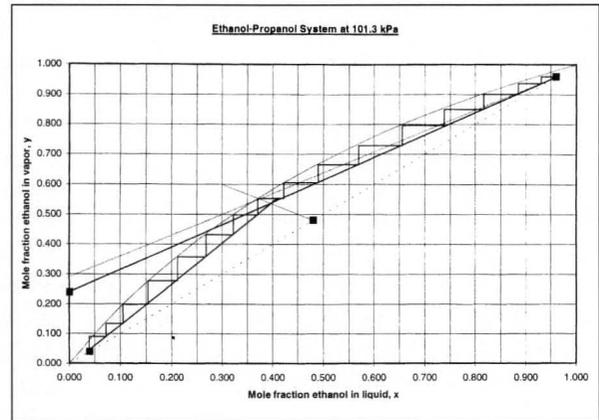
**Figure 3**

$$\frac{h(\vartheta,T,p)=0}{\vartheta \in (0,1)} \text{ Solution is } \{\vartheta=.37704\}$$

**Figure 4**

## EXAMPLE 3

Find the number of stages, the best feed location, and the minimum reflux ratio for a distillation column that separates ethanol and propanol at 101.3 kPa. The ratio of the vapor pressure of ethanol to the vapor pressure of propanol is approximately constant at 2.10. The feed is 48 mole % ethanol and 40 mole % liquid. The distillate and bottoms compositions are to be 96 mole % and 4 mole % ethanol respectively. There is to be a total condenser overhead with no sub-cooling. The reflux ratio is 3.0. The graphical construction is shown in the figure in Excel format.



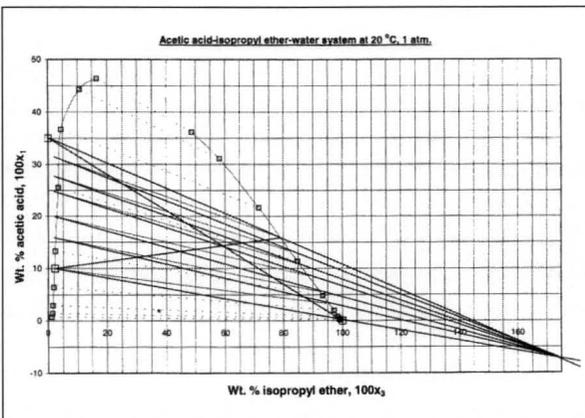
## EXAMPLE 4

Acetic acid (species 1) is to be extracted from water (species 2) using isopropyl ether (species 3) as the solvent at  $20^\circ C$  and 1.0 atm. The feed rate is 1000 kg/hr and contains 35 wt % acid in water. The solvent flow rate is 1475 kg/hr and is essentially pure ether. The raffinate is to contain no more than 10 wt % acid. Find (a) the minimum solvent flow rate, (b) the number of equilibrium stages required for the separation, and (c) the outlet concentrations and flow rates. Equilibrium data at the operating conditions are given in the Table and the graphical construction in Excel is shown in the figure.

Water Layer		Ether Layer	
$X_3$	$X_1$	$X_3$	$X_1$
1.2	0.69	99.3	0.18
1.5	1.41	98.9	0.37
1.6	2.89	98.4	0.79
1.9	6.42	97.1	1.93
2.3	13.3	93.3	4.82
3.4	25.5	84.7	11.4
4.4	36.7	71.5	21.6
10.6	44.3	58.1	31.1
16.5	46.4	48.7	36.2

TABLE  
Phase Equilibrium  
Data

FIGURE  
Excel Constuction for  
Example 4



## FILE HANDLING

An extraordinary amount of time is required to open files to learn the source and/or the contents. This is especially true if more than one course is underway. Consequently, labeling of files is very important. Points are deducted from assignments and examinations (which may not even be accepted in some cases) if the established procedures are not followed. No files are accepted unless adherence to the Honor Code is pledged by the students at the end of the file.

Homework files are prepared weekly by students working in groups. The assignments are numbered and are generally specific problems in specific chapters of the text. Solutions to individual problems are labeled as gxpy-zc210.(tex, rap, doc, xls,...) where x is the group number, y is the chapter, and z is the problem number. The individual solution files are then assembled in a single archive, with WinZip for example. The archive is labeled gxayc210.zip where x is the group number and y is the assignment number. The archive is attached to an e-mail message with an informative subject entry and mailed to the instructor. The archives are placed in a directory named with the group numbers. Solution files for each problem are posted for downloading after the due date for the assignment.

Examination files include a reference to the individual student: exmc210qnabz.(tex, rap, doc, xls,...), where m is the examination number, n is the question number, ab are the student initials, and z is the group number. We have not encountered students with the same initials in the same group yet, but many modifications are possible to handle such an event. The examination files are then grouped in an archive labeled exmc210abz.zip and attached to a relevantly labeled e-mail message to the instructor. The archives are then placed in a directory named with the examination number.

Copies of files received by the instructor are forwarded by e-mail to the grader. The grader is not permitted to accept files directly from the students. The grader has a set of directories similar to those used by the instructor, described above. The grader uses several additional subdirectories associated with the grading process. One directory is for graded files, one for ungraded files, and one for the archive in process of being graded. After the files are graded and the comments and points included, the files are returned directly to the students, the grader retains a copy, and a copy of the file is sent to the instructor. The same file name is retained so that the instructor can replace the previously ungraded file with the graded one in his directory. It has always been possible to track down "missing" files with this procedure.

The grader is responsible for posting grades in WebCT, but a separate grade file is maintained by the instructor and updated with each new assignment or examination. The grade file maintained by the instructor is the official one so that grades, once recorded, cannot be changed without the

instructor updating this file. Grade access is limited to the student, the grader, and the instructor, but statistical information is generally available.

## PROJECT

The objectives of the project are for the student to gain a special familiarity with a specific chemical process or a category of chemical process equipment and a significant experience with web-based presentation of technical materials. The students are also required to present their projects to the class, electronically if desired.

The bases on which the sites are initiated or enhanced are summarized below.

### A) Process equipment (nine sites at present covering major equipment categories):

- 1) Purpose and operating principle(s)
- 2) Historical background
- 3) Construction—schematic/illustrations
- 4) Pictures of actual equipment
- 5) Range of duties—sizes
- 6) Maintenance required
- 7) Utilities required
- 8) (Some) design equations
- 9) References

### B) Chemical Processes (nine sites at present spanning range of top 50 chemicals):

- 1) Chemical formula and form/state of product
- 2) Uses and market price
- 3) Historical industry development
- 4) Common methods of production with raw material sources and side products
- 5) Major companies, production methods, and production levels
- 6) Details for a common production method: process chemistry with implications for most favorable process conditions; flow sheet(s); operating conditions and problems; environmental considerations; production costs; utility requirements; hazards; handling of waste and side products
- 7) References

### C) Grading (Engineers from EXXON Research and Engineering and experienced faculty outside the department contribute to site assessment):

- 1) Content (see above)
- 2) Layout/format
- 3) User friendliness
- 4) Use of colors and graphics
- 5) Use of relevant hyperlinks and other resources

Html files are prepared or edited with software that is generally available to the students, such as Microsoft Word, or that is the individual preference of the students. Scanning hardware is used for some picture files, which can be edited with Photopaint. The completed project files, including images (gif, jpeg,...) are collected in an archive and mailed to the instructor as described above.

## DISCUSSION

The students very quickly become accustomed to the electronic communication features of the course and the file-handling procedures. It is, however, helpful to deduct points for improper file labeling as well as to not answer exam questions online unless posted for viewing by the entire class. Off-campus students find the electronic version helpful and students generally like the option of transferring files and posing questions at their convenience. Such items appear at all hours of the day. For the solutions to assignments, the availability of examples for downloading by the students is crucial for each new application.

The use of SNB for material balances has greatly improved the sophistication and ability of the students to write an independent set of material-balance equations and to be acutely aware of the degrees of freedom. They are also able to spot-check their solutions with quick calculations using time components, inerts, etc. Most students begin with doing the solution on paper and transferring it to SNB. They soon progress, some to doing the solution completely online. A series of user sessions would be helpful at the beginning for learning the software. Some students have prior experience in mathematics classes, which is beneficial. Students have voiced a preference for SNB to similar software packages, but these alternatives have not been explored in a formal way.

The use of Excel for graphical multistage constructions has been very successful and well accepted by students. Errors can be quickly corrected. The students cannot imagine doing liquid-liquid extraction constructions by hand.

When not required, the computer-aided instruction modules in MicroMENTOR are not extensively used. Use of the modules is greatly increased if the students are held accountable, for example, in class discussions on the Bulletin Board of WebCT. The modules, once used, are considered helpful.

Distill is viewed as inconvenient by the students, although the results are very elucidating for comparison purposes. For this reason and for broader objectives, it may be worthwhile to introduce Aspen in a limited way at this stage.

ChemWindows is viewed primarily as a cosmetic add-on for problem assignments when not required. It is used for all examination drawings and for some project work. As it significantly enhances the quality of the presentation, we are introducing some limited requirements for its use.

The class projects have been most successful and well received by the students. The project and equipment sites they have developed are being made an integral part of the course. The students are extremely creative and enthusiastic about finding relevant materials on the Web and using other resources to develop or enhance their site. The technical content of the class presentations attests to the learning component that is present in the projects. The students very

easily adopt a full range of software to suit their personal needs for developing the required html files and exploit the extensive range of picture files available on the Web.

The electronic approach used in Process Analysis has been repeated with much less effort by the author in Transport Phenomena, a course offered in the following semester. The approach has not yet been extended further across the chemical engineering curriculum. Software is, however, used in all of the courses to some extent and coding is required in several classes. The students have been observed using the specific skills (especially the graphical solution to multistage equilibrium separations) and exhibiting the electronic dexterity they gained in Process Analysis in subsequent courses.

The time commitment and the background that must be acquired on the part of faculty in order to develop an electronic version of a course as defined here are important related issues and tied very much to the available support and the electronic environment. It must be generally recognized, however, that significant effort is required which must be explicitly recognized and supported within the local educational context and the electronic capabilities of its constituencies. The benefits include presentation of a course in an environment that anticipates the workplace, that is more adaptable to the different life styles of the students, and that can be conveniently modified and maintained with no more effort than a conventional course. The electronic version is more supportive of the learning process and allows more spontaneity and interaction, especially when the students are networked with their own computers. A greater focus on problem structure and formulation can be realized as well as a pronounced increase in the specific and general electronic skills of the students.

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# DEMONSTRATING SIMULTANEOUS HEAT AND MASS TRANSFER WITH MICROWAVE DRYING

CHERI C. STEIDLE, KEVIN J. MYERS  
University of Dayton • Dayton, OH 45469-0246

In a recent article, Nirdosh and Baird<sup>[1]</sup> emphasized the critical role that the laboratory plays in the undergraduate engineering experience. It is crucial that laboratory experiments provide practical reinforcement of the theoretical chemical engineering concepts developed in lecture courses, but due to budget constraints, it is often also necessary to develop inexpensive experiments or to make use of existing equipment. This paper describes an effective and inexpensive microwave drying experiment that can be used on a variety of levels. On the introductory level, the data analysis associated with this experiment illustrates the numerical approximation of derivatives from discrete data, while on the advanced level, the experiment develops an understanding of simultaneous heat and mass transfer.

## BACKGROUND

Of all the chemical engineering unit operations, drying is one of the most widely used, with applications in various processing industries such as food processing, pulp and paper, pharmaceuticals, etc. Because of its widespread use and the fact that it may account for up to ten percent of industrial energy consumption,<sup>[2]</sup> it is therefore essential that the fundamentals of the drying process be encountered and understood by undergraduate chemical engineering students.

There are a variety of drying techniques, such as vacuum drying and spray drying,<sup>[3]</sup> each with its own operational characteristics. Conventional dryers include both direct and indirect methods of heat transfer.<sup>[4]</sup> Direct dryers (also called convection dryers) use contact between the wet solid and a hot gas to accomplish heat transfer, with the vaporized liquid being carried away by the drying gas. In indirect dryers, heat for drying is transferred through a wall that separates the wet solid and the heating medium, with the vaporized liquid being removed independently of the heating medium. Indi-

rect dryers are also called conduction, or contact, dryers.

The driving force for heat transfer in both direct and indirect dryers is the temperature difference between the drying medium and the wet solid. In the case of microwave drying, a magnetron produces a pulsing electromagnetic field. Polar molecules such as water align with this field, and as the field direction changes, the molecules are forced to realign. These molecular oscillations create friction that generates heat, raising the temperature and causing liquid evaporation.<sup>[5]</sup> Thus, although supplied from an external source, the energy for microwave drying is often thought of as being generated *within* the wet solid.

Although the mechanism of delivering energy to the wet solid in microwave drying is different than in conventional drying, since microwave energy does not penetrate very far below the surface of the exposed material,<sup>[6]</sup> the transport processes occurring during microwave drying are very similar to those that occur during conventional drying. As liquid evaporates from the surface of the solid-liquid mixture, liq-

*Cheri C. Steidle received her Bachelor of Chemical Engineering degree in 1995 and her MS in Chemical Engineering in 1998, both from the University of Dayton. She is currently working as a process engineer in the glass industry and is responsible for implementation of new process control equipment for the manufacture of glass tumblers and tableware.*



*Kevin Myers is a professor in the Department of Chemical and Materials Engineering at the University of Dayton. He received his BChE degree from the University of Dayton and his DSChE from Washington University in St. Louis. His research interests are in multiphase agitation and chemical reactors.*

***This experiment demonstrates the drying process effectively. It is an extremely flexible, safe, and inexpensive experiment that can be incorporated into the undergraduate laboratory curriculum. The experiment is easy to set up and run. Typically, meaningful experimental data for higher power settings can be collected in about thirty minutes.***

uid from within the solid migrates to the surface because of concentration gradients. Thus, drying, either by conventional or microwave devices, inherently involves simultaneous heat and mass transfer.

The primary data obtained during a drying experiment are the moisture content as a function of time (on a dry basis the moisture content equals the liquid mass divided by the solid mass). Curve 1 in Figure 1 presents a typical moisture content curve. The moisture content data can be differentiated to yield the drying rate curve, Curve 2 in Figure 1.

$$\text{Drying Rate} = \left( \frac{-1}{m_s} \right) \left( \frac{dm}{dt} \right) \quad (1)$$

Typically, drying rate curves for materials with a thoroughly wetted surface exhibit three periods.<sup>[7]</sup> The first stage is the warming-up period. This stage is characterized by increasing the material temperature to that of the evaporation temperature of the wetting liquid. Also, the drying rate increases as the liquid begins to vaporize. This is followed by a period of constant-rate drying where the surface moisture evaporates and moisture is steadily brought to the surface to maintain a continuous liquid film over the surface. The third, and last, period in the drying-rate curve, called the falling-rate period, is characterized by a nonlinear decrease of the drying rate due to the increasingly uneven moisture distribution over the surface. The constant-rate and falling-rate stages of the drying-rate curve are separated by the point of critical moisture content. This point marks the instant

when the liquid no longer forms a continuous film over the entire surface because the rate of moisture transport to the surface is less than the rate of evaporation from the surface. The critical moisture content is not a material property. It varies with drying rate, thickness of the material, particle size, and other factors that affect moisture movement. Critical moisture content is best determined by experiment.

## APPARATUS

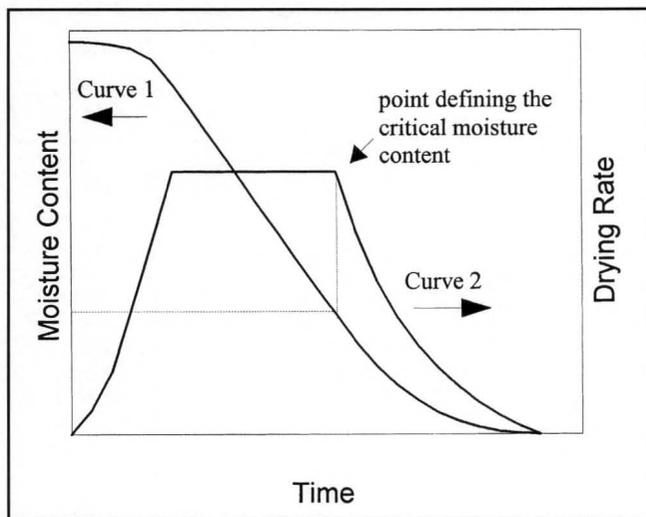
The equipment required for this experiment is inexpensive and easy to operate. Specifically, an off-the-shelf Frigidare MC-1100M microwave with ten power settings ranging from 72 W to 720 W was used. The power settings of the oven are in terms of percentage of the maximum power. This microwave oven is rather old, but a comparable current model could be purchased for less than \$200. Other required items include a digital balance accurate to the nearest gram, a stopwatch (or the microwave timer), microwaveable trays or Pyrex glass beakers, and a thermocouple (specifically, a type T was used). Sand wetted with water was studied, with the nominal diameter of the sand particles being 600 microns.

## METHOD

Wet sand in the ratio of approximately 1 kg of sand to 0.2 kg of water was used. This ratio provided the condition that all of the sand was completely wetted, but no standing pools of water were present. The sand and water were thoroughly mixed together. The mixture was weighed, spread into an even layer approximately 0.025 m deep in a 0.15x0.15x0.05 m tray that was placed in the center of the microwave oven. The microwave was started at a desired power level. The weight of the mixture was recorded every minute until the sample was dry. In addition, the surface temperature of the sand could also be monitored with a thermocouple when the sample was removed from the oven for weighing. The effect of removing the sample from the oven for weighing was examined by using various drying intervals, such as 30 seconds, 1 minute, 5 minutes, and 10 minutes. Only minor changes in the sample weight were observed for these different drying intervals. Appropriate safety precautions include wearing safety glasses and oven mitts when handling the hot tray.

## RESULTS

Figure 2 presents experimental moisture content and drying rate data for the highest power setting of the microwave oven (720 W), while Figure 3 compares the drying rate



**Figure 1.** Typical moisture content and drying-rate curves for a solid with a thoroughly wetted surface.

curves obtained at three power settings (720 W, 540 W, and 360 W). All of the experimental data are very similar to the idealized data of Figure 1, clearly illustrating the three stages of drying. Table 1 demonstrates the influence of power setting on the critical moisture content. Recall that the critical moisture content is not a material property; rather, it is dependent on operating conditions. The trend of increasing critical moisture content with increasing power setting is typical.<sup>[4]</sup> As the drying rate is increased (by increasing the power setting), it becomes progressively more difficult for the rate of moisture transport to the surface to remain as high as the rate of surface evaporation. Thus, the falling-rate period, which begins when the critical moisture content is reached, occurs at a higher moisture content.

During the constant-drying-rate period, a pseudo-steady state is achieved, with the power input going to the latent heat of evaporation of the liquid and energy losses. Table 2 presents the efficiency of the constant drying-rate period assuming a latent heat of evaporation of 2300 kJ/kg (corresponding to approximately 80°C). The efficiency is calculated as the energy required for water evaporation (equal to the evaporation rate, kg/s, times the latent heat of evaporation, kJ/kg) divided by the rate of energy input (kW = kJ/s). The observed efficiencies are rather high, ranging from 74% to 87%. Given the advanced age of our microwave oven, its power output is probably less than the nominal value (we accepted the nominal power outputs and did not actually measure the oven's power output). If this is true, the actual efficiencies are higher than those calculated here. The high efficiencies of microwave drying are partially due to the energy-transfer mechanism. Since energy is supplied directly to the wet solid, there is no large energy requirement for heating the drying medium as in conventional drying devices.

The efficiency decreases with increasing power level. Initially this was thought to be due to increased energy losses to the lower portions of the wet solid by conduction. At low power inputs, the temperature of the wet solid might be

relatively uniform at the start of the constant-drying-rate period as conduction has had sufficient time to transport energy from the surface to the interior of the wet solid. At high power inputs, conduction may be unable to transport energy from the surface to the interior regions of the wet solid rapidly enough to achieve temperature uniformity at the start of the constant-drying-rate period. If this were the

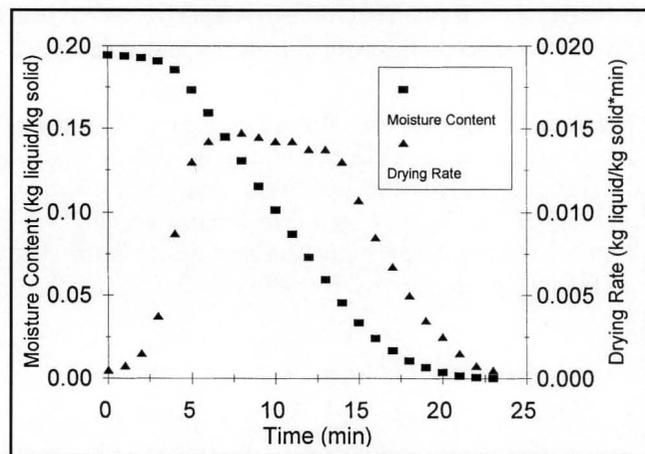


Figure 2. Moisture content and drying-rate curves for a power level of 720 W.

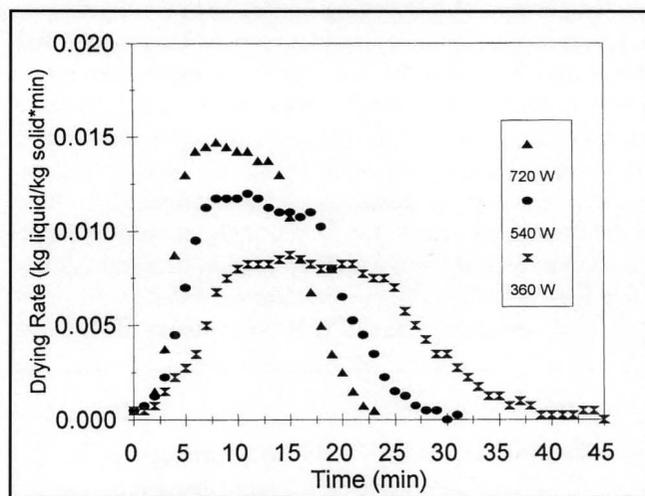


Figure 3. Comparison of drying-rate curves for power levels of 720 W, 540 W, and 360 W.

**TABLE 1**  
Influence of Power Level  
on Critical Moisture  
Content for Drying Sand

Power Level	Critical Moisture Content
720 W	7.4%
540 W	7.1%
360 W	6.2%
144 W	5.7%
Literature value <sup>[4]</sup> (unknown power level)	5.9%

**TABLE 2**  
Influence of Power Level on  
Constant Drying-Rate Period Efficiency  
(from Figure 3 drying-rate curves)

Power Level (kW = kJ/s)	Evaporation Rate (kg/s)	Evaporation Energy (kJ/s)	Efficiency
0.360	$1.36 \times 10^{-4}$	0.313	87%
0.540	$1.90 \times 10^{-4}$	0.437	81%
0.720	$2.33 \times 10^{-4}$	0.536	74%

case, conduction would still be removing some of the energy input from the surface to the interior during the constant-drying-rate period. This energy "loss" would lead to decreased efficiencies at high power levels. This explanation, however, loses its appeal when the energy inputs during the warming-up period are compared. These energy inputs are about 240 kJ, independent of power level. This constancy of energy input during the warming-up period indicates that energy losses due to conduction are likely to be the same for all power levels. The reason for decreasing efficiency with increasing power level requires another explanation that requires further investigation.

The drying-rate curves of Figures 2 and 3 were generated from the moisture-content curves through numerical differentiation using a central-difference method. The central-difference method is best used in cases involving large time intervals<sup>[8]</sup> as is the case with this experiment. Assuming evenly spaced data, at some time,  $t_i$ , the central difference

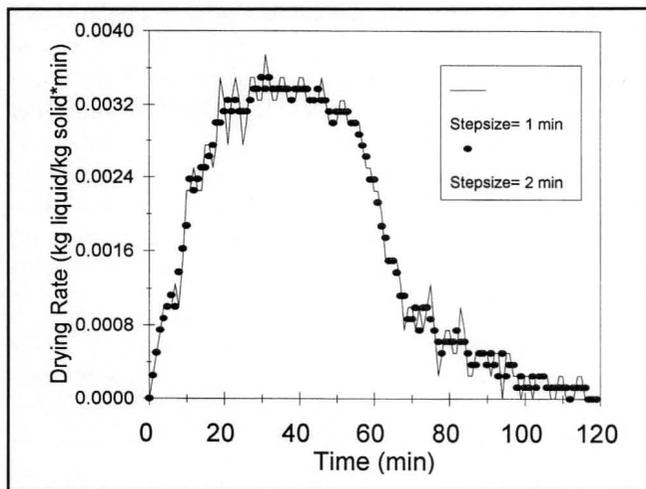


Figure 4. Effect of step size on numerical differentiation at a power level of 144W.

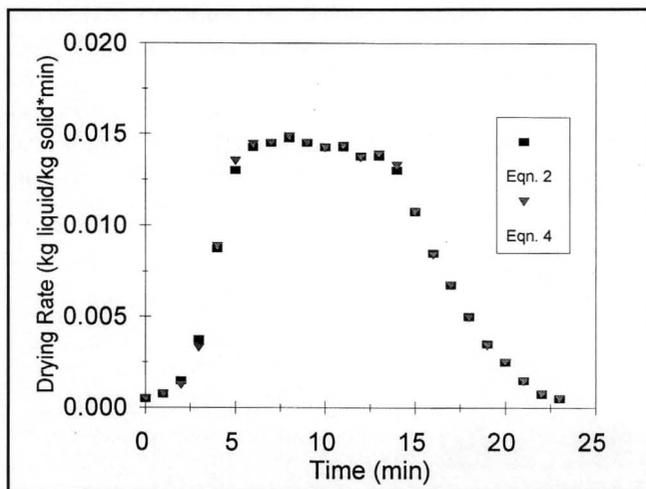


Figure 5. Effect of truncation on numerical differentiation at a power level of 720 W.

approximation to the drying rate is

$$\text{Drying Rate} = \left[ \left( \frac{-1}{m_s} \right) \left( \frac{dm}{dt} \right) \right]_{t_i} \cong -\frac{1}{m_s} \left[ \frac{(m_{i+1} - m_{i-1}))}{2(t_{i+1} - t_i)} \right] \quad (2)$$

The drying rates at the first and last points were generated using related forward and backward difference approximations as shown in the following equations:

First Point:

$$\text{Drying Rate} = \left[ \left( \frac{-1}{m_s} \right) \left( \frac{dm}{dt} \right) \right]_{t_0} \cong -\frac{1}{m_s} \left[ \frac{(-m_2 + 4m_1 - 3m_0)}{2(t_1 - t_0)} \right] \quad (3a)$$

Last Point:

$$\text{Drying Rate} = \left[ \left( \frac{-1}{m_s} \right) \left( \frac{dm}{dt} \right) \right]_{t_n} \cong -\frac{1}{m_s} \left[ \frac{(m_{n-2} - 4m_{n-1} + 3m_n)}{2(t_n - t_{n-1})} \right] \quad (3b)$$

Figure 4 illustrates the importance of sampling interval on the numerical differentiation process. These data were taken at a low power setting (144 W), and the drying-rate curve was generated using step sizes of both one and two minutes. The drying-rate curve obtained using a step size of two minutes is relatively smooth, while the drying-rate curve obtained using a step size of one minute fluctuates, particularly during the constant-rate drying period and as the drying rate falls to zero. At this low power setting, the amount of water evaporated in a one-minute interval was approaching the accuracy of the scale, introducing significant round-off error into the calculations.

Figure 5 examines the effect of truncation error on numerical differentiation of the data. This figure compares the central difference approximation of Eq. (2) to the following, more accurate, central-difference approximation:

Drying Rate =

$$\left[ \left( \frac{-1}{m_s} \right) \left( \frac{dm}{dt} \right) \right]_{t_i} \cong -\frac{1}{m_s} \left[ \frac{(-m_{i+2} + 8m_{i+1} - 8m_{i-1} + m_{i-2}))}{12(t_{i+1} - t_i)} \right] \quad (4)$$

The minimal difference between the derivatives generated by the two differentiation formulas is indicative that truncation error is not significant in this instance and the numerical differentiation formula of Eq. (2) is sufficiently accurate.

## EXTENSIONS

This experiment offers great flexibility and can be extended to examine other concepts, including temperature profiles, particle size and geometry effects, and drying characteristics of different materials.

- Temperature profiles of the solid surface can be produced by recording the surface temperature with a thermocouple when the sample is removed for weighing. Surface

Continued on page 71.

# MEDICAL SURVEILLANCE AND THE UNDERGRADUATE THESIS

IAN A. FURZER

*University of Sydney • Sydney, New South Wales 2006, Australia*

The Department of Chemical Engineering at the University of Sydney has a thesis as a core unit of study in the final year of the chemical engineering curriculum. Students are required to complete fifty credit units in their final year, and the undergraduate thesis is worth eight of them. It normally takes place in Semester 1 and may overflow into the vacation break before the second semester begins.

The thesis discussed in this article is an experimental thesis concerned with the operation of a distillation column to collect composition data on the trays for a ternary mixture of ethyl acetate-ethanol-water. The same thesis, however, can incorporate a significant new component that is designed to make students more aware of occupational exposure to hazardous substances.

This insight can also be valuable in other chemical engineering courses, including risk engineering, hazards and hazops, environmental pollution, and chemical engineering design. The awareness of the dangers of human exposure to hazardous substances is becoming evermore important due to the long-term health effects on workers in the oil, chemical, and biotechnology industries, as well as on the general public. Chemical engineering students need to be aware of alternative process flowsheets that avoid hazardous substances and a general chemical reduction-use program. Several popular books have brought the effect of chemicals on human health into the public consciousness.<sup>[1]</sup>

## MEDICAL SURVEILLANCE

The World Health Organization has a medical surveillance program for the early detection of occupational diseases. It is a prevention program that should be brought to

the attention of chemical engineering students. The information from such program can help students reduce the risk of exposure to hazardous substances. While medical treatment procedures are still not well developed for exposure that leads to cancer several decades ahead, numerous medical treatment procedures are outlined on Internet web sites, including osha.gov in the USA and worksafe.gov.au in Australia. There is also a CD-ROM<sup>[2]</sup> that contains outlines of medical treatment and surveillance programs for a wide range of hazardous substances.

Another CD-ROM search for ethyl acetate provides a wide range of information, including an eight-hour time-weighted average (TWA) exposure of 200 ppm in many countries and an outline of the proper medical treatment for it. This information confirms the low risk to students of exposure to ethyl acetate during a series of distillation experiments conducted for their undergraduate thesis. But chemical engineering students should be made aware of important and relevant sections of the subject's toxicology and epidemiology. Benzene is a substance that has undergone a reduced TWA over the years and is now recognized as being carcinogenic to humans. Details on background levels of benzene, a series of epidemiological studies, and cancer mortalities can be found in reference 3. The environ-



*Ian Furzer has been a faculty member in the Department of Chemical Engineering at the University of Sydney for over twenty-five years. He has extensive teaching and research interests that include computing, process simulation, and chemical engineering plant design. He is the author of over eighty research publications and the textbook Distillation for University Students.*

mental effects of benzene<sup>[4]</sup> in wastewater and aircraft engine exhausts and their connective pathways to humans need to be carefully considered by chemical engineering students in the design of plants that produce benzene or fuels which produce benzene upon combustion. Can we expect a reduction in the TWA value for ethyl acetate in the future if there is medical evidence of an adverse health effect?

In New South Wales, 1966 legislation on Occupational Health and Safety (Hazardous Substances) Regulation has a separate division on an employer's duties relating to health surveillance. The employer must provide workplace health surveillance if any exposure to a hazardous substance results in a reasonable likelihood of a disease or other effect on health. This health surveillance must be under the supervision of an approved medical practitioner. The type of surveillance is listed in some detail for eleven hazardous substances, including acrylonitrile, asbestos, isocyanates, organophosphate pesticides, polycyclic aromatics, and vinyl chloride. The medical tests include the standard respiratory function tests such as FEV1 and FVC.

## **OCCUPATIONAL HEALTH AND EXPOSURE IN THE LABORATORY**

The distillation column for the undergraduate thesis experiment involves medium quantities of solvent. The choice of solvents to be distilled by students should be based on occupational health, safety, ease of analysis, shape of the x-y diagram for binary systems, and the ability to extract knowledge on separation systems. Alcohol-and-water is a commonly used system. The occupational health risks to students of exposure to ethanol, by inhalation, need to be considered. How often are laboratory demonstrators advising students of the need to minimize the inhalation of ethanol?

For an undergraduate thesis or special project, it is useful to consider the ternary mixture of ethyl acetate, ethanol, and water. This mixture provides a good working environment to extract knowledge on ternary and binary azeotropes, distillation paths, and the appearance of a two-liquid-phase region in the distillation column. The following method has been used to actively reduce the exposure to ethyl acetate and ethanol over the students' extended period of work for the undergraduate thesis.

The most important aspect of occupational health is to introduce the subject to the students who will be involved, to notify them of the low hazard of ethyl acetate and ethanol, and to discuss with them the methods of reducing the mass inhaled. This introduces to them the psychological component of occupational health, leading each student to develop his or her own concern about the toxic nature of the inhaled substances. This component will play an important part in

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*The awareness of the dangers of human exposure to hazardous substances is becoming evermore important due to the long-term health effects on workers in the oil, chemical, and biotechnology industries, as well as on the general public.*

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assessing their own exposure estimates. An approach to primary prevention of exposure is to increase ventilation in the laboratory, thus diluting the inhaled air and reducing the composition of the solvent in the air. The mass of inhaled solvent per breath can be reduced and the risk factor in occupational health could also be expected to be reduced. This involves starting exhaust fans and opening doors and windows to increase air circulation.

The next aspect of occupational health is associated with safety and is concerned with the release of solvent vapors due to a laboratory fire. Students should be advised on the safety procedures to be used in the event of a fire. They should be told to evacuate the laboratory immediately and not to attempt putting out the fire, but to notify the safety officer instead. This is extremely important for minimizing the risk of exposure.

Good laboratory practice is important for occupational health. There is a direct association between hazard identification, hazard analysis, and good occupational health. When release of solvent vapors is the hazard to be minimized, a hazard identification program must be carefully conducted on the distillation equipment, identifying all possibilities of vapor release and listing all actions needed to prevent such a release.

For example, vapor could be released by a failure of the cooling water, a mechanical failure of a glass column piece, a gasket failure, or a low level in the reboiler. Special attention should also be given to the cooling water supply. Safety labels on the cooling water supply switches are essential to prevent an insufficient supply of cooling water and to minimize the release of solvent vapor.

Also associated with good laboratory practice is the need for the student to be present in the laboratory while the distillation equipment is operating. Students should be well trained in emergency procedures such as turning off the steam supply to the reboiler in the event of a solvent release.

## **STUDENT EXPOSURE TO ETHYL ACETATE**

Students can be exposed to ethyl acetate in a number of the

laboratory experiment phases. The first is concerned with calibration of the gas-chromatograph (GC) equipment for analysis of the ethanol-water-ethyl acetate mixture. This can involve exposure while transferring ethyl acetate from a 20-L drum to smaller glass vessels, the preparation of standards, and during the running of the GC. Student exposure to ethyl acetate during this phase is generally low. An internal standard is used in the GC calibration. In this case it was 1-propanol, and students should be aware of its occupational health characteristics.

Filling the distillation column with the ternary mixture involves transferring and measuring about 20 L of the mixture and often involves mild exposure to ethyl acetate. The distillation column, which had been tested for leaks with water, will now be found to have a smell of ethyl acetate, but no visible liquid leaks. The laboratory is equipped with a gas alarm system with a sensor adjacent to the distillation column. This alarm is continuously on but is not activated by this mild smell of ethyl acetate.

Running the distillation column with good ventilation until steady state is reached may require one hour and result in mild exposure to ethyl acetate. Additional exposure could occur when liquid samples are withdrawn from the nine column trays. Further mild exposure would take place for each distillation run.

## BLOOD TESTS AND STUDENT PRIVACY

Students may be exposed to ethyl acetate before entering the unit operations laboratory. Ethyl acetate is a well-known solvent and is often used in the cosmetic industry as a nail polish remover, so female students who use this substance might be expected to have a higher ethyl acetate content in their blood. The body may also generate ethyl acetate from the complex biochemical pathways in the body.

The initial ethyl acetate content of students' blood is important before they enter the solvent environment of the unit operations laboratory, but this can pose some problems with privacy. Students have a right to privacy concerning analysis of their blood. Voluntary agreement must be obtained from the student for a blood test for ethyl acetate. Students are advised to contact the student medical center for this blood test.

The background level of ethyl acetate in the blood should be around 0.5 mg/L. One female student, however, had an initial level of 1.4 mg/L of ethyl acetate. This highlights the importance

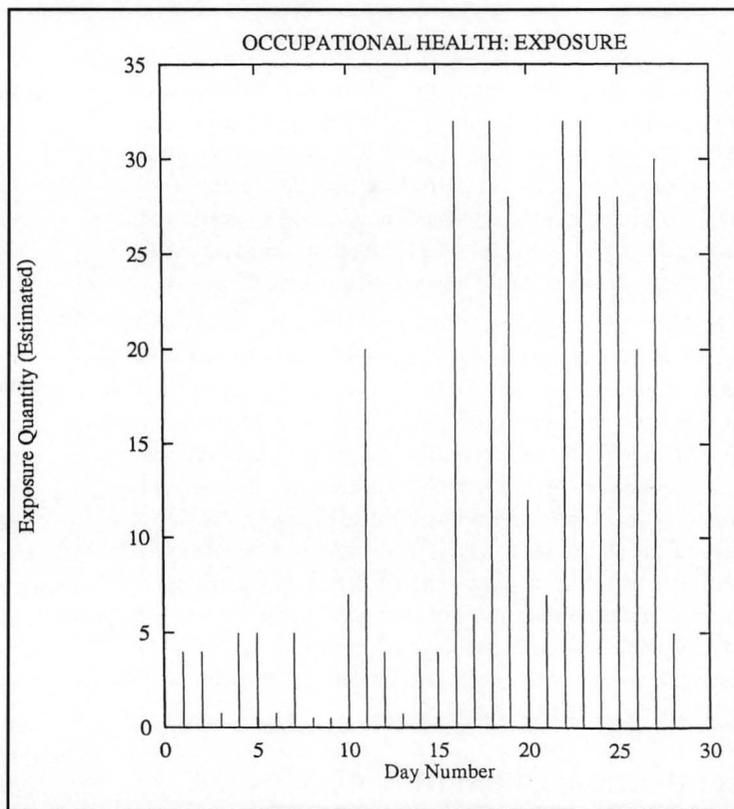


Figure 1. Estimated impulse exposure to ethyl acetate (male student).

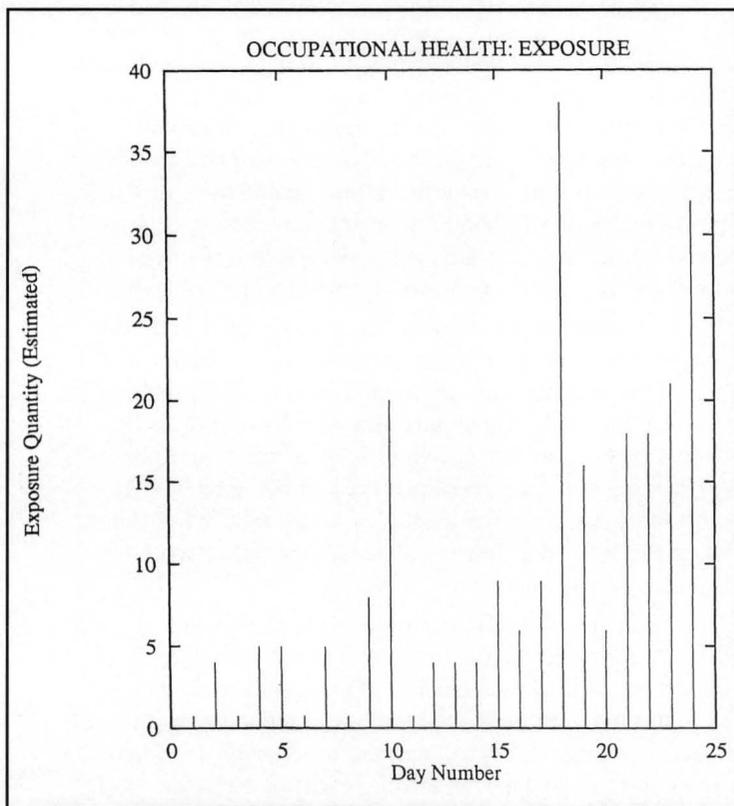


Figure 2. Estimated impulse exposure to ethyl acetate (female student).

of a blood test *before* conducting the distillation experiment.

Students were then asked to estimate their exposure to ethyl acetate in the qualitative terms of low, medium, and high and to estimate the number of hours at these exposure levels on each exposure day. This raw data represents a series of impulses of exposure to ethyl acetate, the height of the impulse being a measure of the perceived intensity of exposure.

The body reacts to these impulses by exhaling ethyl acetate, by generating enzymes to convert ethyl acetate to other substances for rejection, or by storing ethyl acetate in fatty tissue. The complex response is similar to the simple impulse response taught in chemical engineering mathematics and process control.

The process could be made more quantitative if the inhaled dose of ethyl acetate per impulse could be measured. This would require personal monitoring devices attached to the student and subsequent analysis of the sample tubes. These devices are useful in providing an integration of the impulse of ethyl acetate. Other methods, which are not practical in a unit operations laboratory, would involve a composition measurement of ethyl acetate in the air and a profile of the rate of inhalation of air.

Medical surveillance is introduced to the students through blood tests both before and after the full laboratory period covering the undergraduate thesis. Students conducted a calibration, distillation runs, and analyses over a period of four months, with the number of exposure days limited to about thirty days. The period of zero exposure to ethyl acetate between exposure days may have provided time for the body dynamics to remove excess ethyl acetate from the blood.

Figures 1 and 2 show the estimated impulse exposure to ethyl acetate on the exposure days for a male and a female student, respectively. The data for these figures were obtained from the student's own impression of the level of exposure as low, medium, or high, and the hours of exposure. The differences in the two figures is due mainly to the different perceived exposure by each student. The two figures provide important qualitative information on the problem of estimating exposure without a personal monitor. The chemical engineering student will meet this type of occupational health problem when employed in the workplace. The unit operations laboratory environment treated as a local workplace can be valuable in introducing students to exposure, occupational health, and perceived impressions of exposure.

The end of the laboratory experiments, with the column

**The unit operations laboratory environment treated as a local workplace can be valuable in introducing students to exposure, occupational health, and perceived impressions of exposure.**

**TABLE 1**  
Blood Analyses  
Ethyl Acetate (mg/L)

	<i>Before</i>	<i>After</i>
Male	0.5	0.5
Female	1.4	0.5

drained and the solvents returned to the solvent store, marks the end of the occupational health exposure period. Students are then advised to have a second blood test for ethyl acetate. Table 1 shows the ethyl acetate content of the blood before and after the distillation experiments.

The blood results are most encouraging, with both students having background levels of ethyl acetate at 0.5 mg/L. One might conclude that student awareness of the occupational health study reduced their exposure, or that the ventilation of the laboratory was adequate, or that the interval between exposures was sufficient for the body to remove any excess ethyl acetate.

## OCCUPATIONAL HEALTH GOALS

- To use the undergraduate thesis experiment on distillation to introduce students to the concept of medical surveillance.
- To introduce students to the psychological response of exposure limits to inhaled chemicals when introduced to the Material Safety Data Sheets (MSDS).
- To obtain essential information on the previous history of exposure to a chemical through a voluntary blood test *before* the experiment begins.
- To monitor the daily exposure to a chemical in a qualitative manner, thus introducing perceived exposures to a chemical and an improved awareness of occupational health.
- To introduce ventilation as a key measure in reducing exposure to a chemical.
- To have a repeat blood test *after* the laboratory experiment to ensure that preventive methods for reducing occupational health exposure have been successful.
- To expect students to perform better in the occupational health area of chemical engineering design and that they have an improved concept of occupational health, both in the workplace and in general.

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# LABORATORY EXPERIMENT IN BIOCHEMICAL ENGINEERING

## *Ethanol Fermentation*

ALBERTO COLLI BADINO, JR., CARLOS OSAMU HOKKA  
*Universidade Federal de São Carlos • São Carlos, Brazil*

The need for didactic experiments that will prepare our students for their professional futures, together with the importance of the ethanol industry in Brazil, led us to design and construct an experimental bench-scale kit for determining the kinetic parameters related to the ethanol fermentation process.

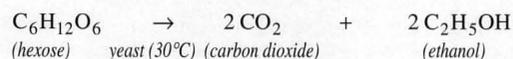
The experiment's design was based on the principles that guided construction of the Didactic Laboratory of Chemical and Biochemical Reactions at our university, which included a laboratory composed of didactic kits for short experiments prepared by the students that would complement classroom knowledge.

A set of three bench-scale fermentors was designed and constructed that would support groups of five students per fermentor. To standardize the experiments, one of them was used in two types of cultivation: the first at low substrate concentration ( $\approx 16.7 \text{ gL}^{-1}$  of glucose) and the

second at a concentration of  $60 \text{ gL}^{-1}$  to allow fitting of traditional kinetic models without and with inhibition by the product, respectively.

### THEORY

We know that in a favorable environment, simple sugars (monosaccharides) are transformed in ethanol and carbon dioxide ( $\text{CO}_2$ ) by the action of yeasts as follows:



It can be seen that for each mole of hexose, equal molar amounts of ethanol and carbon dioxide are produced.

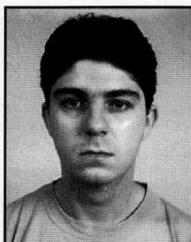
In fermentation processes that synthesize primary metabolites such as ethanol, cell growth and product generation take place simultaneously. Here the cellular growth and the product synthesis are directly related. Therefore, the ethanol production can be predicted from the cellular growth kinetics. From the hypothesis that the concentration of cells is a good measure of the enzymatic system responsible for the transformation of the substrate into product, it is convenient to define the specific growth rate ( $\mu$ ) as

$$\mu = \frac{1}{X} \frac{dX}{dt} \quad (1)$$

where  $dX/dt$  is the variation of the cellular concentration ( $X$ ) with time ( $t$ ).

Several models have been proposed to relate the specific growth rate ( $\mu$ ) to the limiting nutrient and inhibitor concentrations. A classic kinetic model relating the specific growth rate to the limiting substrate was proposed by Monod.<sup>(1,2)</sup> Working in a continuous process, he obtained the following relationship, also applied to batch processes:

**Alberto Colli Badino, Jr.**, is Associate Professor of Chemical Engineering at the Universidade Federal de S. Carlos. He received his Master's from the Federal University of S. Carlos in 1991 and his Doctorate in Biochemical Engineering from the State University of S. Paulo in 1997. His research interests are in mass transfer in conventional fermentation processes, rheology of fermentation broths, and power requirements in conventional fermentors.



**Carlos Osamu Hokka** is Associate Professor of Chemical Engineering at the Universidade Federal de S. Carlos. He received his Master's from Osaka University in 1976, and his Doctorate in Biochemical Engineering from the State University of Campinas in 1983. His research interests are in ethanol production in non-conventional continuous processes and beta-lactam antibiotic production processes in non-conventional reactors.

**The equipment allowed us to perform short-duration didactic experiments  
(4.5 and 3.0 hours) using low-cost raw materials.**

$$\mu = \mu_{\max} \frac{S}{K_S + S} \quad (2)$$

where  $\mu_{\max}$  is the maximum specific growth rate achievable when  $S \gg K_S$ ,  $S$  is the concentration of growth-limiting nutrient, and  $K_S$  is the saturation constant or the value of the limiting nutrient concentration at which the specific growth rate is half of  $\mu_{\max}$ . It is known that this model is valid for cultivations using low initial limiting substrate concentrations ( $S_0$ ).

In ethanol fermentation, high initial substrate concentrations ( $S_0$ ) generate high product concentrations ( $P$ ) that inhibit cellular growth and, consequently, the production of ethanol. Various relationships relating the effect of ethanol concentration ( $P$ ) to the specific growth rate ( $\mu$ ) of the organism have been reported.<sup>[3-5]</sup>

One type of relationship that presents similarity to the non-competitive inhibition in enzyme kinetics has been proposed<sup>[3]</sup> for modeling ethanol inhibition of *Saccharomyces cerevisiae*. A term accounting for ethanol inhibition is added to the simple Monod kinetic model, giving

$$\mu = \mu_{\max} \frac{S}{K_S + S} \frac{K_p}{K_p + P} \quad (3)$$

where  $P$  is the ethanol concentration and  $K_p$  is the product inhibition constant. From Eq. (3), we see that the higher the ethanol concentration, the higher its negative effect will be on the specific growth rate ( $\mu$ ).

Still, in a fermentation process, the concentration of cells ( $X$ ) and product ( $P$ ) can be related to the limiting substrate concentration ( $S$ ) by the yield coefficients

$$Y_{X/S} = \frac{dX}{dS} = \frac{X - X_0}{S_0 - S} \quad (4)$$

$$Y_{P/S} = \frac{dP}{dS} = \frac{P - P_0}{S_0 - S} \quad (5)$$

**MATERIAL AND METHODS:**

● **Microorganism** *Saccharomyces cerevisiae* (commercial Fleischmann's baker's yeast) was grown in two different media for ethanol production.

● **Media** Two different media have been used in the experiments: media 1 and 2 in ASSAYS 1 and 2, respectively.

● **Medium 1** (low substrate concentration) in  $gL^{-1}$ : commercial corn glucose (90% w/w in glucose), 20.0;  $KH_2PO_4$ ,

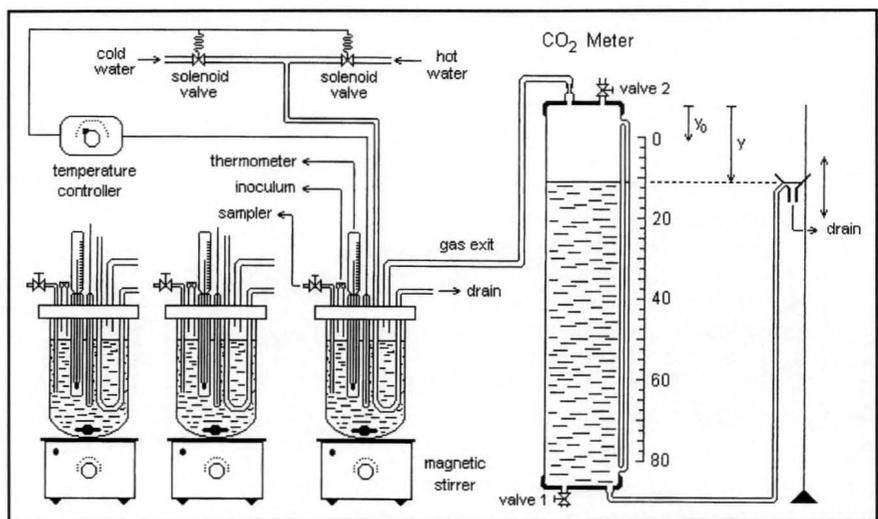
5.0;  $MgSO_4 \cdot 7 H_2O$ , 0.4; yeast extract, 3.0;  $(NH_4)_2SO_4$ , 1.8; commercial antifoam (dilution 1:10), 5 drops; pH=4.6; solvent, distilled water.

● **Medium 2** (high substrate concentration) in  $gL^{-1}$ : commercial corn glucose, 66.0;  $KH_2PO_4$ , 5.0;  $MgSO_4 \cdot 7 H_2O$ , 0.4; yeast extract, 3.0;  $NH_4Cl$ , 2.5; commercial antifoam (dilution 1:10), 5 drops; pH=4.6; solvent, distilled water.

● **Experimental Equipment** The fermentors were made of glass, adapting 1000-mL "kettle"-type (Pyrex) recipients with flat bottoms. Fermentor lids were made of "technyl" (nylon) and adapted to the opening of the recipients. Agitation was accomplished using magnetic stirrers adapted to the base of the fermentors. The temperature was controlled through solenoid valves activated by bulb and capillary controllers. Wells for controlling and monitoring temperature, and tubes for heat transfer ("U" tubes), sampling, inoculation, and gas exit, were made of stainless steel and connected to the lids of the fermentors.

Devices for determining the volume of  $CO_2$  liberated by the fermentation were constructed of PVC (polyvinylchloride) pipes with internal diameters of 10 cm and heights of 100 cm and connected to the gas exits of the fermentors, based on equipment proposed by Nilsson, et al.<sup>[6]</sup> A scheme of the experimental apparatus is shown in Figure 1.

● **Analytical Methods** Cell concentration was evaluated as dry weight. Broth samples were centrifuged, washed twice, and resuspended with distilled water. Aliquots were diluted and the absorbance of the suspension was measured at 650 nm with a spectrophotometer (Micronal B-395). The concen-



**Figure 1.** Schematic of the experimental apparatus.

tration of the yeast suspension (X) in  $\text{gL}^{-1}$  was related to the absorbance according to the following calibration curve:  $X=0.817 \text{ Abs}$ , valid for  $X < 0,45 \text{ gL}^{-1}$ . Glucose concentration (S) was determined as total reduction sugars by the colorimetric Somogyi method<sup>[7]</sup> using the same spectrophotometer. Ethanol concentration (P) was determined by the method of oxidation by potassium dichromate after distillation and indirectly relating to the volume of  $\text{CO}_2$  formed.

**Measurement of  $\text{CO}_2$  Volume Produced by Fermentation** According to the stoichiometry of the microbial reaction, for each mole of consumed glucose, two moles of ethanol and  $\text{CO}_2$  are produced. Therefore, if it is possible to measure the amount of  $\text{CO}_2$  produced by the reaction, this can be related to the concentration of ethanol present in the fermentation broth. Such a procedure facilitates the didactic experimental routine as ethanol analysis by the method of oxidation by potassium dichromate or other conventional method is time consuming, requiring the supernatant of the centrifuged sample to be distilled and diluted for titration.

Measurements of the  $\text{CO}_2$  volume produced by the fermentation process were accomplished in the following manner. Initially, the pipe was filled with water from the bottom (valve 1) up to the level  $y_0$  measured from the top of the pipe, maintaining valve 2 open. Before cultivation was started, valves 1 and 2 were closed. The  $\text{CO}_2$  produced left the fermentor through the gas exit tube and entered from the top of the pipe, pushing the water level down. The water level was monitored by a transparent tube connected vertically to the PVC pipe. According to hydrostatic principles, in order to maintain constant atmospheric pressure in the head of the fermentor, the water level in a thin tube connected to the base of the PVC pipe was controlled manually by draining the water.

The number of moles of  $\text{CO}_2$  produced during fermentation can be calculated at any time by the ideal gas law

$$n_i = \frac{P_{\text{atm}} V_i}{RT} = \frac{P_{\text{atm}} \pi D^2 (y_i - y_0)}{4 RT} \quad (6)$$

where

- $n_i$  number of moles of  $\text{CO}_2$  evolved at time  $t=i$
- $V_i$  gas volume at time  $t=i$
- R gas constant [ $R=82.04 \text{ atm cm}^3/(\text{g-mole K})$ ]
- T gas temperature [K]
- D internal diameter of the PVC pipe [ $D=10 \text{ cm}$ ]
- $y_i$  distance from the top of the PVC tube to the water level at time  $t=i$
- $y_0$  Distance from the top of the PVC tube to the water level at  $t=0$

**Experimental Procedure** Two fermentation assays were carried out at  $30^\circ\text{C}$  using the culture media previously presented. First, the 1000-mL fermentors containing 700 mL of culture media were sterilized in an autoclave at  $121^\circ\text{C}$  for thirty minutes. After sterilization, the temperature was main-

tained at  $30^\circ\text{C}$ . Then, 100 mL of inoculum activated in a shaker with different cell concentrations ( $X_0$ ) was added, completing 800 mL of initial working volume. The inoculum is activated prior to its addition to the culture medium in order to eliminate the adaptation stage of the microorganism to the culture medium (the "lag" phase of the process). Samples of 10 mL were withdrawn approximately every half hour, right after inoculation up to complete depletion of the glucose (end of fermentation). At the moment of sample withdrawal, the distance between the top of the PVC pipe and the water level ( $y_i$ ) was measured. Samples were divided into two aliquots of 5 mL for analysis of the concentrations of substrate (S), ethanol (P), and cellular mass (X). The assays carried out at low and high initial substrate concentrations ( $S_0$ ) were designated as ASSAY 1 and ASSAY 2, respectively. Ethanol concentrations were determined analytically only in ASSAY 2 to be related to the  $\text{CO}_2$  volume produced. In ASSAY 1, the ethanol concentrations were determined indirectly by the  $\text{CO}_2$  volume produced.

## RESULTS AND DISCUSSION

The results obtained in ASSAYS 1 and 2 are shown in Table 1. Usually, fermentation processes are relatively too time-consuming to be used in didactic experiments, but standardization of the assays provided reasonably short experiments of 4.5 and 3.0 hours, respectively.

From the experimental data of ASSAY 2, it was possible to relate the numbers of moles of ethanol and  $\text{CO}_2$  generated by the ethanol fermentation. The number of moles of  $\text{CO}_2$  evolved ( $n_{\text{CO}_2}$ ) was calculated by Eq. (6) and the number of ethanol moles ( $n_{\text{ethanol}}$ ) formed was estimated as

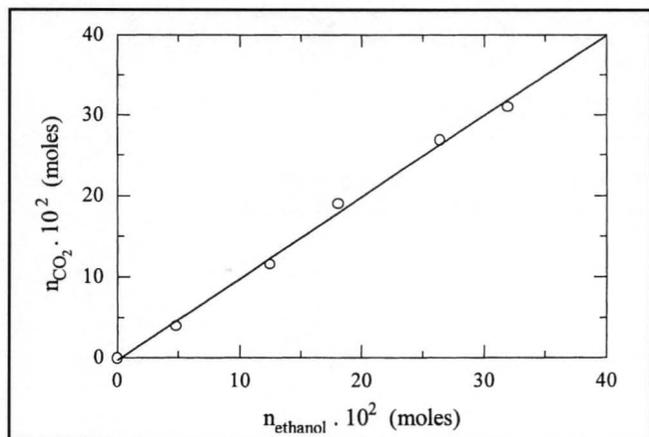
$$n_{\text{ethanol}} = PVM_{\text{ethanol}} \quad (7)$$

where P is the ethanol concentration in the broth (in  $\text{gL}^{-1}$ ), V is the broth's volume (in L), and  $M_{\text{ethanol}}$  is the ethanol molecular weight ( $M_{\text{ethanol}}=46$ ).

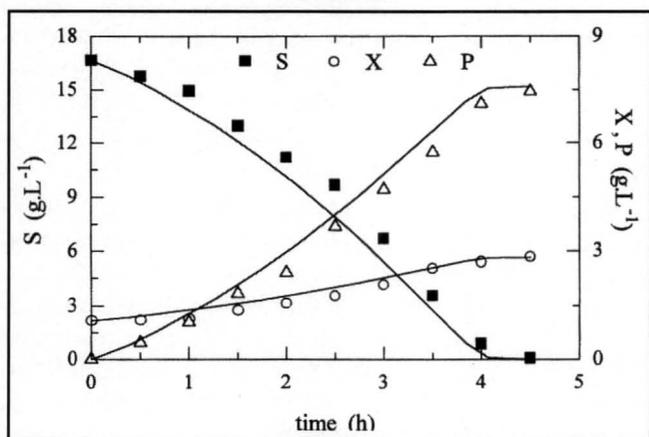
**TABLE 1**  
Experimental Results Obtained in ASSAYS 1 and 2

time (h)	ASSAY 1			ASSAY 2			
	S( $\text{gL}^{-1}$ )	x( $\text{gL}^{-1}$ )	P( $\text{gL}^{-1}$ )	time (h)	S( $\text{gL}^{-1}$ )	x( $\text{gL}^{-1}$ )	P( $\text{gL}^{-1}$ )
0.0	16.66	1.08	0.00	0.00	60.00	18.38	0.00
0.5	15.78	1.09	0.46	0.58	48.25	19.80	2.79
1.0	14.94	1.15	1.03	1.17	35.73	22.51	7.18
1.5	12.97	1.37	1.83	1.75	26.60	23.78	10.37
2.0	11.19	1.56	2.40	2.33	15.38	24.43	15.16
2.5	9.68	1.76	3.66	2.92	5.86	25.83	18.35
3.0	6.69	2.06	4.69				
3.5	3.52	2.52	5.72				
4.0	0.88	2.72	7.10				
4.5	0.10	2.84	7.44				

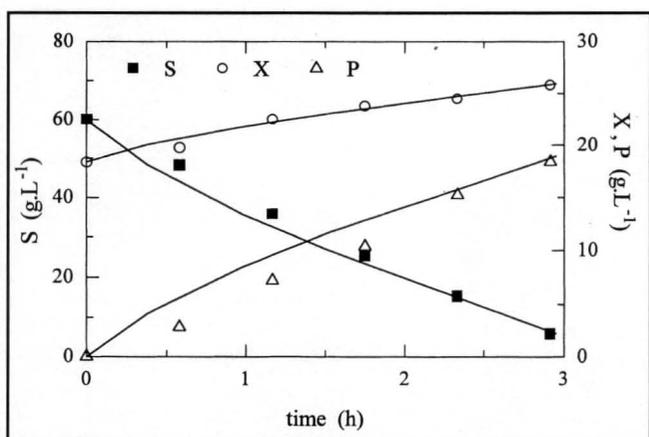
Figure 2 illustrates the good linear relationship between values of  $n_{\text{ethanol}}$  and  $n_{\text{CO}_2}$ . The linear regression of the experimental data resulted in a slope of 1.006 and a regression coefficient ( $R^2$ ) of 0.994, showing that the theoretical-experimental methods, proposed to determine the ethanol con-



**Figure 2.** Relationship between the number of moles of ethanol formed ( $n_{\text{ethanol}}$ ) and  $\text{CO}_2$  evolved ( $n_{\text{CO}_2}$ ) during ASSAY 2.



**Figure 3.** Fit of Monod's model to the experimental data of ASSAY 1.



**Figure 4.** Fit of the Aiba, et al., model<sup>[3]</sup> to experimental data of ASSAY 2.

centration indirectly in the broth by the volume of  $\text{CO}_2$  produced, generated very good results.

Yield coefficients  $Y_{X/S}$  and  $Y_{P/S}$  were determined by experimental data (Table 1) as being:  $Y_{X/S}=0.11$ — $Y_{P/S}=0.46$  (ASSAY 1) and  $Y_{X/S}=0.14$ — $Y_{P/S}=0.35$  (ASSAY2), respectively.

Experimental results were analyzed based on two classical kinetic models. Initially, Monod's model (Eq. 2) was fitted to the experimental data of ASSAY 1. The specific growth rate ( $\mu$ ) was estimated by Eq. (1) where  $dX/dt$  was calculated from the polynomial equation fitted to the curve  $X(t)$ . The kinetic parameters,  $\mu_{\text{max}}=0.32 \text{ h}^{-1}$  and  $K_S=0.63 \text{ gL}^{-1}$ , were obtained by nonlinear regression of  $\mu$  and  $S$  values according to Eq. (2) using Marquardt's algorithm.

In the same way, the kinetic model proposed by Aiba, et al.,<sup>[3]</sup> was fitted to the experimental values of ASSAY 2, considering the kinetic parameters,  $\mu_{\text{max}}$  and  $K_S$ , obtained previously (ASSAY 1). The product inhibition constant ( $K_p$ ) was estimated as being 6.29.

Figures 3 and 4 illustrate the good fits of the kinetic models of Monod and Aiba, et al., to the experimental values of the assays carried out at low and high initial substrate concentration, ASSAY 1 and ASSAY 2, respectively. A fourth-order Runge-Kutta technique was applied to simulate the predicted curves of  $S$ ,  $X$ , and  $P$  as a function of time.

For comparison, Table 2 shows the values of the kinetic parameters evaluated from the data of other workers.<sup>[8]</sup> It can be seen that the values of the kinetic parameters obtained by the present work are within the range of values encountered in the literature showing that the proposed methodology can be of great value for educational and research purposes.

## CONCLUSIONS

The equipment allowed us to perform short-duration didactic experiments (4.5 and 3.0 hours) using low-cost raw materials. The relationship of ethanol/ $\text{CO}_2$  produced by the fermentation was very close to unity (1.006), showing the precision of the equipment. Use of the  $\text{CO}_2$  meter in didactic

*Continued on page 70.*

**TABLE 2**  
Kinetic Parameters

	T (°C)	$\mu_{\text{max}}$ ( $\text{h}^{-1}$ )	$K_S$ ( $\text{gL}^{-1}$ )	$K_p$ ( $\text{gL}^{-1}$ )	$Y_{P/S}$ (-)
Egamberdiev and Ierusalimskii <sup>[8]</sup>	28	0.31	-	20.6	0.39
Aiba and Shoda <sup>[8]</sup>	30	0.43	-	55	0.35
Pironti <sup>[8]</sup>	30	0.26	15.5	13.7	0.47
Cysewski <sup>[8]</sup>	35	0.58	4.9	5.0	0.44
Bazua and Wilke <sup>[8]</sup>	35	0.64	0.24	40	0.52
Hoppe and Hansford <sup>[8]</sup>	30	0.64	3.3	5.2	0.43
This work	30	0.32	0.63	6.29	0.35-0.46

# PERMEATION OF GASES IN ASYMMETRIC CERAMIC MEMBRANES

CARLOS FINOL, JOAQUÍN CORONAS  
*University of Zaragoza • 50009 Zaragoza, Spain*

Interest in and applications of inorganic membranes have been growing exponentially for the last fifteen years.<sup>[1]</sup> Inorganic membranes can be classified into two categories: dense and porous. Dense membranes are dominated by palladium and its alloys (metal membranes) and solid electrolyte membranes (commonly, simple or complex oxides or oxide-solid solutions). Porous membranes are made of oxides, carbon, glass, metals, zeolites, etc. The most unusual commercial porous ceramic membranes have an asymmetric structure consisting of a support layer (generally, alpha-alumina) with large pores and a separation layer made of a different material (gamma-alumina, zirconia, silica, etc.) that controls the permeation flux.

The industrial development of inorganic membranes started in the 1940s with the purification of nuclear fuels. This process is based on the separation of  $U^{235}F_6/U^{238}F_6$  by Knudsen diffusion. Knudsen diffusion occurs when the mean-free-path of the gas molecules is much larger than the average pore dimensions of a porous material through which the molecules diffuse, and permeate will be enriched in the molecule of the lower molecular weight.

In this short article, we will describe an easy experiment that helps to understand the transport through ceramic membranes when Knudsen diffusion occurs.

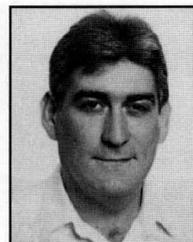
## THEORY

In general, transport through porous ceramic membranes can be related to the pore diameter,  $dp$ , according to IUPAC definitions:<sup>[2]</sup> macropores with  $dp > 50$  nm, where basically viscous flow (in this case, no separation of mixtures is possible) and Knudsen diffusion occur; mesopores with  $dp$  between 2 and 50 nm, where Knudsen diffusion and multilayer diffusion/capillary condensation take place; and micropores

with  $dp < 2$  nm, where molecular sieving effects can be expected. Surface-multilayer diffusion and capillary condensation are achieved when the permeating molecule preferentially adsorbs on the membrane pores or condenses within the pores due to capillary forces, respectively. Both transport mechanisms, which allow the separation of mixtures with very high selectivities, are especially important at relatively low temperatures and with small pores, mesopores, and even micropores.

When permeances through mesoporous membranes are studied for permanent gas or vapors at low relative pressures, the transport mechanism is controlled by the Knudsen diffusion. Sometimes laminar flow (viscous flow at laminar regime) can appear if the membrane has defects of macropore size, decreasing the separation power of the membrane. Considering both the laminar and Knudsen flow contributions, the transport equation can be written as

*Carlos Finol is a PhD student in the Department of Chemical and Environmental Engineering at the University of Zaragoza. His research interests are in using special reactors for partial oxidation of hydrocarbons.*



*Joaquín Coronas is Assistant Professor in Environmental Engineering at the University of Zaragoza. He received his PhD in chemistry in 1995 from Zaragoza University. His research interests are in developing membranes for separation and ceramic membrane reactors.*

$$F_T = F_K + F_{OV}P = \frac{4}{3} \sqrt{\frac{2}{\pi}} \frac{\varepsilon r}{L\tau\sqrt{RTM}} + \frac{\varepsilon r^2}{8 L\tau\mu RT} P \quad (1)$$

where

- $F_T$  total permeance [mol/(m<sup>2</sup> s Pa)]
- $F_K$  is the Knudsen contribution
- $F_{OV}$  factor that multiplied by  $P$  gives the laminar contribution to the total permeance
- $P$  average pressure across the membrane [Pa]
- $\varepsilon$  porosity of the membrane
- $r$  pore radius [m]
- $L$  membrane thickness [m]
- $\tau$  tortuosity of the medium
- $R$  gas constant [8.314 m<sup>3</sup>Pa/(mol K)]
- $T$  absolute temperature [K]
- $\mu$  viscosity of the gas [Pa s]

A plot of  $F_T$  vs.  $P$  allows one to estimate the relative contributions of both transport mechanisms: the higher the slope of such a plot, the higher the laminar contribution and vice versa. On the other hand, for a certain membrane material, if the laminar contribution is not important, or  $P=0$ , it is possible to calculate the Knudsen separation factor for two gases, A and B, by using the first term of Eq. (1)

$$\alpha_{A/B} = \frac{F_K^A}{F_K^B} = \sqrt{\frac{M_B}{M_A}} \quad (2)$$

Since Knudsen diffusion occurs when the mean-free-path of the molecules ( $\lambda$ ) is much larger than the mean pore radius ( $r$ ) of the membrane, the Knudsen number, defined by the equation

$$Kn = \frac{\lambda}{r} = \frac{16\mu}{5\pi P} \sqrt{\frac{\pi RT}{2M}} \quad (3)$$

is a convenient dimensionless group to quickly estimate if Knudsen diffusion will likely be the dominant transport mechanism. When  $Kn > 1$ , the molecules collide with the pore wall much more often than with each other.

## EXPERIMENTAL

The membrane used was a commercial ceramic tube 10 cm long and 0.7 cm i.d. purchased at SCT (Société des Céramiques Techniques, a subsidiary of US Filter). The ceramic tube had an asymmetric structure consisting of a support layer of  $\alpha$ -alumina and an inner layer of  $\gamma$ -alumina with 5-nm diameter pores. The ends of the membrane were non-permeable, restricting the permeation area to a length of 5 cm.

Figure 1 shows the permeation system. The membrane was sealed in a stainless-steel module by silicone o-rings, and the pressure at the feed site (or retentate) was measured by a pressure transducer. At the permeate side, the permeation flux was measured using a bubble flowmeter and, finally, an electric furnace allowed modification of the mem-

**A very simple system can be used with a commercial ceramic membrane of  $\gamma$ -alumina to measure permeances of single gases (e.g.,  $N_2$  and He) at several total pressures and temperatures.**

brane temperature. The permeate side was open to the atmosphere, and permeate pressure was always the atmospheric one. The permeance  $F$  in mol/(m<sup>2</sup> s Pa) was calculated as

$$F = \frac{Q}{A\Delta P} \quad (4)$$

where

- $Q$  molar flux [mol/s]
- $A$  permeation area referred to the internal side of the ceramic tube (1.1x10<sup>-3</sup>m<sup>2</sup>)
- $\Delta P$  pressure drop [bar] between retentate and permeate sides

## RESULTS AND DISCUSSION

The variation of He and  $N_2$  single-gas permeances vs. the total pressure (calculated as  $[P_1 + P_2]/2$ , where  $P_1$  and  $P_2$  are the pressures at the permeate and retentate sides, respectively) through an alumina membrane was studied at 298 and 473K. Figure 2 shows that the He permeances at 298 and 473K did not change with total pressure, and the same can be stated for the  $N_2$  permeances (Figure 3), at least in the pressure range tested, which means that the viscous contribution is not important, and in the equation (Eq. 1) that governs transport through the membrane, the second term

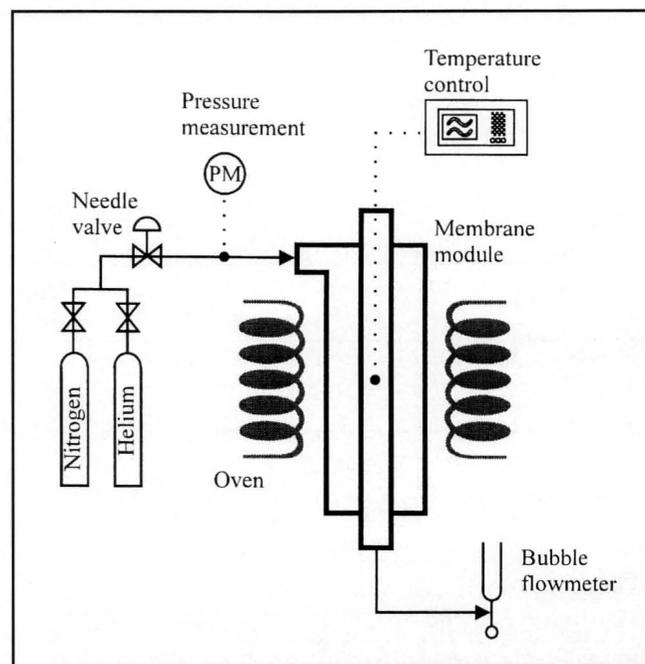


Figure 1. Experimental system.

( $F_{OV}$ ) can be neglected.

The Knudsen number calculated using Eq. (3) for He and  $N_2$  in the temperature and pressure ranges tested is 44-124 and 14-30, respectively (it decreases with increasing pressure and decreasing temperature), *i.e.*, in this case, this number is always higher than one, which means (as seen above) that Knudsen diffusion will dominate over viscous flow. Moreover, permeances decreased with increasing tempera-

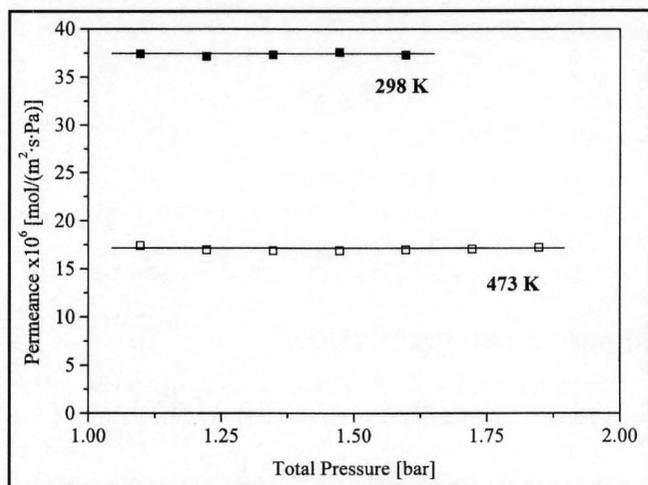


Figure 2. He permeance as a function of total pressure at 298 and 473 K.

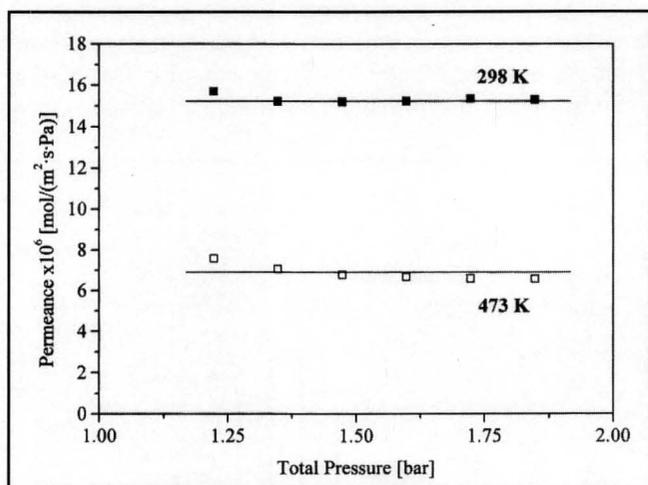


Figure 3.  $N_2$  permeance as a function of total pressure at 298 and 473K.

TABLE 1

He and  $N_2$  permeances and  $\alpha_{He/N_2}$  at 298 and 473 K

Temperature [K]	Permeance [mol/(m <sup>2</sup> sPa)]		$\alpha_{He/N_2}$	
	He	$N_2$	Theoretical	Experimental
298	$37.2 \times 10^{-6}$	$15.3 \times 10^{-6}$	2.65	2.43
473	$17.2 \times 10^{-6}$	$6.81 \times 10^{-6}$	2.65	2.53

ture, as expected after analyzing Eq. (1). Table 1 lists the averages of  $N_2$  and He permeances. From these permeances, the experimental separation factor  $\alpha_{He/N_2}$  can be calculated as the ratio of He and  $N_2$  permeances. The  $\alpha_{He/N_2}$  is 2.43 at 298K and 2.53 at 473, converging with increasing temperature to the theoretical value of 2.65 calculated by using Eq. (2). Probably,  $N_2$  absorbs weakly, but stronger than He at low temperature, contributing to the total  $N_2$  flux. This contribution will decrease at higher temperature, increasing the separation factor slightly.

Finally, the ratio of pure gas permeances is also known as the ideal separation factor, and very often ideal separation factors do not allow extrapolation to mixtures. To carry out separation of mixtures of compounds with selectivities higher than those of Knudsen, microporous membranes (silica, zeolite, carbon) can be employed. Zeolite membranes have recently received increasing attention (because of their great potential for use in industrial applications, especially under high temperature conditions) and have been used for gas or liquid-phase separations of non-adsorbing compounds,<sup>[3]</sup> organic/organic,<sup>[4]</sup> permanent gas/vapor,<sup>[5]</sup> and water or polar molecules/organic<sup>[6]</sup> mixtures. Although molecular sieving is mainly invoked to justify the separation of permanent gas mixtures with significant differences in their molecular size, the majority of separations using zeolite membranes can be explained in terms of surface diffusion and, sometimes, capillary condensation.

## CONCLUSIONS

A very simple system can be used with a commercial ceramic membrane of  $\gamma$ -alumina to measure permeances of single gases (*e.g.*,  $N_2$  and He) at several total pressures and temperatures. The experiment gives the student a complete and easy analysis of the permeation measurements in terms of Knudsen transport.

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□

# Discontinuities

Continued from page 25.

$\langle c_{A\gamma} \rangle^\gamma$	intrinsic volume averaged concentration of species A, mole/m <sup>3</sup>
$\tilde{c}_{A\gamma}$	spatial deviation concentration, mole/m <sup>3</sup>
$c_p$	constant pressure heat capacity, J/kgK
$c$	speed of sound, m/s
<b>D</b>	dispersion tensor, m <sup>2</sup> /s
<b>F</b>	force acting on a particle, N
<b>g</b>	gravity vector, m/s <sup>2</sup>
<b>k</b>	thermal conductivity, J/msK
$L_\mu$	viscous length, m
$L_p$	inertial length, m
$L$	length associated with the pressure change, $\Delta p$ , m
$M$	$u_o/c$ , Mach number
$m$	mass of a particle, kg
$n$	number of moles
<b>n</b>	unit normal vector
$\mathbf{n}_{\gamma\sigma}$	unit normal vector directed from the $\gamma$ - phase toward the $\sigma$ - phase
$p$	pressure, N/m <sup>2</sup>
$p_m$	pressure for an incompressible flow, N/m <sup>2</sup>
<b>r</b>	position vector, m
<b>R</b>	gas constant, Nm/mole K
$Re$	$\rho u_o L_\mu / \mu$ , Reynolds number
$R_A$	molar rate of production of species A owing to homogeneous reaction, mole/m <sup>3</sup> s
$R_{A\gamma}$	molar rate of production of species A in the $\gamma$ - phase owing to homogeneous reaction, mole/m <sup>3</sup> s
<b>T</b>	temperature, K
$T_m$	temperature for an incompressible flow, K
<b>t</b>	time, s
$\mathbf{t}_{(n)}$	stress vector, N/m <sup>2</sup>
<b>T</b>	stress tensor, N/m <sup>2</sup>
$u_o$	characteristic velocity, m/s
<b>v</b>	mass average velocity vector, m/s
$\mathbf{v}_m$	velocity for an incompressible flow, m/s
$\mathbf{v}_A$	velocity of species A, m/s
$\mathbf{v}_{A\gamma}$	velocity of species A in the $\gamma$ - phase, m/s
$\mathbf{v}_\gamma$	mass average velocity in the $\gamma$ - phase, m/s
$\langle \mathbf{v}_\gamma \rangle$	superficial mass average velocity in the $\gamma$ - phase, m/s
$\langle \mathbf{v}_\gamma \rangle^\gamma$	intrinsic mass average velocity in the $\gamma$ - phase, m/s
$\tilde{\mathbf{v}}_\gamma$	spatial deviation velocity, m/s
<b>V</b>	volume, m <sup>3</sup>
$\mathcal{V}$	averaging volume, m <sup>3</sup>
$V_\gamma(\mathbf{x}, t)$	volume of the $\gamma$ - phase contained in the averaging volume, m <sup>3</sup>
<b>w</b>	arbitrary velocity, m/s
<b>x</b>	position vector locating the centroid of an averaging volume, m

## Greek Letters

$\varepsilon_\gamma$	$V_\gamma(\mathbf{x}, t)/\mathcal{V}$ , volume fraction of the $\gamma$ - phase
$\lambda$	unit vector
$\mu$	fluid viscosity, Ns/m <sup>2</sup>
$\rho$	mass density, kg/m <sup>3</sup>

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# A JOINT CHEMICAL/ELECTRICAL ENGINEERING COURSE IN ADVANCED DIGITAL PROCESS CONTROL

JOSEPH J. FEELEY, LOUIS L. EDWARDS  
*University of Idaho • Moscow, ID 83843*

This article describes a course in the digital control of industrial processes jointly offered by the Departments of Chemical Engineering and Electrical Engineering at the University of Idaho. The course grew out of a perceived need for engineers with the ability to design multi-input multi-output (MIMO) digital controllers for industrial processes, especially in the pulp and paper industry. Evidence for this need lies in the numerous opportunities for improved process performance offered by advanced multi-variable digital control techniques.

The primary goals of the course are to

- Teach students how to design MIMO controllers for industrial processes
- Give students laboratory experience with representative industrial processes and control systems
- Introduce students to the use of state-of-the-art computer-aided design software for control-system design
- Provide an opportunity for chemical and electrical engineering students to work together in interdisciplinary teams.

The following sections describe how the course attempts to achieve these goals, highlights some of the distinctive features of the course, and discusses some plans for the future.

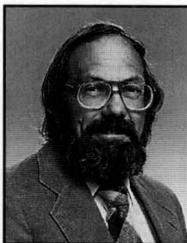
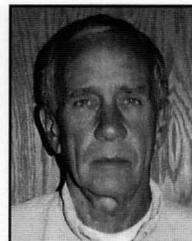
## COURSE DESCRIPTION

Digital Process Control is a three semester-credit hour course jointly offered by the chemical and electrical engineering departments. It is a required course for chemical engineering (ChemE) seniors and an elective course that

satisfies a breadth requirement in the control-systems area for electrical engineering (EE) seniors. ChemE students have previously had a course in chemical process control using classical control-system design methods. The prerequisite for EE students is a junior-level course in signals and systems. Some EE students, however, have had a prior course in classical control-system design as applied, primarily, to electro-mechanical systems. All of the EE students and many of the ChemE students have had a prior course in linear algebra or have had some exposure to vectors and matrices in previous courses.

Computer-aided design is an essential part of the course, and all students have had prior experience with Matlab,<sup>[1]</sup> the main computer program used in the course. The course is taken by about twenty-five ChemE students and fifteen EE students each year and is jointly taught by a faculty member from each department.

**Joseph J. Feeley** is Associate Professor of Electrical Engineering at the University of Idaho. He received his BS from the New Jersey Institute of Technology, and his MS and PhD degrees from the University of Idaho, all in electrical engineering. He is currently writing a textbook on digital process control.



**Louis L. Edwards** has been Professor of Chemical Engineering at the University of Idaho since 1971. He teaches process control and his research focuses on simulation of pulp and paper processes. He has published over fifty papers and has consulted with more than thirty pulp- and paper-related companies worldwide.

The course is organized around three major laboratory experiments of progressive difficulty. Each of the experiments is a laboratory-scale simulation representative of a typical industrial process. The lecture material and the laboratories are coordinated so that when a lecture sequence describing a new design technique is completed, it is followed immediately by a laboratory experiment using that technique.

The choice of an appropriate design method, or methods, for this class is not easy. Current practice in the process control community is focused on some form of internal model control (IMC),<sup>[2,3]</sup> often model predictive control (MPC) or dynamic matrix control (DMC). On the other hand, methods based on the linear quadratic regulator (LQR)<sup>[4]</sup> and its extensions to incorporate state estimation via linear quadratic estimation (LQE), recover stability margins via loop-transfer recovery (LTR), and design for robustness directly through  $H_\infty$  and  $\mu$ -synthesis<sup>[5]</sup> have been more popular in the electro-mechanical control community. The distinctions are not, of course, that clear, and there are many successful LQR applications in the process industry<sup>[6]</sup> and many PID applications in the electro-mechanical area.<sup>[7]</sup>

A compromise, of sorts, has been reached by using the discrete-time version of the linear quadratic regulator (DLQR) as the main design tool used and pointing out the relationships among DLQR, DLQG, PID, and MPC as the occasions arise. DLQR is used because of its generality, the availability of Matlab design tools and the familiarity of most of the students with Matlab, and the simplicity of the resulting control algorithm. Once a suitable process model is developed, the design can be efficiently completed in an interactive computer session using Matlab, Simulink,<sup>[8]</sup> and the Control Systems Toolbox.<sup>[9]</sup> Students quickly learn the relationship between performance index weightings on the one hand and state performance and control effort on the other hand, and are able to find control gains that yield satisfactory system performance.

After an introduction to sampling and development of a discrete-time model, the DLQR method is introduced through a scalar single-input single-output (SISO) example. The example concerns a simple nonlinear process model associated with the liquid-level control problem addressed in the first

laboratory experiment. The model is linearized at an operating point and discretized at a selected sampling rate to form the basis for the controller design. The control problem is presented as an optimization problem, trading off control effort for state performance. The dynamic programming approach is used to develop the Riccati equation, and its steady-state solution is used to find the optimal DLQR gain. By beginning with this scalar example, students get a good understanding of the basic DLQR approach before moving to the multivariable problem, with the additional complexity

of vector-matrix notation, studied later. The effect of state variable feedback in changing the system time constant is also clearly seen in this simple example. Students solve this control problem by hand and then use Matlab to verify their calculations. Simulink is then used to simulate the continuous-time nonlinear process model under DLQR control.

### Experiment 1

The first experiment is a simple water-level control problem that illustrates the application of DLQR state variable feedback control

methods to a first-order system. It allows the chemical engineering students to become familiar with the notion of sampling and digital-control-system hardware and familiarizes the electrical engineering students with the relatively long time scale and nonlinearity of process systems. The relationship of scalar DLQR control to traditional proportional control is pointed out, and the need for integral augmentation to eliminate steady-state error is clearly illustrated. The integrator-augmented DLQR controller is then shown to be equivalent to a traditional PI controller.

### Experiment 2

The second experiment involves a second-order process consisting of two cascaded tanks simulating a bioreactor system. The objective of this experiment is to control the level in the second tank, in spite of disturbances caused by a fluctuating flow from the first tank into the bottom of the second tank. Both tank levels are measured so that full state-feedback can be used. The control input is the position of an outlet valve on the second tank. A schematic of the experimental setup is shown in Figure 1. The system is modeled as a two-state discrete-time SISO process and the vector-matrix form of the state and output equations is introduced. The controller for this process is designed using the integrator-

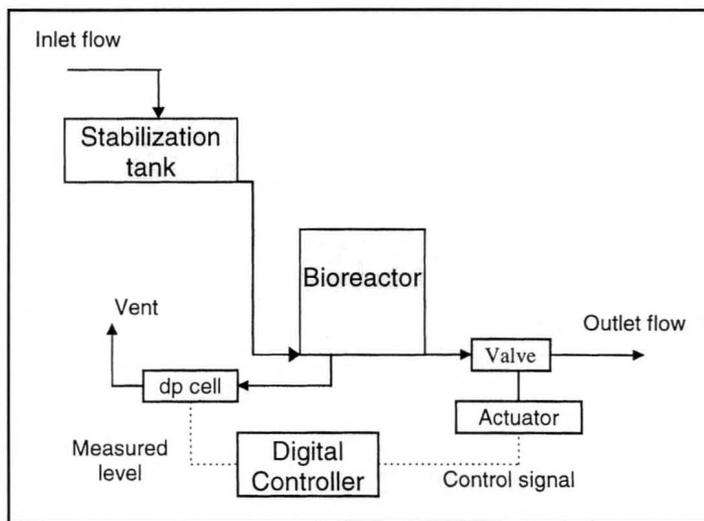


Figure 1. Experiment 2: a simulated bioreactor system consisting of two cascaded tanks.

augmented DLQR method<sup>[10]</sup> extended to accommodate level set-point changes and zero steady-state error. The necessity of using vector-matrix notation and computer-aided design tools begins to become evident to students when solving this relatively simple second-order problem. The relationship of this simple DLQR controller to the classical PID controller is also examined.

### Experiment 3

The third experiment requires the design of a two-input/two-output controller to simultaneously control the water level and total head in a laboratory-scale model of a paper machine head box. A schematic diagram of the process is shown in Figure 2 and details of its construction are available from the second author. Zero steady-state error and set-point control are required for both controlled variables. This is the most challenging of the control problems and involves four states, two inputs, and two outputs. Nevertheless, most students are now familiar with the DLQR design-iteration procedure and are able to complete the controller design with little difficulty. In the laboratory, students are encouraged to attempt this MIMO control manually to fully appreciate the difficulty of the task and the power of the DLQR design method. The control design is carried out on a full state feedback basis.

### COURSE STRUCTURE

Daily homework assignments are focused on the upcoming laboratory experiment. Each assignment addresses a different phase of the design effort, with the last assignment before a given lab producing the controller algorithm required for that experiment.

Student performance is assessed through the homework, two one-hour tests, a two-hour final exam, and reports on each of the laboratory experiments. The lab reports are a crucial part of the course requirements and account for about one-third of the course grade. Lab groups generally consist of three students, two from chemical engineering and one from electrical engineering. Students pick their own lab partners, but "bonus points" are awarded to interdisciplinary lab groups to encourage interaction between the electrical and chemical engineering students. Individual lab reports in the form of a technical memo with supporting appendices are required of each student.

### STUDENT REACTION

Student reaction to the course has been quite favorable. The ability to test controller designs in the laboratory is mentioned by most students as the most positive feature of the course. Many students comment on the power of the computer-aided design tools to facilitate control system design. A smaller number view the computer approach as "magic."

### DISTINCTIVE FEATURES OF THE COURSE

This course includes a number of distinctive features. The most obvious is the combination of chemical and electrical engineering students in a joint class. This helps bridge the disciplinary gap and teaches the students how to work with specialists in another field on challenging interdisciplinary

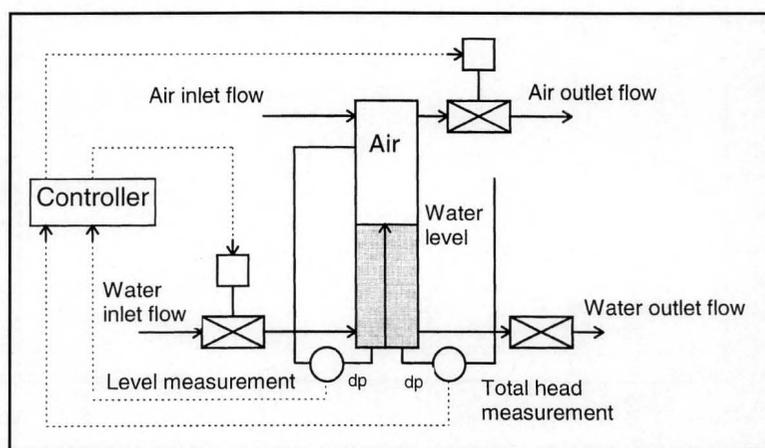


Figure 2. Experiment 3: a laboratory-scale model of a paper-machine headbox.

problems. The student-to-student learning process generally involves the ChemE students teaching the EE students about process dynamics and modeling, while the EE students take the lead on computer and digital controller topics. The fact that the class is jointly taught by a faculty member from each department also gives the students complementary views of a given control or modeling issue. Both instructors attend each class,

with the EE instructor primarily addressing the control theory and design topics and the ChemE instructor focusing on process modeling and the relationship of the labs to actual industrial processes.

A second key feature of the course is that it approaches the digital control-design problem from the "direct digital design" perspective and uses the DLQR design method as the basic design approach. This approach is taken for a number of reasons. First, the DLQR method approaches controller design as an optimization problem, trading off control effort for state performance. This is a crucial concept that is often overlooked, or addressed after the fact, in other design methods. Second, currently available CAD tools, such as Matlab, Simulink, and associated toolboxes, simplify computations so that students can focus on design objectives and not become bogged down in mathematical complexities. Students are taught the advantages of testing controller designs by nonlinear simulations on a desktop computer before trying them out on the actual process. Third, the DLQR approach seems more direct in that a good design can be accomplished almost entirely in the discrete-time domain,

avoiding, for the most part, the complexities introduced by transform mathematics. Finally, we realize that students completing this course will not be experts in DLQR design methods. They will, however, have had a practical introduction to the topic that will alert them to the power and potential of advanced control techniques. They will also be aware of some of the relationships among three control methods representative of the electro-mechanical, process, and traditional control communities, *i.e.*, DLQR, MPC, and PID.

The final important aspect of the course is the laboratories and their integration with the lecture material. In a sense, the course is driven by the laboratory experiments and the students are motivated to master the lecture material so that they can perform the laboratory experiments satisfactorily. Homework assignments are carefully chosen so that satisfactory completion of the last assignment before a lab should fully prepare the student to carry out the experiment properly.

### PLANS FOR FUTURE DEVELOPMENT

A number of plans are underway for further development of the course. New laboratory experiments are always under consideration. We plan to include an experiment involving system identification to develop an empirical model of the headbox process next year. Longer-range plans include adding a third input and a third output to the headbox experiment and developing a new experiment using a distillation column as the process to be controlled. The lecture material is also being continually refined and updated to find more logical and consistent ways to introduce this relatively advanced material to students at this stage in their development. More emphasis will be given to IMC methods such as MPC and DMC in future versions of the course. The course notes currently being used as the course text are being readied for publication and should be submitted to a publisher this year.

### ACKNOWLEDGMENT

The authors are very grateful to Barry King for constructing and maintaining the laboratory experiments and for his assistance with the students in the laboratory.

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## BOOK REVIEW: *Numeric Computation*

*Continued from page 11.*

The next three chapters are devoted to function interpolation and differentiation (Chapter 6), numerical integration (Chapter 7), and approximation of functions, lines, and surfaces (Chapter 8). In the final chapters, the author discusses the solution of ordinary differential equations and initial value problems (Chapter 9), boundary-value, eigenvalue, and free-boundary problems (Chapter 10), and finite-difference methods for partial differential equations (Chapter 11).

Finally, the author provides four appendices. In Appendix A, he provides a brief calculus refresher, with a table of various series approximations to a variety of functions. In Appendix B, he discusses orthogonal polynomials. Again, he includes a number of tables of various orthogonal polynomials, including Legendre, Chebyshev, Jacobi, Radau, Lobatto Laguerre, Hermite, and Gram, and their properties.

Developing the ability to proficiently use the computer and interface with the operating system is one of the main hurdles often encountered by students in a numerical methods course. Appendix C provides this essential background information, including an introduction to the c-shell, to the unix file system, to the vi editor, and to the compilation and linking of typical programs. Finally, Appendix D provides a Fortran primer, while an index to the publicly available programs discussed above is provided in Appendix E.

Although they are covered briefly in Chapter 10, I would have liked additional coverage of weighted residual techniques. These methods provide a powerful tool for the solution of ordinary differential equations and provide the basis of finite element methods for the solution of partial differential equations. In devoting only seventeen pages to this topic, the author has given the students only a brief glimpse of the power of such methods and may leave students thinking that they are not as useful as others that are covered in much more detail. Further, as is often the case, the coverage of techniques for solving partial differential equations is quite limited. I assume that this is because the author expects this materials to be covered in a later course.

In general, Pozrikidis has met his goals and has produced a usable text in which he covers the fundamentals of numerical methods, while at the same time enabling the reader to understand how to use the various techniques to solve physical problems in science and engineering. □

# INTRODUCING PROCESS-DESIGN ELEMENTS IN THE UNIT OPERATIONS LAB

CHRISTINE L. McCALLUM, L. ANTONIO ESTÉVEZ\*  
Cornell University • Ithaca, NY 14853-5201

One of the main problems of the classical chemical engineering or unit operations laboratory is the danger of its becoming repetitive and boring. This paper will address that problem and show how a simple laboratory experiment can be turned into an interesting experience for both the students and the instructor by giving it a slight flavor of process design. This was accomplished by adding to the requirements of the final lab report the solution of a design problem related to the experiment done in the lab. The problem combined scale-up elements and changes to the material's chemical nature, or to the physical characteristics of the laboratory setup.

This paper describes our approach to a classical stripping experiment where air was used to remove toluene from water in a packed column. Although the approach is described in the context of this specific experiment, it can be applied to any classical experiment.

## THE UNIT OPERATIONS LAB AT CORNELL

To better understand the approach presented in this paper, we will first give a brief description of how our lab is organized. The senior class is divided into five groups (Monday, Tuesday, Wednesday, Thursday, and Friday), with four teams in each group. Six experiments are carried out in four rotations. During the first week, all groups work on a short, introductory experiment. Then the first rotation starts on the second week and lasts four weeks, as do all rotations: a rotation involves preparation, experiments (2 weeks), and a report. (The report on one rotation and the preparation in next rotation may overlap.) Two shorter experiments are done in one rotation. The stripping experiment (described in this paper) is done in one full rotation. The Unit Operations Laboratory at Cornell has a page on the world

\* Present Address: University of Puerto Rico, Mayagüez, Puerto Rico 00681-9046

wide web, currently at

<http://speedrcr.cheme.cornell.edu/Uo/>

that can be consulted for additional details on the course organization.

## ABOUT THE EXPERIMENT

The essence of this experiment is to remove a trace amount of pollutant (a volatile organic compound) from water by stripping it with air. The experimental apparatus and basic operating procedure are as follows.

**Apparatus** • In this experiment, air and a toluene-contaminated water stream are brought into counter-current contact in a stripping column. The experimental apparatus is shown in Figure 1. The column is 15 cm (0.5') in diameter, packed with 5/8" plastic Pall rings. The approximate packing height is 1.15 m (3.75'). A 0.5-m<sup>3</sup> (135-gal) tank with an electric mixer is used to homogenize the feed supply. Rotameters are used to read liquid and air-flow rates, and the thermocouples are used to read tank and column temperatures. The liquid feed flows by gravity at low flow rates and is driven by a centrifugal pump at higher flow rates. Samples are collected at the water-stream inlet and outlet and analyzed using a Gow-Mac gas chromatograph equipped with a flame ionization detector and Spectra-Physics integrator.

**Christine L. McCallum** received her MS in chemical engineering at Cornell University, where she conducted research in the area of molecular simulation and thermodynamics. She received her BS from Bucknell University, also in chemical engineering. She currently works for Intel Corporation in Phoenix, Arizona.

**L. Antonio Estévez** received his PhD from the University of California, Davis. He holds a BS degree from the University of Santiago, Chile, and a MS from the Central University of Venezuela. He has been on the faculty of the University of Puerto Rico since 1987, having previously taught at the University of Santiago, Chile, and the Simón Bolívar University in Caracas. He was on sabbatical leave at Cornell University during the academic year 1996-97. His research interests are supercritical fluids, separation processes, and multiphase reactors.

**Procedure** • The toluene/water feed is prepared at least one hour before the lab begins by filling the feed tank with water and adding an amount of toluene to produce the desired concentration. The mixer runs until the lab period begins. After verifying proper valve settings, air is allowed to flow through the system by opening valve V4, and its flow rate is regulated with valve V3. The water is then introduced by opening valve V2. A water seal is maintained by keeping the water depth at the bottom of the column within 3 to 5 cm. Steady-state conditions are reached after about five minutes. Water samples are collected at ports S1 and S2 (drain pipe) in glass vials. Corks wrapped with aluminum foil are used to seal the samples, which are then labeled and stored on ice. The samples are analyzed using the gas chromatograph. Pressure drop, gauge pressure at the bottom of the column, and column temperature are also measured.

## THE NEW APPROACH

As explained previously, the students have four weeks to complete the experiment and submit a final report. In the first week, the TA meets with the group for a brief explanation of the experiment's objectives and operation of the apparatus. A memo with the requirements is distributed at this

***This paper presents a simple way to enhance the learning experience in the unit operations laboratory by adding a related design problem to the lab requirements.***

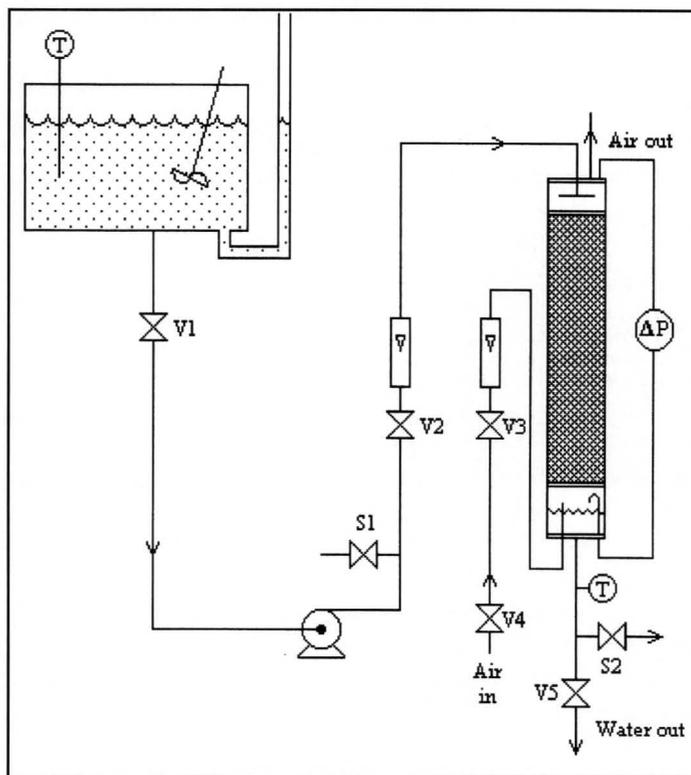


Figure 1. Apparatus for the stripping experiment.

**TABLE 1**  
Design Problem

Clearwaters and Associates is a company that produces bottled drinking water on a large scale. In their process they chlorinate their source using standard processes, and therefore the level of chloroform (and of other trihalomethanes, THMs) goes beyond specifications. They are considering reducing the THM level by stripping with air in a packed column. The water after chlorination may contain up to 400 ppb (by mole) of THM, 30% of which is chloroform, 70% bromodichloromethane, and negligible amounts of bromoform and dibromochloromethane. Their typical daily production is about 60,000 5-gal bottles. As the engineering team of Clearwaters and Associates your assignment is to design the THM-removal system using stripping. They plan to use a column packed with 5/8" plastic Pall rings. The final THM level must be less than 50 ppb (by mole). Typically, the operation will take place at 77°F.

meeting. The students are also referred to the experiment's reference manual, which is available on the world wide web at <http://cheme.cornell.edu/~lae/432/stripping.htm>.

Using the traditional approach, the students would figure out what variables to measure to determine the overall mass-transfer coefficient and would probably present some plots showing the effect of, say, flow rates on mass-transfer coefficient and on the height of a transfer unit. With this new approach, the students must also solve a design problem and include the solution in their final lab report. In this particular design problem, the students use the information collected in the lab to compute the height of the column. In addition to scale-up, they must also consider a difference in the chemical composition/nature of the inlet stream or the size/type of the column packing. The students need to determine whether or not that difference is important, and if so, how to account for it.

## A SAMPLE DESIGN PROBLEM

Table 1 shows a sample design problem given to the students in one of the fall 1996 rotations. Each team was responsible for providing a final design for the company. This task required determination of the packing height and the column diameter. The students were given guidelines to help achieve this goal, and in this particular case they were referred to Velázquez and

Estévez<sup>[1]</sup> to find the needed THM's properties. Additionally, they were asked to submit three pieces of documentation: a pre-experimentation memo, a preliminary-calculations memo, and a final report. Each of these parts had a specific objective and helped break up the student workload during the four-week lab period. The three parts are discussed in detail in the following section.

## REPORTING REQUIREMENTS

### *Pre-Experimentation Memo*

To help meet the final objectives of the design problem, the students were asked to first prepare an experimental plan, including a factorial design of experiments, to measure the mass-transfer coefficients and the height of a transfer unit in the laboratory. The plan was to be submitted to the TA in a short memo at least two days before the day the experiment was to begin. The next day, a copy of the memo would be returned to the team with comments.

Some of the questions to be answered in this memo were: What is the problem being addressed? What variables will be measured? Which flow rates will be run? How much toluene is needed to prepare the feed solution? What procedure will be followed? What calculations will be performed? How will the results be presented?

The pre-experimentation memo was an important part of the lab, as it required the team to become familiar with the apparatus and to carefully plan the experiment. The group also needed to figure out how to do the necessary calculations ahead of time so they could record all the relevant data.

### *Preliminary Calculations*

On the second lab day, each team had to submit calculations of the height of a transfer unit and the mass-transfer coefficient for each experimental point taken on the first lab day. Results had to be presented in a short memo (2 or 3 pages) along with a table showing  $L$  and  $V$  in lab units, and  $G_x$ ,  $G_y$ ,  $m$ ,  $S$ ,  $x_a/x_b$ ,  $N_{Ox}$ ,  $H_{Ox}$ , and  $K_x a$  in SI units. A brief description of the procedure that would be used to solve the design problem also had to be included in the memo.

In the preliminary-calculations memo, the students had to use the actual data they collected on the first lab day. At this point, they will realize if they are doing something wrong, or if they have failed to measure a variable they need (e.g., atmospheric pressure, column temperature). This also takes part of the load of writing the lab report from the last week and spreads out report writing over two weeks rather than just one.

### *Final Report*

In addition to the traditional final lab report components, the students were asked to use a correlation for their data of the form

$$K_x a = \psi G_x^\alpha G_y^\beta \quad (1)$$

where  $\psi$ ,  $\alpha$ , and  $\beta$  are constants. To find these constants, they used the linear-regression option of any standard spreadsheet, with three contiguous columns containing  $\log K_x a$ ,  $\log G_x$ , and  $\log G_y$ . Each team also had to prepare a plot of the height of an overall transfer unit and the overall mass-transfer coefficient versus the liquid mass velocity (liquid mass flow rate per unit cross-sectional area) at various gas mass velocities. Experimental results, and the values predicted by Eq. (1) must also be included. Finally, the students had to prepare a parity plot with their results. This is a plot of the experimental  $K_x a$  (or  $H_{Ox}$ ) versus the values computed by Eq. (1). Included as a reference were the diagonal line and constant-error lines (e.g., +5% and -5% lines).

The solution to the design problem was to be discussed in a separate section of the laboratory report. Using the correlations proposed in the earlier section of the report, duly corrected for chloroform and bromodichloromethane, the required packing height and column diameter (for a gas-flow rate equivalent to 1.6 times the minimum gas-flow rate) had to be computed. In the calculation of the diameter, a gas-flow rate equivalent to 50% of the flooding value should be used. After performing all the calculations, the team had to report on the recommended design and the criterion or criteria they used.

A company-type format of about ten pages was suggested for the final report. This required the students to evaluate the process by which they used actual lab data to solve an industrial design problem and to justify their final design proposal.

## RESULTS OF THE EXPERIMENTS

We found it interesting to present the results of this experiment. Although this is not directly related to the main objective of the paper, we realized that correlations for these types of systems are less abundant than originally thought. To present the results in a compact manner, all the data collected during the course of the semester (four rotations, 219 points) were consolidated in a single spreadsheet. Then, a correlation of the form suggested above in Eq. (1) was obtained. The result was

$$K_x a = 8.7 G_x^{0.778} G_y^{-0.05} \quad (2)$$

The correlation coefficient ( $R^2$ ) for this fit was 0.908. With Eq. (2), a parity plot was prepared to show the goodness of fit for the correlation obtained (shown in Figure 2). In a parity plot, the points should align along the diagonal, which represents the perfect fit. Although the exponent for  $G_y$  is small, its standard error determined that it is statistically significant.

## ON THE SOLUTION OF THE DESIGN PROBLEM

The design problem presented here requires the computation of mass-transfer coefficients for trihalomethanes in a system similar to the one used in the lab. The calculation of the packing height and column diameter is relatively straightforward. If the data obtained for toluene are used, however, the students have to determine how to correct for the fact that the solutes in the lab and in the problem are different. To stimulate creativity, no guidelines were given on how to approach this aspect of the problem. Perhaps the most elegant way to do this is to obtain a dimensionless correlation to fit the experimental data, *i.e.*,

$$Sh_{Ox} = \phi Re_x^\alpha Re_y^\beta Sc_x^\gamma \quad (3)$$

The exponent for  $Sc$  cannot be obtained from the experimental data since only one solute is used. A value taken from the literature can be used instead. The students can determine the exponents  $\alpha$  and  $\beta$  from the experimental data and then use the correlation to obtain the mass-transfer coefficient for the design problem. The five groups in this rotation used a similar, but somewhat lengthier, approach. They took a dimensionless correlation from the literature<sup>[2]</sup> and used it to figure out a "corrected" value of  $\psi$  in Eq. (1) (one for chloroform and one for dichlorobromomethane). Then they used the "corrected" Eq. (1) for the corresponding trihalomethane. The important thing here is that all the groups could find their way in solving the problem correctly. This contributes more to the learning process than guiding them through a solution that could be more to the instructor's liking.

## OTHER DESIGN PROBLEMS

During the fall 1996 semester, we prepared four design problems, one for each rotation. The goal was to encourage independent thinking about how to use a routine lab experiment to solve a real-life problem. To provide some ideas of how this approach can be implemented, we highlight here the main features of the other three problems.

- **Problem 1.** Here the students were asked to design a

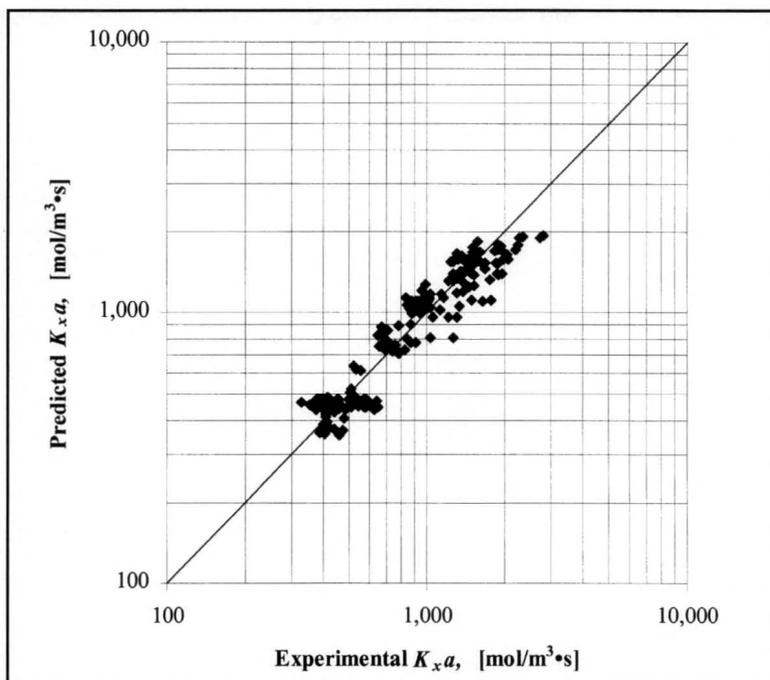


Figure 2. Parity plot for the mass-transfer coefficient.

stripping system to remove toluene from a wastewater stream. The packing available was 1.5" Pall rings. Gas flow rate to be used was 1.5 times the minimum value. The students had to figure out how to correct for the different packing size.

- **Problem 2.** Additionally, the students had to find the value gas-flow rate (relative to the minimum value) that minimized the amount of packing in the column.
- **Problem 3.** Similar to the problem presented *in extenso*, but with just one trihalomethane (chloroform).

## STUDENT FEEDBACK

No formal specific survey to explore the students' impression of the approach was conducted because the idea of writing this paper came after the term was over. But a three-page course-evaluation questionnaire was distributed to give the students an opportunity to comment generally on the course. One of the questions was, "Please comment on each experiment in terms of its value as a chemical engineering learning experience." We also informally asked some students what they thought of the new approach. The feedback was highly positive. The most praised fact was the opportunity to connect an isolated lab experiment with a real-world problem.

Some of the actual responses were:

- "This was the most valuable learning experience. I got a lot out of it in terms of learning what it takes to design a real column..."
- "I really like this lab. It was complicated, but not impossible. Overall, I learned a lot."
- "I liked this experiment. The lab itself is simple, but understanding and utilizing the data is very complex."
- "Of all the experiments, I feel that this one was the one I learned the most in."
- "Good learning experience in terms of scale-up design."

## CONCLUSIONS

This paper presents a simple way to enhance the learning experience in the unit operations laboratory by adding a related design problem to the lab requirements. This idea can be implemented in any classical unit operations experiment such as distillation, absorption, liquid-liquid extraction, or even in a heat-exchanger experiment.

By implementing this approach, the students connect lab work to real-life problems, their creativity is stimulated, and the concepts are learned enduringly. The feedback from the students confirms this. It is apparent that they felt more comfortable the following term when they had to apply these concepts to design absorption, stripping, and even distillation columns as part of the task in the senior design course.

## NOMENCLATURE

$a$	gas-liquid interfacial area per unit total volume [ $\text{m}^2/\text{m}^3$ ]
$G_x$	liquid-phase flow rate per unit cross-sectional surface area [m]
$G_y$	gas-phase flow rate per unit cross-sectional surface area [m]
$H_{OL}$	height of an overall transfer unit based on liquid-phase concentrations [m]

$K_x$	overall mass-transfer coefficient [m/s]
$L$	liquid-phase flow rate [kg/s]
$m$	Henry's constant expressed as a ratio of mole fractions
$N_{Ox}$	number of overall transfer units based on liquid-phase concentrations
$Re_x$	liquid-phase Reynolds number
$Re_y$	gas-phase Reynolds number
$S$	stripping (desorption) factor
$Sc_x$	liquid-phase Schmidt number
$Sh_{Ox}$	liquid-phase Sherwood number based on $K_L$
$V$	gas-phase flow rate [kg/s]
$x_a$	mole fraction of solute in the liquid phase at the inlet
$x_b$	mole fraction of solute in the liquid phase at the outlet

### Greek Symbols

$\alpha$	exponent in Eqs. (1) and (3)
$\beta$	exponent in Eqs. (1) and (3)
$\gamma$	exponent in Eq. (3)
$\phi$	coefficient in Eq. (3)
$\psi$	coefficient in Eq. (1)

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## Ethanol Fermentation

Continued from page 57.

experiments of ethanol fermentation dispensed with the distillation of the sample and the chemical analysis of ethanol. The experimental data obtained in the assays allowed fits of a simple kinetic model (Monod) and of one that takes into account the inhibition by the product.<sup>[3]</sup> Comparison of the kinetic parameters obtained in the present work with others in the literature showed that the experimental device has attained the expected aim.

## NOMENCLATURE

$D$	internal diameter of the PVC pipe [ $D=10$ cm]
$K_p$	product inhibition constant [ $\text{gL}^{-1}$ ]
$K_S$	saturation constant [ $\text{gL}^{-1}$ ]
$M_{\text{ethanol}}$	ethanol molecular weight [ $M_{\text{ethanol}}=46$ ]
$n_{\text{CO}_2}$	number of moles of ethanol formed
$n_i$	number of moles of $\text{CO}_2$ evolved at time $t=i$
$P$	product concentration [ $\text{gL}^{-1}$ ]
$P_{\text{atm}}$	local atmospheric pressure or barometric pressure [atm]
$R$	gas constant [ $R=82.04$ atm $\text{cm}^3/(\text{g-mole K})$ ]
$R^2$	regression coefficient [-]
$S$	limiting substrate concentration [ $\text{gL}^{-1}$ ]
$T$	gas temperature [K]
$t$	time [h]
$V$	broth's volume [L]
$V_i$	gas volume at time $t=i$ [mL or $\text{cm}^3$ ]
$X$	cellular concentration [ $\text{gL}^{-1}$ ]
$y_0$	distance from top of PVC tube to water level at $t=0$ [cm]

$y_i$	distance from top of PVC tube to water level at $t=i$ [cm]
$Y_{X/S}$	cell yield coefficient [ $\text{gg}^{-1}$ ]
$Y_{P/S}$	product yield coefficient [ $\text{gg}^{-1}$ ]

### Greek

$\mu$	specific growth rate [ $\text{h}^{-1}$ ]
$\mu_{\text{max}}$	maximum specific growth rate [ $\text{h}^{-1}$ ]

### Subscripts

0	refers to the time $t=0$
i	refers to the time $t=i$

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## Microwave Drying

Continued from page 49.

temperatures show trends similar to the drying-rate curves (see Figure 6). The temperature profiles demonstrate the warming-up period, a constant-temperature period, as well as a rapid falling-off period. Due to the difficult nature of temperature measurement in microwave drying, these data are applicable only for representing trends in the temperature profile. It should be noted that the surface-temperature values of Figure 6 did not reach 100°C, the boiling point of water at atmospheric pressure. This can be accounted for by the effect of surface evaporation<sup>[5]</sup> and by the measurement technique that allowed for some cooling of the sample upon removal from the microwave. In general, during microwave drying, the surface temperature falls between the wet-bulb temperature in the oven and the boiling temperature.<sup>[4]</sup> Our microwave oven was not equipped with a carousel, and given the uneven nature of the energy field in a microwave oven, the temperature probably varied with position. We did not study this phenomenon, however, and only measured the surface temperature near the middle of the sample.

- Students can be asked to design an experiment that illustrates that mass transport effects are responsible for the falling-rate period. Evaporation of water with no solid present can be used to do this. In this instance, the falling-rate period is eliminated, with the constant-drying-rate period ending abruptly as the last of the water is evaporated.
- Particle-size effects can be examined by using sand that has been sifted into different particle sizes. Critical moisture content increases with decreasing particle size since smaller particles pack closer together, slowing the movement of moisture to the surface.<sup>[4]</sup>
- Datta<sup>[5]</sup> states that geometry plays a role in microwave processing. This effect can be explored by changing the shapes of the containers and the thickness of the bed height while maintaining a constant mass.
- The analysis presented here does not yield detailed information about the fundamental mechanisms of heat and mass transfer during the drying process. It is possible, however, to estimate interphase heat and mass transfer coefficients and effective liquid diffusivities using methods presented in the literature.<sup>[4]</sup> Also, complex mathematical models of the drying process have been developed.<sup>[9]</sup>
- Drying characteristics of different materials can be compared. Various materials have been used in our laboratory, including calcium carbonate, sponges, bread, and fruit.

## CONCLUSIONS

This experiment demonstrates the drying process effectively. It is an extremely flexible, safe, and inexpensive experiment that can be incorporated into the undergraduate laboratory curriculum. The experiment is easy to set up and run. Typically, meaningful experimental data for higher power

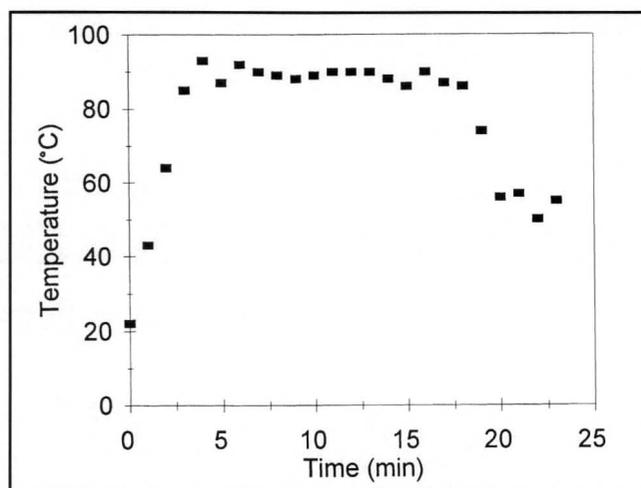


Figure 6. Surface temperature profile for a power level of 720 W.

settings can be collected in about thirty minutes. This experiment also involves data analysis that introduces students to the various methods of treating data and the errors associated with each method.

## ACKNOWLEDGMENTS

We would like to thank the reviewers of this paper for their positive comments and pertinent suggestions that improved it.

## NOMENCLATURE

- i index for numerical differentiation (unitless)
- m mass of liquid (kilograms)
- $m_s$  mass of solid (kilograms)
- t time (minutes)
- $t_0$  time of first data point (minutes)
- $t_n$  time of last data point (minutes)

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# RANKING GRADUATE PROGRAMS

## *Alternative Measures of Quality*

JOHN C. ANGUS, ROBERT V. EDWARDS, BRIAN D. SCHULTZ  
*Case Western Reserve University • Cleveland, OH 44106-7217*

Assessing the relative quality of graduate programs is of great interest to policy makers, academic administrators, prospective students, employers of graduates, alumni, and the general public. Rankings by federal advisory panels<sup>[1]</sup> and the popular press<sup>[2]</sup> are widely quoted, but despite the importance assigned to the rankings, there has been little critical, detailed analysis of their relevance and accuracy. In this paper we will present an analysis of the most prominent of these reports,<sup>[1]</sup> especially as it relates to chemical engineering programs. Although our discussion is confined to chemical engineering, we believe that the general conclusions and methods are also relevant to the other engineering disciplines.

The National Research Council (NRC) in 1995 released a massive study<sup>[1]</sup> of research doctorate programs in the U.S. It was the product of a committee of eighteen academics from

various disciplines and is a follow-on study of a similar report issued in 1982. The report contains reputational rankings, based on a survey of graduate faculty, as well as an impressive amount of factual data from several independent sources. Unfortunately, most attention has been focused on the survey results—in particular the reputational ranking based on perceived faculty quality. This is apparently due, at least in part, to the method by which the data were displayed in the report and the normal tendency to simplify complex data sets into a single, easily understood, quality index.

Several aspects of the NRC report have caused concern. (See, for example, the summary article by Mervis.<sup>[3]</sup>) One striking feature of the results, noted by the authors, was the “remarkable stability among programs rated in the top and bottom quarter” between the 1982 and 1995 reports. Another striking feature was the heavy reliance on the survey

### *Editorial Comment . . .*

A strength of the engineering education system in the United States is its diversity. It is evident in such characteristics as student demographics, college missions and sources of funding, enrollment levels, research strengths, collaborations, and curricula. A positive outcome of our system is the diverse pool of graduates produced to meet the varied and dynamic workforce needs of the world. Choices, however, are being made that can significantly impact programs. Industry selects schools for recruiting visits; students commit to pursue graduate or undergraduate degrees at specific schools, and private and public foundations and agencies award grants, contracts and gifts to selected institutions. The perceived quality of an institution is often an important factor in these decisions, and rankings by institution, college, or degree program contribute to defining perceptions.

In recent years, chemical engineering departments have been asked to assess the quality of their programs to direct improvement strategies. This movement is being driven internally as well as externally by regional and national accreditation entities and by funding agencies (e.g., state governments). Ideally, rankings would directly assess the quality of graduates and the improvement in students while they were enrolled. Since no method to do this has been devised, ranking schemes typically use a combination of numerical program data and peer ranking to determine a score instead of doing a direct assessment. Although the efficacy of this approach is still being debated, it has increased the importance of peer comparison and the availability of program data. This issue of *CEE* presents a paper by Angus, Edwards, and Schultz that proposes alternative measures of graduate program quality. Not surprisingly, an extensive review process revealed that the subject of rankings is a

contentious issue. The reviewers as well as the authors identified many of the shortfalls in assessing the quality of something as complex, multidimensional, and subjective as graduate programs. Identified issues included the establishment of false goals, for example publishing papers in smaller segments or of lesser quality, or hiring faculty in publication-intensive research areas simply to increase the publication count, all of which would increase ranking but could likely decrease program quality. Another issue was that inaccurate or inappropriate data would undermine the conclusions. Examples include the counting of non-competitive research funding (e.g., state funding) and the use of a limited set of journals for citation searching or a limited set of societies in award counting that would not recognize programs with an emphasis on emerging research areas.

This paper presents a sound analysis of the recent NRC ranking, and many of the conclusions as well as the analytical approach can be extended to other ranking schemes. Although the proposed alternative measures of quality may be open to criticism, the authors clearly show the sensitivity of rank order to the selected set of measures and to weighting algorithms (e.g., intensive vs. extensive). We hope that this paper will increase awareness of the shortfalls of any approach to ranking and help one gauge what can and cannot be ascertained from a ranking. We do not believe that a composite index can be developed to accurately measure the relative quality of chemical engineering degree programs in our complex graduate education system, nor is it desirable to drive programs to conformity. We recognize, however, that ranking schemes have increased their presence in our profession and to ignore their impact would be a mistake. We hope that this article will stimulate serious discussion in the community. □

results, which were used to generate reputational rankings rather than "quantitative" measures of quality. Another concern, quite apparent to engineers and scientists, was the minimal distinction drawn between intensive (size independent) and extensive (size dependent) measures of quality. Although the report included a number of statistical tests of the data, no detailed analysis of sources of error in the data sets was provided. Finally, there was no assessment of program quality based on student outcomes in their subsequent professional life. The committee was

aware of many of these concerns and, in fact, was unable to address some of them for lack of time and resources. The committee was also aware that the report might be used in superficial ways that were not intended.

The NRC report is being used by deans, legislators, and foundations in the allocation of resources and in other critical decisions. It is therefore useful to understand the report and to critically examine its conclusions. In this paper we will give an analysis of the data for the chemical engineering programs covered in the report. We will also give alternative rankings using data from the NRC report and other sources. *We emphasize that the rankings presented here are meant only to illustrate the methods employed and to reach general conclusions. Because of limitations in the data available to us, the position of a particular individual program in the rankings should be treated with caution.*

**TABLE 1**  
**Survey Questions Used for the NRC Report<sup>(1)</sup>**

**B1 Familiarity with work of Program Faculty**

1. \_\_\_ Considerable familiarity
2. \_\_\_ Some familiarity
3. \_\_\_ Little or no familiarity

**B2 Scholarly Quality of Program Faculty**

1. \_\_\_ Distinguished
2. \_\_\_ Strong
3. \_\_\_ Good
4. \_\_\_ Adequate
5. \_\_\_ Marginal
6. \_\_\_ Not sufficient for doctoral education
- 
9. \_\_\_ Don't know well enough to evaluate

**B3. Familiarity with Graduates of this Program**

1. \_\_\_ Considerable familiarity
2. \_\_\_ Some familiarity
3. \_\_\_ Little or no familiarity

**B4 Effectiveness of Program in Educating Research Scholars/Scientists**

1. \_\_\_ Extremely effective
2. \_\_\_ Reasonable effective
3. \_\_\_ Minimally effective
4. \_\_\_ Not effective
- 
9. \_\_\_ Don't know well enough to evaluate

**B5 Change in Program Quality in Last Five Years**

1. \_\_\_ Better than five years ago
2. \_\_\_ Little or no change in the last five years
3. \_\_\_ Poorer than five years ago
- 
9. Don't know well enough to evaluate

**PART 1**  
**THE NATIONAL RESEARCH COUNCIL REPORT**

**Methods** • The most discussed part of the NRC report is the faculty survey conducted in 1993. Questionnaires were sent to randomly selected faculty and each participant was asked to rank approximately fifty programs. Other than a list of faculty, the participants were provided no other information about the programs. The survey questions are shown in Table 1.

Forty-one graduate fields of study were covered in the NRC report, one of which was chemical engineering. For chemical engineering programs, 206 usable responses were obtained from 361 questionnaires, a 57% response rate. Within chemical engineering, 93 of the 121 engineering departments awarding PhD degrees during the 1986-92 time period were included. These 93 departments produced 96% of the chemical engineering PhDs awarded during that period.

The results of the survey were tabulated in the Appendices to the NRC report. The programs were listed in order in the tables according to the results of the first survey question (the average ranking of faculty quality). This procedure was used in response to complaints that data in the 1982 report were difficult to interpret because programs were listed alphabetically. The result, however, has been to focus on this one single measure of quality, despite the fact that rankings in the other categories (e.g., program effectiveness and visibility) are also provided in the report.

One of the purposes of the committee that compiled the 1995 NRC Report was to expand the "objective" measures developed by prior committees. Some program statistics were provided: number of faculty, number of PhDs granted, number of PhDs awarded to female and minority students and non-citizens, and the average length of time to receive a PhD. Quantitative measures of quality were also provided: 1) percentage of faculty with research support (%SUPP), 2) percentage of faculty publishing during 1986-92 (%PUB), 3) total publications during 1986-92 (PUB), and 4) total citations to published work during 1986-92 (TC). The latter two were also reported on an intensive (normalized per faculty) basis, i.e., PUB/TF and TC/TF (see Table 2 for a description of

**John C. Angus** is Professor of Chemical Engineering at Case Western Reserve University. He received his BS, MS, and PhD degrees from the University of Michigan. He worked on thermoelectric materials at the 3M Company for three years before joining the faculty at Case. He has worked on the growth of diamond by chemical vapor deposition and various electrochemical problems for almost forty years.

**Robert V. Edwards** received his PhD from Johns Hopkins University in 1968 and took a post-doctoral position at Case Western Reserve University to work on the then-new field of laser light scattering for transport measurements. He joined the Case faculty in 1970 and has subsequently made numerous contributions to the theory and practice of laser light scattering with collaborators, both here and abroad.

**Brian D. Schultz** obtained his BS in chemical engineering from Case Western Reserve University in 1977. He won a National Science Foundation Fellowship, which he used to pursue his Master's degree at Case, and in the fall of 1998, he began working toward his PhD at the University of Minnesota. Research interests include ternary phase diagrams for low-pressure crystal growth as well as the thermochemical behavior of group III nitrides.

the terms in the NRC report).

**Survey Results** • In Table 3 we give the acronyms used in subsequent tables for identification of universities, and in Table 4 we list the graduate programs in chemical engineering as they were rank-ordered by perceived faculty quality (93Q) in the NRC report. This is the order in which the programs are listed in Appendix P of the NRC report.

A striking, but not widely appreciated, feature of the NRC report is shown in Figure 1,<sup>\*</sup> which is a plot of the survey results for faculty quality (93Q) versus program effectiveness (93E). A very strong correlation is evident. For example,  $R^2=0.97$  when the data are fit with the equality  $(93Q)=(93E)$ . This strong correlation can arise simply because high-quality faculty will produce effective graduate programs. We believe it is far more likely that the respondents did not discriminate between faculty quality and program effectiveness and treated both questions the same. This strong correlation was noted in the NRC report in Appendix O-8 where a Pearson product-moment correlation coefficient of 0.98 between 93Q and 93E was given for chemical engineering. Similar strong correlations between 93Q and 93E were observed for the

<sup>\*</sup> In Figure 1 and subsequent figures we indicate the square of the degree of correlation by  $R^2$ , the coefficient of determination. The magnitude of  $R^2$  is simply described as the fraction of the raw variance in the data set accounted for by using the fitted equation. The plots and values of  $R^2$  were obtained using an Excel spreadsheet.

**TABLE 2**  
Definition of Terms Used in this Paper

NOTE: In the NRC report, the symbols for the variables referred to both the rank order, and, where applicable, to the average score of the ratings on the scale of 1 to 5. We give both definitions in the list below. The definitions are taken from Appendix P, page 469, and Table 2-4, page 25, of the NRC report. Not all of the categories used in the NRC report were used in this paper. The terms below the dashed line were not used in the NRC report.

93Q	Rank order of "scholarly quality of program faculty." (Average score on a scale of 0 to 5, with 5 representing "Distinguished.")
93E	Rank order of "program effectiveness in educating research scholars and scientists." (Average score on a scale of 0 to 5, with 5 representing "Extremely Effective.")
VIS	Rank order of visibility of the doctoral program (Percentage of the questionnaires that reported some knowledge of the program by an answer other than "Don't know well enough to evaluate" or "Little or no familiarity" to one or more of the five questions.)
TC	Rank order of the total number of citations attributed to program faculty in the period 1988-92. (Total number of citations attributed to program faculty.) Source: Institute of Scientific Information.
C/F	Rank order of the citation density for the program faculty (Total number of citations (TC) divided by the number of program faculty (TF)). Source: Institute of Scientific Information.
PUB	Total number of publications attributed to program faculty for the period 1988-92.
TF	Number of program faculty in fall 1992. NRC Report for calculating PUB/TF and TC/TF; AICHE <sup>(9)</sup> for calculating HON/TF and SUPP/TF.
HON	Number of honors received by faculty. <sup>[6-8]</sup> See text for details
SUPP	Total research support from all sources. Source: National Science Foundation. <sup>[4]</sup>

**TABLE 3**  
Acronyms Used to Identify Universities

ASU	Arizona State University	NEU	Northeastern University	UAZ	University of Arizona	UMOC	University of Missouri-Columbia
AUB	Auburn University	NJIT	New Jersey Inst. of Technology	UCB	University of California-Berkeley	UMOR	University of Missouri-Rolla
BYU	Brigham Young University	NWU	Northwestern University	UCD	University of California-Davis	UMS	University of Mississippi
CIT	California Inst. of Technology	OHU	Ohio University	UCIN	University of Cincinnati	UOK	University of Oklahoma
CLAR	Clarkson University	OKSU	Oklahoma State University	UCLA	Univ. of California-Los Angeles	UPA	University of Pennsylvania
CLMN	Clemson University	ORSU	Oregon State University	UCO	University of Colorado	URI	University of Rhode Island
CMU	Carnegie Mellon University	OSU	Ohio State University	UCSB	Univ of California-Santa Barbara	USC	Univ. of Southern California
COL	Columbia University	PITT	University of Pittsburgh	UCT	University of Connecticut	UTA	University of Texas-Austin
CORN	Cornell University	PLYU	Polytechnic University	UDE	University of Delaware	UTN	Univ. of Tennessee-Knoxville
CSM	Colorado School of Mines	PRU	Princeton University	UFL	University of Florida	UTUL	University of Tulsa
CUNY	CUNY-Grad Sch & Univ Center	PSU	Pennsylvania State University	UH	University of Houston	UUT	University of Utah
CWRU	Case Western Reserve Univ.	PUR	Purdue University	UIA	University of Iowa	UVA	University of Virginia
DUKE	Duke University	RICE	Rice University	UIC	University of Illinois-Chicago	UWA	University of Washington
GIT	Georgia Institute of Technology	ROCH	University of Rochester	UID	University of Idaho	UWI	Univ. of Wisconsin-Madison
IIT	Illinois Institute of Technology	RPI	Rensselaer Polytechnic Institute	UIL	Univ of Illinois,Urbana-Champaign	UWY	University of Wyoming
ISU	Iowa State University	RSU	Rutgers St. Univ-New Brunswick	UKS	University of Kansas	VAND	Vanderbilt University
JHU	Johns Hopkins University	SIT	Stevens Institute of Technology	UKY	University of Kentucky	VPI	Virginia Polytech Inst & State Univ
KSU	Kansas State University	STAN	Stanford University	ULV	University of Louisville	WASU	Washington State University
LEH	Lehigh University	SUNY	State Univ of New York-Buffalo	UMA	Univ. of Massachusetts-Amherst	WPI	Worcester Polytechnic Institute
LSU	Louisiana St. U & A&M College	SYR	Syracuse University	UMD	Univ. of Maryland-College Park	WSU	Wayne State University
MIT	Massachusetts Inst. of Tech.	TAM	Texas A&M University	UME	University of Maine	WU	Washington University
MSU	Michigan State University	TUL	Tulane University	UMI	University of Michigan	WVU	West Virginia University
NCSU	North Carolina State University	UAKR	University of Akron	UMN	University of Minnesota	YALE	Yale University
ND	University of Notre Dame						

other engineering programs. This level of correlation strongly suggests that these two of the five survey questions gave indistinguishable results.

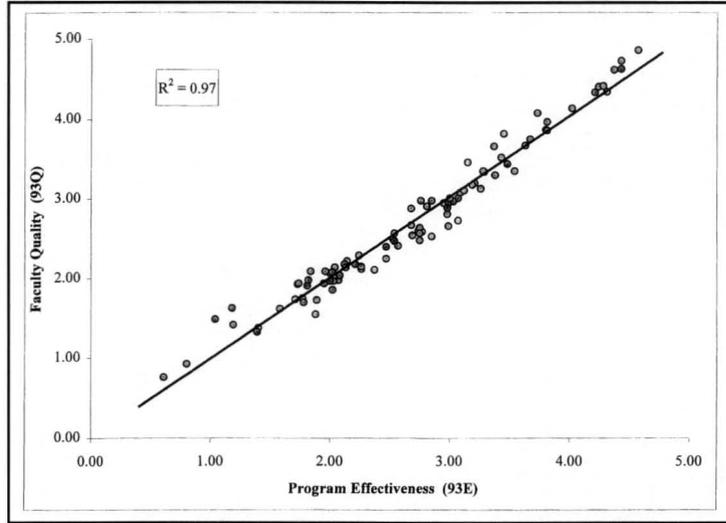
In Figure 2a, we show a plot of perceived

**TABLE 4**  
**Rank Order of ChE Faculty**  
**Quality Survey Results (93Q) Given**  
**in the NRC Report**

Rank	Order	University
1		University of Minnesota
2		Massachusetts Institute of Technology
3		University of California-Berkeley
4		University of Wisconsin-Madison
5		Univ of Illinois, Urbana-Champaign
6		California Institute of Technology
7		Stanford University
8		University of Delaware
9		Princeton University
10		University of Texas at Austin
11		University of Pennsylvania
12		Carnegie Mellon University
13		Cornell University
14		Univ of California-Santa Barbara
15		Northwestern University
16		Purdue University
17		University of Houston
18		University of Michigan
19		CUNY-Grad Sch & Univ Center
20		University of Washington
21.5		Univ of Massachusetts-Amherst
21.5		Rice University
23		Pennsylvania State University
24		University of Notre Dame
25		North Carolina State University
26		University of Colorado
27		Lehigh University
28		University of California-Davis
29		State University of New York-Buffalo
30.5		University of Virginia
30.5		Georgia Institute of Technology
32.5		Yale University
32.5		Iowa State University
34		University of Florida
35.5		Rensselaer Polytechnic Institute
35.5		Johns Hopkins University
37		Texas A&M University
38		Washington University
39		University of California-Los Angeles
40		University of Rochester
41		Ohio State University
42		Virginia Polytech Inst & State Univ
43		Rutgers State Univ.-New Brunswick
44		University of Pittsburgh
45		Michigan State University
46		Case Western Reserve University
47.5		Syracuse University
47.5		Illinois Institute of Technology
49		Clarkson University
50		Brigham Young University

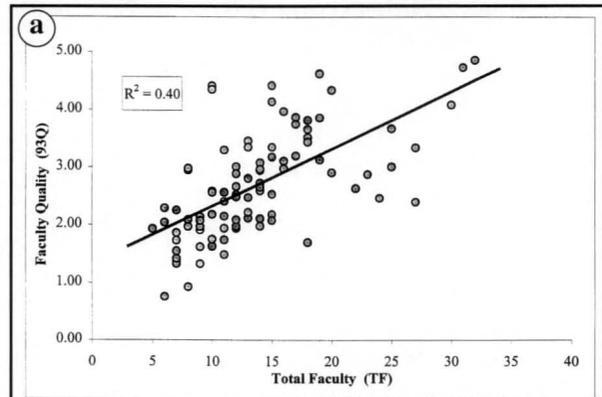
faculty quality (93Q) versus faculty size (TF). The value of  $R^2$  is 0.40, suggesting that the survey results for faculty quality are influenced to some extent by program size, but that other factors are also important.

The program visibility (VIS) was defined as the percentage of respondents who reported some knowledge of the program. In Figure 2b we plot the faculty quality (93Q) versus the visibility (VIS). A strong correlation,  $R^2=0.84$ , is observed. One cannot prove cause-and-effect relationships through correlation alone; however, these results suggest that the perceived faculty quality (93Q) scores arise, at least in part, because respondents rate highly those faculty with

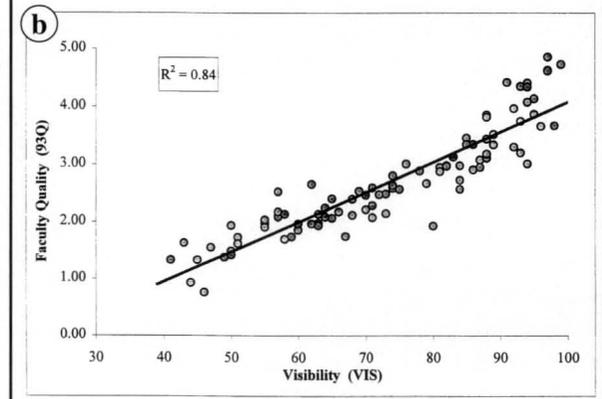


**Figure 1.** Survey results of program effectiveness (93E) versus faculty quality score (93Q).  $R^2=0.97$  when fit with  $(93E)=(93Q)$ .

**Figure 2.**  
**(a)** Survey results of faculty quality (93Q) versus total faculty (TF).  $R^2=0.40$  for linear fit,  $y=mx+b$ .



**(b)** Survey results of faculty quality (93Q) versus visibility (VIS).  $R^2=0.84$  for linear fit,  $y=mx+b$ .



whom they are familiar. If this familiarity arises solely because of the true quality of the faculty, this result is benign; otherwise it is not.

A relatively strong correlation is observed between rank order of visibility and rank order of total citations ( $R^2=0.67$ ), and a weaker correlation between rank order of visibility and total number of faculty ( $R^2=0.39$ ). These results are encouraging because they show that smaller departments can have an impact by virtue of their research output. Significant correlations are also found between perceived faculty quality (93Q) and the number of publications ( $R^2=0.73$ ), number of publications per faculty ( $R^2=0.64$ ), total citations ( $R^2=0.71$ ), and citations per faculty ( $R^2=0.56$ ).

In summary, it appears that the respondents made no distinction between the survey questions on faculty quality (93Q) and program effectiveness (93E). To some extent, sheer size influenced the quality rankings and respondents gave high ranks to programs with which they were familiar. Strong positive correlations exist between the survey results of faculty quality and the publication and citation rates.

**PART 2  
ALTERNATIVE METHODS OF  
RANKING**

**Alternative Measures of Quality** • Four extensive measures of program quality are used: 1) Number of publications, 2) number of citations to publications, 3) research funding, and 4) faculty honors. In addition, each of these extensive measures is normalized by the number of faculty to provide four intensive measures of quality. We use these data to develop alternative rankings of programs based on both the extensive and intensive criteria. We also provide a final composite ranking based on the extensive and intensive rankings. We are quite aware that these so-called "objective" measures are imperfect, and we will attempt to point out potential problems with each of the measures we use.

Quantitative measures of quality are not new. Some were used in the NRC Report as mentioned above. Also, the often-maligned *U.S. News and World Report*<sup>[2]</sup> used a lumped score in which

**TABLE 5  
Programs not Considered in Final Rankings  
Because of Lack of Data on Research Support**

Brigham Young University	University of Louisville
City University of New York	University of Maine
Duke University	University of Mississippi
Illinois Institute of Technology	University of Notre Dame
Northeastern University	University of Rhode Island
Rice University	University of Tulsa
University of Akron	University of Wyoming
University of Idaho	Washington University
University of Kansas	Worcester Polytechnic University

**TABLE 6  
Rank Order and Scaled Scores of ChE Graduate Programs  
Using Extensive Criteria**

University	Publications		Citations		Support		Honors		Extensive Composite	
	Score	Rank	Score	Rank	Score	Rank	Score	Rank	Score	Rank
UMN	100.0	1	100.0	1	76.6	3	77.9	2	354.5	1
MIT	79.2	2	65.0	3	100.0	1	100.0	1	344.2	2
UTA	76.6	3	76.6	2	55.6	5	72.6	3	281.4	3
UCB	50.3	4	45.2	4	13.4	41	56.1	6	165.0	4
UDE	34.2	6	23.3	8	30.7	12	68.3	4	156.6	5
UWI	34.1	7	16.2	19	41.6	7	58.6	5	150.6	6
TAM	22.8	24	6.4	45	77.8	2	21.8	27	128.7	7
PSU	25.7	17	13.0	24	23.0	19	54.0	7	115.7	8
UCLA	43.4	5	39.6	5	12.2	44	18.7	35	114.0	9
UCSB	27.6	13	24.9	7	28.2	13	32.5	16	113.2	10
PRU	21.0	27	17.5	16	25.7	16	46.9	10	111.1	11
NCSU	22.6	25	16.8	17	35.9	9	35.0	12	110.4	12
NWU	24.7	20	13.7	23	13.1	42	52.8	8	104.3	13
PUR	34.0	8	21.4	9	26.0	15	20.3	32	101.6	14
STAN	27.6	13	27.7	6	25.4	17	20.3	31	101.0	15
UMI	28.4	11	18.8	13	21.2	24	32.0	17	100.4	16
CIT	24.0	21	17.9	15	21.7	23	29.8	20	93.4	17
UIL	25.7	17	18.3	14	15.4	34	34.0	15	93.4	18
CORN	30.2	9	19.0	12	21.9	22	21.8	27	92.9	19
LEH	30.2	9	20.3	10	23.9	18	17.2	37	91.5	20
UPA	26.1	16	19.3	11	8.4	56	35.0	12	88.7	21
CMU	18.9	30	9.6	38	10.7	48	47.6	9	86.8	22
GIT	28.2	12	10.3	35	26.7	14	20.8	29	86.0	23
SUNY	23.8	22	14.8	22	10.0	50	34.1	14	82.6	24
CWRU	12.0	50	15.8	21	32.2	11	22.4	25	82.3	25
UMA	19.1	29	12.1	26	11.9	45	35.3	11	78.3	26
LSU	24.9	19	11.1	31	22.1	21	16.5	39	74.8	27
UCO	16.5	33	9.4	39	16.9	31	31.9	18	74.7	28
UTN	3.7	87	0.5	91	61.6	4	8.5	53	74.3	29
UWA	27.6	13	16.5	18	14.4	37	13.8	43	72.3	30
UCD	23.5	23	15.8	20	8.8	53	24.0	24	72.1	31
JHU	15.1	36	11.1	32	34.4	10	11.1	48	71.6	32
UUT	22.5	26	11.1	32	21.2	25	16.5	39	71.3	33
UOK	11.8	51	7.9	44	51.6	6	0.0	83	71.3	34
UH	12.2	48	5.3	52	23.0	20	27.2	21	67.7	35
OSU	18.5	31	9.2	40	11.2	47	26.7	22	65.6	36
RPI	17.3	32	9.9	37	15.3	35	20.2	34	62.7	37
PITT	16.4	34	5.8	48	18.9	29	18.1	36	59.2	38
ISU	12.6	44	12.2	25	8.7	55	22.4	25	55.9	39
UVA	14.3	38	10.0	36	10.4	49	20.3	32	55.0	40

Average of Extensive Composite Scores for All Universities - 71.85

40% was based on a reputational survey of deans and members of the National Academy of Engineering. The remaining 60% was derived from quantitative measures of research support, faculty honors, and student selectivity. The *U.S. News and World* report also included both extensive and intensive measures of quality.

We have included only the top forty programs in the extensive, intensive, and composite rankings. Our purpose is to focus on alternative methods of ranking rather than the rank order itself. We have no wish to identify any program as being of low quality.

**Publications and Citations** • We use both the total number of faculty publications (PUB) and citations to published papers (TC) from the NRC report as extensive measures of research quality. The same variables normalized by the total number of faculty (TF) are used as intensive measures of research quality. We recognize these are imperfect measures. For example, research with the longest range and most profound impact may go unnoticed for decades. Also, it is difficult to agree on what constitutes a publication, and there is a proliferation and duplication of research papers of marginal merit. The number of times a research paper has been cited is a summary judgment, albeit imperfect, of its relevance and importance. But papers with classic errors (for example, cold fusion) may attract numerous citations. More significantly, a single review paper or a paper describing a widely used test or procedure can generate an inordinate number of citations not closely related to research quality. Finally, certain sub-fields within chemical engineering may more easily produce publishable results than others.

**Research Support** • The NRC report contained data on the percentage of faculty that received research support (%SUPP) and the percentage of faculty that published (%PUB). We found these variables provided little discrimination, especially between high-ranked programs, and we did not use them in our analysis. Instead, we elected to use total research support from all sources (SUPP) collected by the National Science Foundation<sup>[4]</sup> as an extensive quality measure. These figures were used without modification.<sup>\*</sup> We emphasize that the compilation reported by the NSF is meant to be complete; it includes state support and support from other federal agencies, industry, and foundations. We also note that total research support is one of the primary measures used in recent scholarly studies of the relative quality of research universities.<sup>[5]</sup>

The data in the NSF report are reported by the individual institutions and may not be reported on a similar basis; research support from ancillary research institutes or unrelated programs may be included in some cases. Also, the amount of

state support for research may not be uniformly reported.

Eighteen chemical engineering programs in the NRC report were not listed in the National Science Foundation report. There is no indication whether this is because no data were submitted by these programs or whether they had too little research income to appear on the table (only the top 100 engineering programs were included in the table). Rather than estimate the research support from other sources, we excluded these programs from our rankings. The programs that were excluded are listed in Table 5.

**Faculty Honors** • Inexplicably, faculty honors were not used as a quality index for engineering and science programs in the NRC report; they were used, however, in the NRC rankings of programs in the arts and humanities. There are certain categories of honors and awards for chemical engineering faculty that can easily be tabulated. For junior faculty we used the number of recipients of NSF Career Development Awards, NSF Young Investigator awards, and Presidential Investigator awards over the period 1988 to 1996;<sup>[6]</sup> for mid-career faculty we used winners of the principal AIChE awards from 1987 to 1996;<sup>[7]</sup> and for senior faculty we use the sum of the current number of National Academy of Engineering members<sup>[8]</sup> plus one-half of the number of Fellows of the AIChE.<sup>[7]</sup> This arbitrary choice is based on the observation that there are approximately twice as many AIChE fellows as NAE members in the departments surveyed. Retired and emeritus faculty were excluded. The three categories (junior, mid-career, senior) were scaled to give each equal weight. We believe that including only AIChE honors and awards over-emphasizes the traditional areas of chemical engineering. In future rankings we suggest including honors and awards from other professional organizations (*e.g.*, the American Chemical Society, the Electrochemical Society, and the Materials Research Society).

**Alternative Rankings** • The numerical data in each extensive category (Publications, Citations, Support, and Honors) were scaled so the maximum value in each category was 100. The total extensive score for each program was obtained by summing the four scores for each extensive category. The overall extensive rank order was determined from these summed scores (see Table 6). The programs are listed in Table 6 in the order of their total extensive score.

The intensive scores in each category for each program were obtained by dividing the extensive scores by the appropriate number of program faculty. For calculation of PUB/TF and TC/TF, all data were taken from the NRC report. For calculation of HON/TF and SUPP/TF, the data were taken from references 4,6,7,8, and 9. The intensive scores were also scaled so that the maximum value in each category was 100. A total intensive score was obtained for each program by summing the scaled intensive scores of the four categories. The programs are listed in Table 7 in the order of their total intensive score.

\* We made one exception to this generalization. For our own university, we removed the expenditures of the Macromolecular Science Department from the NSF figures. This lowered the CWRU extensive ranking and left the intensive ranking unchanged. We were unable to make a similar correction for other programs.

It is tempting to use the intensive rankings in Table 7 as a measure of the average, individual quality of the program faculty. But one should be cautious in doing so, especially for the smaller programs. In some cases the average intensive score is heavily influenced by the activities of one or two particularly strong individuals. This effect was measured in the NRC report by the Gini coefficient, which is a measure of the non-uniformity of the distribution of scores among the individuals. Since we did not have access to the raw data, we could not make this estimate.

A composite extensive plus intensive ranking was also calculated. A simple summation of the total extensive plus intensive scores gave undue weight to the intensive scores. We rescaled the intensive total scores to give the same average score as the extensive scores. A composite extensive/intensive score was calculated for each program using the total extensive score and the rescaled intensive total score. For example, for MIT the composite extensive/intensive score was obtained from

$$344.2 + \frac{71.85}{130.66}(312.1) = 515.8$$

This procedure gave the same overall weighting to the extensive and intensive scores. The composite extensive/intensive scores and rankings are given in Table 8.

It is most appropriate to compare programs using the separate extensive and intensive measures in Tables 6 and 7. Nevertheless, the composite extensive/intensive ranking in Table 8 has value. For example, when making a choice of a graduate program, a prospective student will make an integrated assessment of both extensive and intensive measures. Small programs that are rated very highly on a per-faculty basis may have a limited range of course work and research options; large programs with high extensive scores may not have the desired level of individual faculty quality. A composite score also permits comparisons with other lumped scores—for example, the *U.S. News and World* report rankings.

**Sensitivity and Error Analysis** • The sensitivity of the rank ordering to changes in the extensive data sets (Publications, Citations, Support, and Honors) can be calculated by calculating  $\Delta \ln X (\cong \Delta X/X)$  for each of the rank ordered data sets. We show plots of these results in Figure 3. For example, the

value of  $\Delta \ln (TC)$  is the fractional change in number of total citations required to change one place in the rank order. In the middle range, the average fractional change required to move one place in the rank order of citations is approximately 0.03; however, greater fractional changes (over 0.30) are required to move one place in the rank ordering at either extreme. Similar behavior is observed for the other extensive variables, also shown in Figure 3. These results show that while it is relatively easy to move in the middle range of rank orders, it will be more difficult for programs to move

**TABLE 7**  
Rank Order and Scaled Scores of ChE Graduate Programs Using Intensive Criteria

University	Publications/Faculty		Citations/Faculty		Support/Faculty		Honors/Faculty		Intensive Composite	
	Score	Rank	Score	Rank	Score	Rank	Score	Rank	Score	Rank
UMN	100.0	1	100.0	1	56.7	11	69.5	13	326.2	1
UTA	81.7	4	81.7	3	58.3	9	91.8	4	313.5	2
MIT	81.7	4	67.1	5	74.1	6	89.2	6	312.1	3
STAN	88.3	2	88.7	2	63.9	8	61.5	19	302.4	4
UCB	84.8	3	76.2	4	19.8	47	100.0	1	280.8	5
CIT	77.0	6	57.3	6	54.7	12	90.2	5	279.1	6
UWI	57.4	10	27.4	27	58.2	10	98.8	2	241.8	7
JHU	60.4	8	44.3	10	96.2	4	37.4	32	238.3	8
CWRU	38.3	33	50.4	8	73.7	7	61.6	18	224.0	9
UIL	54.8	11	39.0	12	32.3	24	86.0	10	212.0	10
PRU	44.8	25	37.3	14	40.5	15	88.9	8	211.5	11
UDE	54.8	11	37.3	14	30.9	26	82.9	12	205.9	12
SUNY	54.3	13	33.8	19	22.9	40	93.9	3	205.0	13
UCLA	60.4	8	55.1	7	30.8	27	56.7	22	203.1	14
UCSB	49.1	20	44.2	11	41.7	14	58.0	21	193.0	15
NWU	46.5	24	25.9	31	18.3	53	89.0	7	179.6	16
TAM	36.5	37	10.2	62	97.9	3	33.0	38	177.7	17
SYR	61.3	7	36.6	16	39.2	16	40.6	31	177.6	18
UPA	52.2	14	38.6	13	13.2	61	66.4	16	170.3	19
CORN	50.9	17	32.1	21	36.8	19	44.0	29	163.8	20
PSU	30.4	48	15.4	45	30.5	29	86.2	9	162.5	21
UMA	47.0	22	29.9	24	18.7	51	66.8	15	162.3	22
UOK	34.3	43	22.9	35	100.0	1	0.0	83	157.2	23
NCSU	42.6	27	31.7	22	37.7	18	44.2	28	156.3	24
UMI	50.4	19	33.5	20	25.4	34	46.1	27	155.6	25
YALE	51.3	16	48.0	9	19.6	49	36.1	34	155.1	26
UCO	35.2	41	20.0	40	30.5	28	69.2	14	154.8	27
CMU	35.7	40	18.0	41	15.9	56	84.8	11	154.4	28
LEH	50.9	17	34.1	18	33.4	21	28.9	42	147.3	29
OSU	42.2	28	21.1	39	21.7	45	62.3	17	147.3	30
OKSU	20.9	70	7.7	71	98.0	2	19.5	53	146.0	31
UVA	38.3	33	26.7	30	23.7	38	55.9	23	144.6	32
RPI	39.6	30	22.5	36	27.5	30	43.8	30	133.4	33
UWA	49.1	20	29.4	25	22.6	43	26.1	44	127.2	34
UH	21.7	68	9.4	67	38.6	17	55.0	24	124.7	35
PUR	43.5	26	27.4	27	26.2	32	24.6	47	121.6	36
COL	31.7	45	9.8	65	43.1	13	36.3	33	120.9	37
UCD	47.0	22	31.7	23	9.2	69	30.3	39	118.2	38
UTN	7.8	92	1.1	92	86.2	5	14.4	60	109.5	39
LSU	29.6	52	13.2	52	32.8	23	29.5	41	105.1	40

Average of Intensive Composite Scores for all Universities 130.66

**TABLE 8**

**Example of Rank Order of ChE Graduate Programs using a Single, Composite Extensive/Intensive Criterion**

University	Composite Score			University	Composite Score				
	Rescaled <sup>(a)</sup>	Normalized	Deviation <sup>(b)</sup> /Rank		Rescaled <sup>(a)</sup>	Normalized	Deviation <sup>(b)</sup> /Rank		
University of Minnesota	533.9	100.0	4.9	1	Purdue University	168.5	31.6	13.3	25
Massachusetts Inst. of Technology	515.8	96.6	2.1	2	Univ. of Massachusetts, Amherst	167.6	31.4	13.8	26
University of Texas at Austin	453.8	85.0	2.2	3	University of Colorado	159.9	29.9	10.1	27
University of California-Berkeley	319.4	59.8	18.8	4 <sup>(c)</sup>	University of Oklahoma	157.7	29.5	30.4	28 <sup>(d)</sup>
University of Wisconsin-Madison	283.5	53.1	8.2	5	Syracuse University	151.4	28.4	14.2	29
University of Delaware	269.8	50.5	6.7	6	Ohio State University	146.6	27.5	10.9	30
Stanford University	267.3	50.1	9.9	7	University of Washington	142.2	26.6	12.8	31
California Institute of Technology	246.9	46.2	7.3	8	University of California-Davis	137.1	25.7	18.1	32
Princeton University	227.4	42.6	6.6	9	University of Houston	136.2	25.5	21.6	33
Texas A&M University	226.4	42.4	20.4	10 <sup>(d)</sup>	Rensselaer Polytechnic Institute	136.0	25.5	2.9	34
Univ. of California-Los Angeles	225.6	42.3	15.2	11	University of Tennessee-Knoxville	134.6	25.2	37.7	35 <sup>(d)</sup>
Univ. of California-Santa Barbara	219.3	41.1	4.6	12	University of Virginia	134.5	25.2	7.5	36
Univ. of Illinois, Urbana-Champaign	210.0	39.3	8.1	13	Georgia Institute of Technology	134.1	25.1	16.4	37
Case Western Reserve University	205.5	38.5	14.5	14	Louisiana State University	132.5	24.8	13.3	38
Pennsylvania State University	205.1	38.4	15.2	15	Oklahoma State University	131.0	24.5	31.0	39 <sup>(d)</sup>
Northwestern University	203.1	38.0	15.8	16	Yale University	125.8	23.6	18.1	40
Johns Hopkins University	202.7	38.0	16.4	17					
North Carolina State University	196.4	36.8	7.0	18					
State Univ. of New York-Buffalo	195.3	36.6	15.2	19					
University of Michigan	185.9	34.8	7.5	20					
Cornell University	183.0	34.3	6.8	21					
University of Pennsylvania	182.4	34.2	20.9	22 <sup>(c)</sup>					
Lehigh University	172.5	32.3	11.9	23					
Carnegie Mellon University	171.7	32.2	16.7	24					

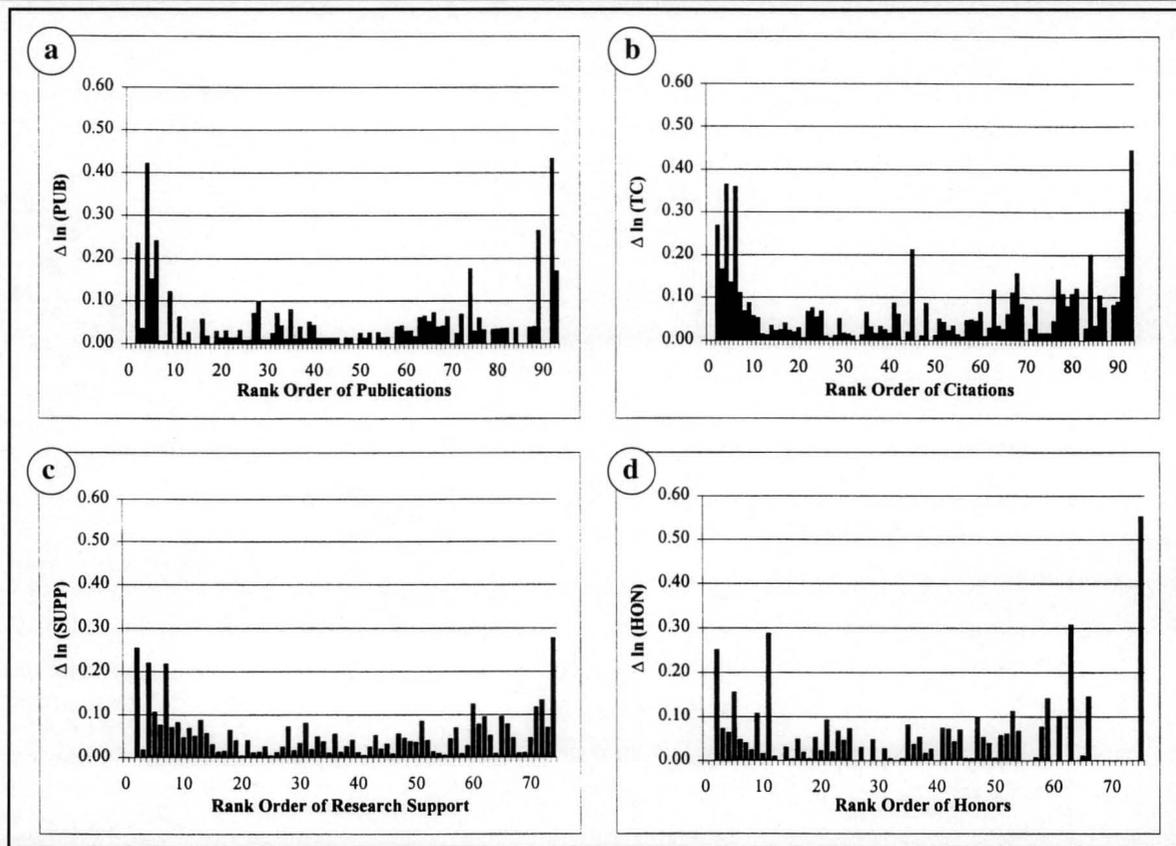
<sup>(a)</sup> Extensive score plus rescaled intensive score as described in text.

<sup>(b)</sup> Standard deviation of the rank order numbers of the eight quality measures as described in text.

<sup>(c)</sup> Ranking may be low because of different basis or error in Research Support category.

<sup>(d)</sup> Ranking may be high because of different basis or error in Research Support category.

**Figure 3. (a)** Fractional change in citations,  $\Delta(TC)/(TC)$ , versus rank order; top-ranked programs are on left. **(b)** Fractional change in publications,  $\Delta(PUB)/(PUB)$ , versus rank order; top-ranked programs are on left. **(c)** Fractional change in research support,  $\Delta(SUPP)/(SUPP)$ , versus rank order; top-ranked programs are on left. **(d)** Fractional change in honors,  $\Delta(HON)/(HON)$ , versus rank order; top-ranked programs are on left.



into the first decile or out of the tenth decile.

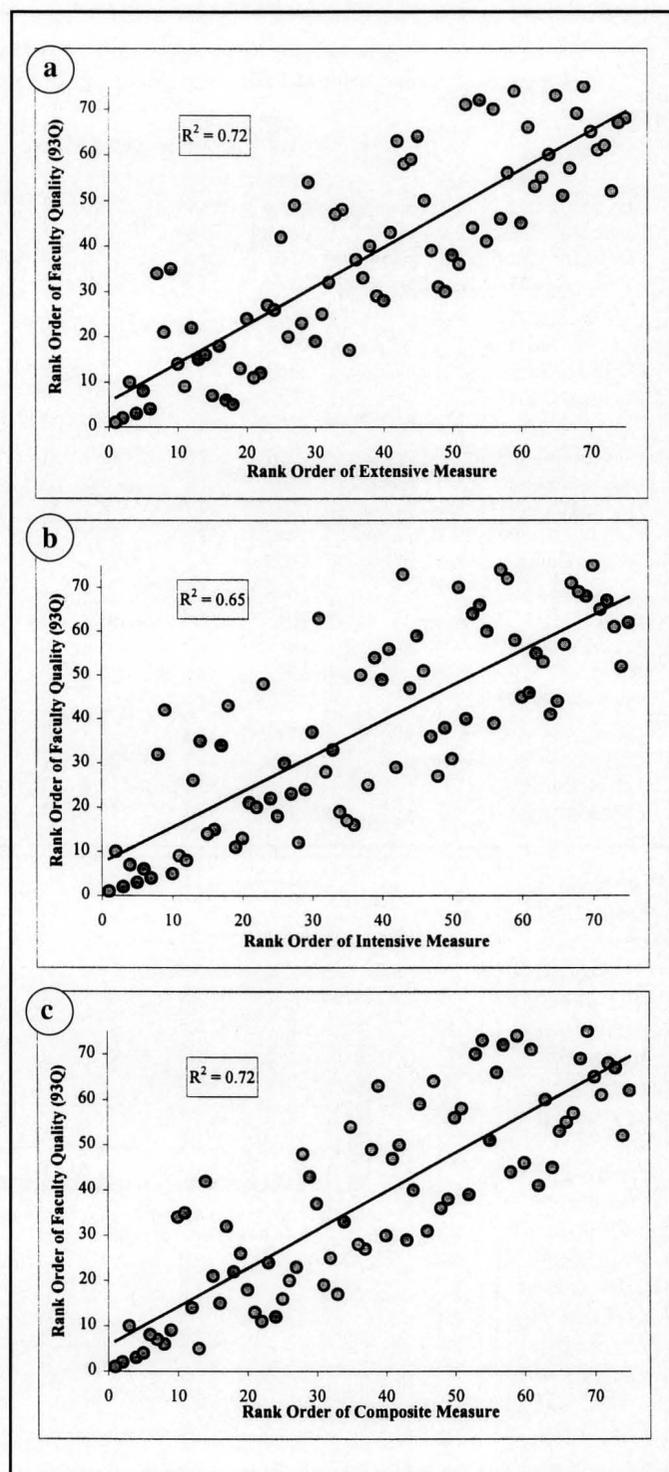
Without knowing details of the data collection, it is not possible to make a rigorous assessment of the uncertainty in the rank ordering. However, a heuristic assessment can be made. We assume, based on experience and for purposes of argument, that there are independent errors of 10% in each of the four extensive numerical data sets: Publications, Citations, Support, and Honors. In the middle range of each of the extensive data sets, the fractional change,  $\Delta X/X$ , required to move one place in the rank order is approximately 0.03 (see Figure 3). A fractional error of 0.10 therefore corresponds to approximately  $0.10/0.03 \approx 3$  places in the rank ordering. Also, if the errors are independent, one would expect an error in the composite rank ordering of extensive criteria to be approximately  $\sqrt{4}(3) = 6$  places. If similar arguments are used for the four intensive data sets, we also find an approximate error of six places. This error is not independent of the error in the extensive rank ordering. We conclude that, in the middle range, programs within 5 to 10 places on the composite extensive/intensive rank ordering are essentially indistinguishable from each other. This estimate is consistent with our common-sense interpretation of the rank ordering, *e.g.*, programs in the second decile are probably superior to programs in the third decile, and so on.

The eight separate (though not completely independent) measures of quality give the rankings a certain degree of robustness that a single criterion would not have. The internal consistency of the eight measures of quality is estimated by computing the standard deviation of the rank order number of the eight separate quality categories for each program (see Table 8). For example, for MIT the average of the eight rank orders is 3.5 and the standard deviation of rank orders is just

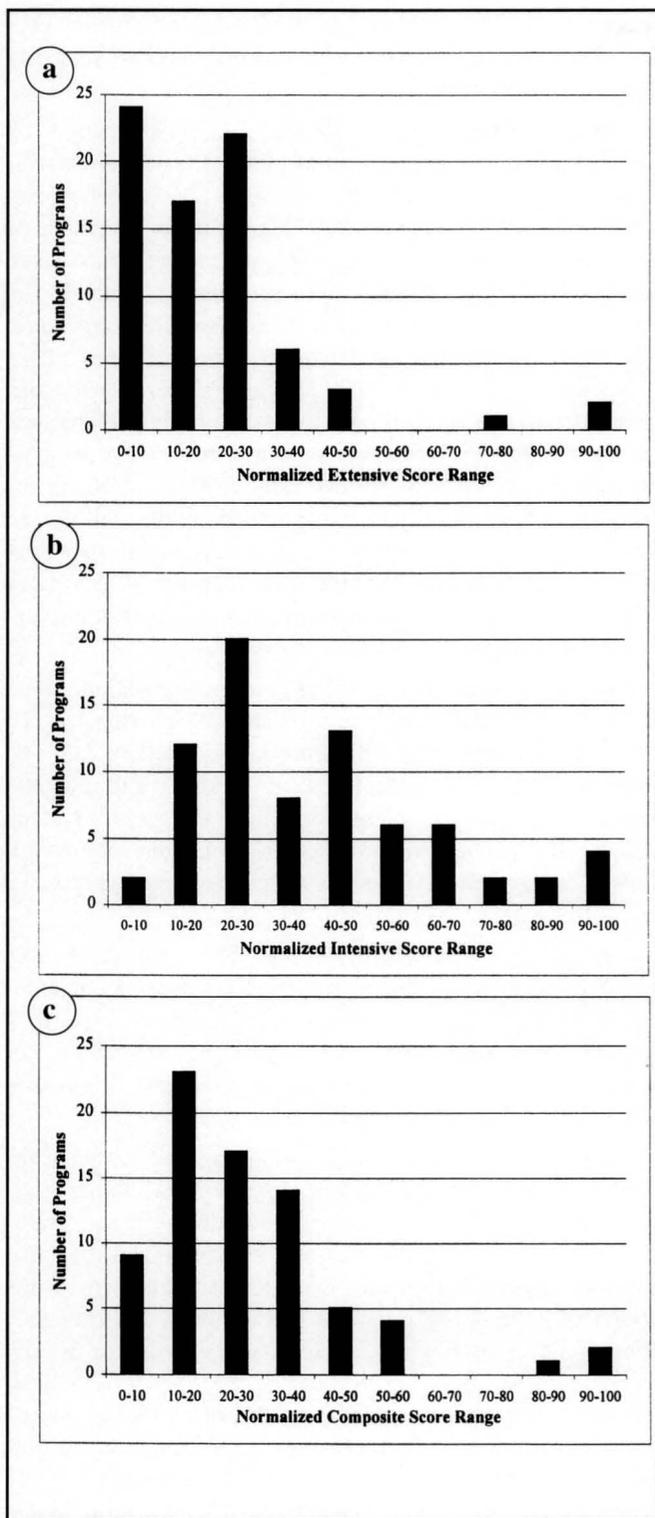
$$\left\{ \frac{(2-3.5)^2 + (3-3.5)^2 + \dots}{8-1} \right\}^{1/2} = 2.07$$

Large values of the deviations indicate programs where indi-

Ranking Category	Fit	$R^2$
PUB	$y = mx + b$	0.7469
PUB/FAC	$y = mx + b$	0.6005
CIT	$y = mx + b$	0.7482
CIT/FAC	$y = mx + b$	0.6028
SUPP	$y = mx + b$	0.2484
SUPP/FAC	$y = mx + b$	0.1351
HON	$y = mx + b$	0.6993
HON/FAC	$y = mx + b$	0.6370



**Figure 4.** (a) Composite extensive rank order versus rank order of faculty quality (93Q); top-ranked programs are near origin.  $R^2=0.72$  for linear fit,  $y=mx+b$ . (b) Composite intensive rank order versus rank order of faculty quality (93Q); top-ranked programs are near origin.  $R^2=0.65$  for linear fit,  $y=mx+b$ . (c) Composite intensive/extensive rank order versus rank order of faculty quality (93Q); top-ranked programs are near origin.  $R^2=0.72$  for linear fit,  $y=mx+b$



**Figure 5.** (a) Histogram showing number of programs versus scaled total extensive score; top-ranked programs are at the right. (b) Histogram showing number of programs versus scaled total intensive score; top-ranked programs are at the right. (c) Histogram showing number of programs versus scaled total composite extensive/intensive score; top-ranked programs are at the right.

vidual quality rankings are the least internally consistent. In many cases, large deviations are associated with small programs that rank higher in intensive than in extensive categories. However, in some cases, large deviations may indicate problems in the data. For example, four programs have much higher rankings in research support than in the other quality categories: Texas A&M, Oklahoma State University, the University of Oklahoma, and the University of Tennessee. On the other hand, the University of California at Berkeley and the University of Pennsylvania have much lower rankings in research support than they have in the other categories. We believe that these disparities likely arise from different reporting bases and may not reflect true differences in research support. Three programs have a much higher ranking in Honors than in the other quality categories: Pennsylvania State University, Carnegie Mellon University, and Northwestern University.

The rank order of perceived faculty quality (93Q) was correlated with the rank order of each of the separate quality categories (see Table 9). The weakest correlations were found with the two support categories, SUPP and SUPP/TF, consistent with our belief that some of these data are not reported on a consistent basis. Nevertheless, we are reluctant to exclude research support from the quality measures. Research support is probably a better current and leading indicator of quality than the other categories. Also, total research support is a primary criterion used for assessing quality of research universities.<sup>[5]</sup> Rather than re-ranking the programs excluding SUPP and SUPP/TF, we believe it is more reasonable to identify programs where different bases for reporting support may have strongly influenced the rankings.

Plots of the rank order from the faculty quality survey (93Q) from the NRC report versus the overall extensive, overall intensive, and composite rankings are given in Figure 4. In the figure, the high-quality programs are near the origin. The figure clearly shows how the quality survey and our methods identify the same several programs as the highest quality.

**PART 3  
DISCUSSION AND RECOMMENDATIONS**

**Interpretation of Rankings** • There is no calibration standard for quality against which any methodology can be tested. Nevertheless, we find it very suggestive that our composite extensive/intensive ranking and the NRC reputational survey identify the same few top programs. For example, comparison of Tables 4 and 8 shows that the same top two programs, MIT and Minnesota, and nine out of the ten top-ranked programs are the same in both the NRC reputational ranking and our numerical ranking. But only three out of ten programs in the second decile and two of ten in the third decile are the same. The NRC reputational

rankings, which rely heavily on anecdotal, word-of-mouth information, will be most accurate for the few, high-profile, extremely good programs, and will be less accurate for smaller, lower-profile, and second-tier institutions. But the numerical measures of quality should remain useful in assessing the relative quality of all institutions. *We conclude, subject to the caveats given about the accuracy of the data itself, that our simple numerical measures do correlate with program quality as it is normally understood.*

Further comparison of Tables 4 and 8 leads to additional insights. One may divide programs into three broad categories. First are the programs that are highly rated on both the NRC reputational survey and the numerical ranking. Prime examples are the University of Minnesota, Massachusetts Institute of Technology, the University of Wisconsin, the University of California at Berkeley, and Stanford University. Second are programs that rank significantly higher in the numerical ranking than in the survey. These programs are often (but not always) associated with smaller, research-intensive programs. Examples are the University of California at Los Angeles, Case Western Reserve University, and Johns Hopkins University. Finally, there are well-known programs, which do well in the reputational ranking, that do not do as well in the numerical measures. These programs may be relying on past, rather than current, performance.

Further insight can be obtained from histograms of the final scores, shown in Figure 5. For ease of interpretation, in the figure the scores from Tables 6, 7, and 8 were scaled to give maximum values of 100. Figure 5a and Table 6 clearly show that three programs (MIT, Minnesota, and Texas) have extensive scores well above all other departments. This disparity is lessened somewhat when the intensive scores are compared (Figure 5b and Table 7). This same uneven distribution of scores is found in Figure 5c, which shows the distribution of composite extensive/intensive scores. The top half of the composite score range contains only seven programs; the remaining programs fall in the lower half. The summary shown in Table 8 and Figure 5 indicates that the highest quality chemical engineering programs are relatively few in number and significantly higher in quality than the rest. Below the top five or six programs there is a wide range of programs with relatively similar quality.

*Finally, while we believe that for most programs the rankings given here are an accurate reflection of quality, we emphasize once again that one should be cautious in drawing conclusions from the absolute position in the rankings of a single program.*

**Limitations of Ranking Systems** • Respondents to the NRC questionnaire were asked to rate fifty separate programs. An individual respondent will only have personal, detailed knowledge about a small fraction of these. The resulting reputational rankings will inevitably be influenced by the network of informal contacts and acquaintances of the

respondents. This will lead to a bias against smaller programs and will also make the reputational rankings a lagging indicator of program quality.

Another major problem with the NRC report, recognized by the committee, was the lack of data on the performance of graduates from the programs. We were unable to find any direct quantitative measure for assessing the performance of graduates of chemical engineering graduate programs. Since one of the principal goals of a graduate program is the education of the next generation of researchers, this is a serious omission indeed. Personnel departments of major corporate employers of PhD chemical engineers often maintain internal ratings of programs based on the performance of their employees. Perhaps this information can be provided in some suitable blind format to future NRC committees. This is a project that could be addressed by the AIChE and the other engineering societies. Another possible measure of performance is the number of graduates that obtain tenure-track appointments at research universities other than their own.

We suggest that future ranking systems also include some measures of the effectiveness of technology transfer. To partially accomplish this, the Publication category could be expanded to include patents issued to faculty and graduate students. Similarly, Citations could include papers or patents cited within patents. More difficult to count, but very useful, would be the number of new businesses formed as a result of activities within the program.

The quality measures used in the NRC report and in this paper are appropriate for doctoral-level, research-based graduate programs. However, master's-level programs, especially practice-oriented programs, are of growing importance. Future ranking systems should attempt to separately measure the quality of these programs.

The difficulty in accounting for the rapidly changing, interdisciplinary nature of modern engineering is another problem encountered when developing ranking systems. Traditional academic boundaries do not always reflect the realities of engineering practice. The NRC report addressed this problem by ranking "programs" rather than "departments." For chemical engineering, these two categories are usually commensurate, but this may not be the case for chemical engineering programs with strong efforts in biotechnology or advanced materials. Ranking programs with major commitments in these fields can be difficult when the academic administrative units do not correspond to the categories used in the ranking scheme. Very strong, interdisciplinary efforts may not appear in the data set, or conversely, remote extraneous efforts can be included. Obtaining a reliable data set, based on uniform criteria, is a formidable task. The NRC committee had great difficulty in defining program boundaries in modern biology and molecular biology, where the pace of change is particularly great.

Neither the NRC report nor this paper uses any measures of the quality of graduate teaching. The lack of quantitative measures of teaching performance is a continuing, long-term problem.

The very long time between the NRC reports (1982 to 1995) is yet another problem. Waiting more than a decade for an assessment is slow, even by the standards of academia. Some form of continuing assessment, for example on a triennial basis, would be more useful. This would give more timely results and would also permit running averages of several years to average out fluctuations in the data.

**Concluding Remarks** • With all of these difficulties, one can legitimately ask why bother with rankings at all? We believe that universities will be under ever-increasing pressure to justify tuition rates and the cost of performing research. Whether we like it or not, ranking of academic programs will continue and will likely increase. It is in the profession's interest to see that the rankings are based on rational, measurable criteria. But there is little reason to continue relying on surveys. *Reputational rankings only confirm the obvious about the top few programs, permit declining programs to remain complacent, and fail to recognize increasing quality where it occurs.*

### Conclusions and Recommendations

- Alternative, measurable quality indices exist that correlate well with graduate program quality as it is normally understood.
- The professional societies, the National Academy of Engineering, and the National Science Foundation should take the lead in developing these quantitative measures of program quality and appropriate data bases to support these measures.
- Special attention should be paid to developing methods for assessing the performance of students after they receive their graduate degrees; this should include using information from employers of graduates.
- Methods of assessing the effectiveness of technology transfer and impact on industry should be developed.
- Assessments should be made on a more frequent schedule, perhaps triennially.

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## BOOK REVIEW: *Alternative Fuels*

*Continued from page 39.*

The use of geothermal energy is presented in Chapter 9. This topical discussion notes that at depths of about six miles from the earth's surface, the temperature is greater than 100°C. This equates to more energy storage than the total thermal energy in all the nuclear and fossil fuel resources—only solar energy is comparable. Along with scientific and technological updates, the advantages and disadvantages of geothermal energy utilization are outlined; this alternative source of energy will potentially become a larger part of the world's energy consumption in the near future because geothermal energy is both available and economical. In the United States, approximately 3 GW of electric power is produced in 20 power plants from geothermal reservoirs. Geothermal energy also has great potential as a practical provider of heat to local areas.

The overall conversion routes of biomass are described in Chapter 10. They include thermal (combustion, gasification, liquefaction, and pyrolysis), anaerobic digestion, and fermentation to liquid ethanol fuel. The descriptions include 15 process diagrams and several tables of data. A selected amount of cost data is provided for ethanol production from lignocellulose.

Chapter 11 presents a comprehensive overview of relatively recent developments in the generation of energy from municipal solid wastes, including spent tires and polymeric materials. Processes include incineration, anaerobic digestion and landfill gas recovery, pyrolysis, thermal cracking, and partial oxidation via supercritical fluids.

In summary, *Alternative Fuels* superbly achieves its purpose by bringing together a wealth of practical information required for a thorough understanding of those chemical process technologies urgently needed for the development of fuels for future use. Dr. Lee is to be commended for his extraordinary efforts in synthesizing all these facts and systems in a clear and consistent manner. Possibly his next book could focus more on the use of biomass, geothermal, and solid waste resources—three areas that are undergoing rapid development. □

This column provides examples of cases in which students have gained knowledge, insight, and experience in the practice of chemical engineering while in an industrial setting. Summer internships and co-op assignments typify such experiences; however, reports of more unusual cases are also welcome. Description of the analytical tools used and the skills developed during the project should be emphasized. These examples should stimulate innovative approaches to bring real world tools and experiences back to campus for integration into the curriculum. Please submit manuscripts to Professor W. J. Koros, Chemical Engineering Department, University of Texas, Austin, Texas 78712.

# FROM THE CLASSROOM TO THE WORKPLACE

## *Motivating Students to Learn in Industry*

A. CHRISTIAN FRICKE

*Rensselaer Polytechnic Institute • Troy, NY 12180*

**W**hat makes a successful engineer? No one would deny that technical expertise is critical to mastering real-world engineering problems. Yet technical mastery is only half the battle; there are also many complex social skills that must be learned in order to make successful use of technical knowledge in a workplace setting.

The purpose of this article is twofold. First, it will note a few examples of specific nontechnical skills that can be useful in managing the day-to-day workplace realities of a BS-level engineer. These skills and strategies are taken from the author's personal experience in working as a process engineer for three years at a mid-sized manufacturing consulting firm, as well as from conversations with and observations of dozens of colleagues working in varied chemical and mechanical product design and manufacturing settings. The majority of these engineers were within six years of graduation and were in the process of learning the social skills necessary for moving up the corporate ladder from technically oriented process positions to more business-oriented managerial functions. It is hoped that these observations will prove useful to engineering professors who have not worked for an appreciable amount of time at the BS level and who therefore have experienced the industrial setting in a much different context.

Second, this article will outline several ways in which the need for acquiring these informal skills can be communicated to the vast majority of students who will end their education at the BS level. The conveyance of technical concepts, skills, and information is undoubtedly what the undergraduate experience is all about, but by suggesting some of the social contexts within which these skills will be mobi-

lized, engineering educators can increase students' effectiveness in putting this technical material to use in the workplace.

There exists a real need to alert undergraduates to the fact that excelling in the classroom, although critical, is only half the equation in preparing to be an effective professional. Otherwise naive students need to be explicitly made aware of the seemingly commonsense notion that one must indeed "learn in industry" in order to be a successful corporate engineer.

### STUDENT PERCEPTIONS

This need is illustrated by a recent survey of seventy-six undergraduate engineers at Rensselaer Polytechnic Institute (RPI) in which 95% indicated they had a "very firm" or at least a "somewhat firm" idea of what the daily work experience of an average engineer is like (see Figure 1). A close look at the numbers indicates that students likely do not have the firm grasp of engineering workplace realities that they profess.

For instance, there was no correlation between students'

**A. Christian Fricke** graduated from North Carolina State University with BS degrees in chemical engineering and biochemistry. He has worked in a Merck Pharmaceuticals production facility, as a research assistant in a molecular genetics laboratory, and as a process engineer for CTC, a manufacturing consulting firm with headquarters in Johnstown, Pennsylvania. He is currently a doctoral candidate in the Science and Technology Studies program at RPI.



***There exists a real need to alert undergraduates to the fact that excelling in the classroom, although critical, is only half the equation in preparing to be an effective professional. . . Success on the job . . . entails learning many complex social behaviors in addition to those necessary for classroom success. It also entails developing an entirely new perspective on what constitutes "engineering."***

reported knowledge of "what it is that engineers do on a daily basis" and their personal relationships. Students who had no close relatives or acquaintances with engineering backgrounds (more than 60% of those surveyed) were just as likely to indicate a firm knowledge of daily working realities as those with engineers "in the family." In the absence of actual engineers to talk with and observe, student conceptions of "workplace realities" are vague and simplistic at best.

This simplistic view can undermine an engineer's effectiveness in accomplishing personal, professional, and societal goals in the workplace. In addition, the apparently prevalent student attitude of believing they already know what professional working realities are all about can seriously limit the benefits to be gained from intern and co-op experiences. These experiences provide the ideal setting for observing the practical day-to-day social skills and strategies necessary for BS-level success. In order to realize this benefit, however, students must be *actively looking* for these potential lessons in the first place.

## **UNDERGRADUATE SOCIALIZATION**

The majority of undergraduate students form their first concrete conception of "engineering" through survey courses and introductory seminars that are structured to help freshman and first-semester sophomore students choose a particular discipline. At RPI, for example, second-semester freshman students take a course, titled "Engineering Seminar," that is designed to "provide the student with information relative to the various engineering fields and curricular areas."<sup>[1]</sup> These types of survey courses generally focus on the end products of engineering work. In other words, they emphasize what it is that the various disciplines accomplish. They leave undergraduates with a feeling that they understand what it is that engineers do, but without an appreciation for the social realities of *how* these tasks are accomplished.

This distinction is significant. Undergraduate coursework fosters the perception that the engineering working experience is one of solving highly conceptual, well-defined, science-based problems in a largely individualized setting, with emphasis on arriving at a single, objectively "correct" solution. But the reality that working engineers encounter is one of solving highly practical, undefined, procedural-based problems in an extremely tight-knit social setting, resulting in

**TABLE 1**  
**Overall Survey Results**  
(76 respondents)

*Response to the question:*

*"Do you have a firm idea of what it is that engineers do on a daily basis?"*

Very Firm Idea:	30%
Somewhat Firm Idea:	65%
No Firm Idea:	5%
No Idea Whatsoever:	0%

multiple potentially "correct" solutions. In his book *Designing Engineers*,<sup>[2]</sup> Louis Bucciarelli characterizes these fundamentally social aspects of engineering design and practice in the following manner:

*[P]articipants in design work within a rich, multidimensional environment that reaches well beyond the narrow confines of their own object worlds. A customer's needs are not given or discovered, but must be created; an operator's capabilities must be defined; building codes need interpretation;*

*costs must be tried out; budget limits must be agreed upon. The task must be organized into subtasks; suppliers must be coaxed to commit to a price and delivery date; the dropout problem at Photoquik must be constructed. All of this is designing. In all of this, choices are being made, decisions foreshadowed, and possibilities discounted.*

In other words, working engineers must create and manage formal and informal social structures in order to generate built products.

Success on the job therefore entails learning many complex social behaviors in addition to those necessary for classroom success. It also entails developing an entirely new perspective on what constitutes "engineering." Without restructuring the entire undergraduate experience to incorporate these workplace lessons, engineering educators can nevertheless prepare students for this impending paradigm shift by at least bringing it to their attention. In addition, there are many specific exercises that can be easily incorporated into the existing undergraduate curriculum to reinforce some of the nontechnical social skills necessary for success in the corporate workplace.

## **WORKPLACE REALITIES**

According to one early '80s study, "technical professionals typically spend over a third of their work week writing, editing, or preparing reports."<sup>[3]</sup> If you also include composing letters, proposals, drafting schedules and procedures, taking field notes, and generating other more informal modes of written communication, then "writing" easily occupies more than half of the typical engineer's work experience. Oral communication also occupies a major portion of the engineer's time. This can include time spent in meetings or on the phone with vendors or customers, time spent on the shop floor interacting with technicians and workers, etc.

Taken together, these two activities comprise by far the bulk of an engineer's work week. In the workplace setting that the vast majority of graduates will enter, typical engineers will likely use only 10% of their technical background 10% or so of the time. Of course, the specific 10% will vary widely for each individual, making technical breadth within the curriculum essential. But the fact remains that most of a working BS-level engineer's time will be spent not actively solving technical problems, but instead communicating potential technical solutions to others. Engineers' effectiveness, reputation, and career success will be based on technical expertise, yet determined by how well they manage to translate this expertise into action through mastering such nontechnical workplace skills as effective communication, organization, and persuasion.

This is, of course, not a one-way flow of information. For every memo that is written or presentation that is given, someone (presumably) reads and listens. The successful engineer also has to take in and interpret an enormous amount of written and verbal information. Organizing and making effective use of this information requires good critical reading and listening skills. Given the enormous amount of information generated in the typical corporate workplace, quickly and effectively separating the wheat from the chaff is an important skill in itself.

The vast majority of a BS engineer's time is taken up with both taking in and communicating information. Success requires possessing the "nontechnical" skills necessary to first recognize and then convince and organize others to act on information that is important.

## CONVEYING WORKPLACE REALITIES

So, how can you alert engineering undergraduates to this reality? One strategy is to suggest that effective communication is an essential engineering skill—one that can be just as important as any technical ability. In the words of historian Henry Petroski,<sup>[4]</sup> "some of the most accomplished engineers of all time have paid as much attention to their words as to their numbers, to their sentences as to their equations, and to their reports as to their designs." Pointing out to students the vital importance of mastering effective writing, reading, speaking, and listening reinforces the notion of engineering practice as a social activity.

Yet there are many other "nontechnical" skills that are also important to success at the BS level. If presented to students at all, these skills are most often communicated in the most general of terms, with successful engineers described as possessing "curiosity," "perseverance," "self-confidence," "common sense," and so forth. What undergraduates need is a resource that highlights the importance of specific skills, motivated by a concrete social context and picture of the day-to-day realities of corporate engineering practice. The key is to motivate students to appreciate the

complex social realities of engineering practice by giving them a tangible feel for the workplace setting that most will find themselves in.

**Using Popular Culture** • One resource for accomplishing this is the comic strip "Dilbert." In many respects, "Dilbert" is an entirely accurate ethnographic account of the typical BS-level engineering experience. According to one leading management consultant,<sup>[5]</sup> "It's not a comic strip, it's a documentary—it provides the best window into the reality of corporate life that I've ever seen." It therefore provides an excellent resource for undergraduates' (or anyone else, for that matter) interested in the daily interactions of practicing corporate engineers. "Dilbert" can be read as providing very specific, contextualized examples of the many workplace issues and challenges that BS-level engineers must confront and overcome in the process of applying their technical knowledge to real-world problems.

Of course, illustration does not imply prescription. "Dilbert" should certainly *not* be taken as illustrating a social ideal or model for how engineering professionals ought to navigate these issues. It can, however, offer a view of what some of these issues are and motivate students to contemplate how they would manage similar circumstances in a more constructive manner. "Dilbert" provides an alternative insider's perspective that, if presented as serious social satire and critique, can be a valuable learning tool for preparing for the reality of the engineering workplace.

Taking "Dilbert" as serious social commentary can prepare students for making the leap from viewing corporate engineering as a purely technical activity to seeing it as a technically mediated, yet essentially social, endeavor. It can also prevent the disillusionment commonly generated by the experience of realizing that daily workplace realities are quite different from naive undergraduate preconceptions.

**Discussing Specific Strategies** • A truly comprehensive list of specific social skills useful for managing "Dilbert"-like situations in a constructive manner would be almost infinite in length. This section merely presents five strategies that can be particularly critical to workplace success. "Newly minted" BS-level corporate engineers usually learn these strategies only after a sometimes painful and potentially damaging period of trial and error. Discussing these important nontechnical skills within the context of appropriate undergraduate coursework can benefit graduates by accelerating their on-the-job learning curve enormously.

1. *Save everything that crosses your desk.* Undergraduate education reinforces the notion that when something is "done," it's over with. With the end of each semester, textbooks are returned to the bookstore and class notes are relegated to recycled paper bins. But in the real world, projects never really come to an end. You never know when, say, a cost analysis done for a long-forgotten proposal might come in handy.

Saving old work (even draft work) can prevent future duplication of effort.

2. *Document everything in writing.* There is no such thing as an unambiguous verbal order.
3. *Learn to use a daily planner.* Some corporations provide a standard dayplanner system free of charge to technical employees, but even if their use is not officially encouraged, dayplanners are an essential tool for maintaining order in personal and project schedules (planning meetings, scheduling travel, keeping notes, maintaining contacts, etc.). Undergraduates are used to having order imposed for them—tests, project deadlines, class times, course materials, etc., are all organized in advance. This leaves novice engineers completely unprepared for the job of creating their own order from the chaos of daily events. A good dayplanner system is an indispensable tool for managing this process.
4. *Use the “plus a fifth” rule.* One of the most difficult things to learn in managing complex technical efforts is how to account for the unexpected. Even the most detailed, well-researched proposal or project plan can be subject to unanticipated delays, setbacks, cost overruns, and instances of Murphy’s Law in action. Planning for the unforeseeable is a management skill that can only be learned through experience. In the meantime, beginning engineers can instead simply assume that all but the most straightforward tasks will take 20% longer and cost at least 20% more than expected. Even if nothing goes wrong, coming in significantly under budget and ahead of schedule can be much preferable to the alternative for all involved.
5. *Learn where and when to compromise.* A critical skill for managing working relationships is knowing when an issue is important enough to battle over. One engineer who is employed by a large tool and home-appliance manufacturer characterizes this as realizing that “the sun doesn’t rise and set on a toaster oven.” Maintaining an uncompromising stance on, say, the color of a new product can make collaboration impossible. But no compromise should ever be made on any aspect of engineering design, production, or management that infringes on the health or social welfare of others. Students should recognize that they will have to make such distinctions for themselves and that the answers will rarely be clear-cut and obvious.

***Practicing Workplace Strategies in the Classroom*** • In

addition to simply discussing the aforementioned strategies, there are also many relatively simple, straightforward teaching techniques that can be employed to help students develop positive social working skills like good communication, organization, planning, patience, etc. Once again, presenting a truly comprehensive list would be impossible—

this is merely a collection of seven specific activities to illustrate the breadth of possibilities.

1. *Performing peer evaluations for student oral presentations.* Having undergraduates evaluate one another’s presentations in a structured manner would focus listening skills and give students practice in recognizing key points, initiating critical discussion, etc.
2. *Practicing giving oral and written equipment operation and sampling procedure directions.* Unit-op labs provide a plethora of opportunities for sharpening interpersonal communication skills. For example, students could actively direct and observe each other rather than passively following TA instructions. Also, students could be required to generate written operation and sampling procedures for subsequent lab groups to follow. These experiences would highlight the importance of precision and clarity in giving both written and verbal direction.
3. *Swapping notes for lab reports.* Another potential unit-ops exercise would be to require groups to exchange notes and generate reports based on each other’s data. This would highlight the importance of preserving data and other information for unexpected future uses while also stressing the necessity of precision and clarity in all forms of engineering communication.
4. *Writing and presenting standard business communications.* Practice in writing and speaking can be combined with aiding students in their job search. First, students could be asked to research and produce a short report and presentation on a particular industry or market. Then students could generate a resume and letter of application to an appropriate company based on their research. This would give students practice in evaluating what is important to individuals working within other organizations, while at the same time reinforcing proper business communications etiquette, sharpening business research skills, etc. Students could also gain valuable experience from attending departmental seminars and producing short memos or similar communications detailing key information presented, summarizing discussions, etc.
5. *Producing detailed project plans.* Senior design courses also provide a wealth of opportunities for practicing nontechnical, “real-world,” social and organizational skills. For example, students could be required to generate detailed project proposals outlining specifically what is to be done and how it will be accomplished, complete with a breakdown of activities, timelines for completion, etc. This would give students experience in organizing work and delegating responsibility in a formal and considered fashion. Coupling this activity with a proposal

presentation would also give students practice in clearly articulating and advocating a proposed course of action. Also, requiring periodic project updates would prompt students to manage delays and setbacks in an organized fashion.

6. *Dealing with vendors.* Another good senior design experience would be to ask students not just to model a process, but to also locate, spec out, and price the specific equipment necessary to make the process run. This could be done by simply giving students access to a Thomas Register (now available on the Internet) and a telephone. This would expose students to the realities of uncertainty and would likely require management of time and (imaginary) cost overruns.

7. *Rotating group members and responsibilities.* Performing well on corporate-engineering project teams means responding constructively to change. This can be simulated in the classroom by requiring students to periodically reshuffle project, lab, and homework groups. Similarly, specific roles such as coordinator, note taker, etc., can be rotated within groups. Having to constantly fill new roles and interact with different individuals would sharpen both leadership and collaborative, cooperative interpersonal skills.

In general, implementing these activities would require some extra TA work and additional time spent in providing more qualitative feedback on assignments. But all of these suggestions can be incorporated into existing coursework with a minimum of curricular disruption.

***Outlining the Positive “Qualities of Success”*** • Finally, simply presenting a few specific contexts of engineering practice can also motivate students to begin thinking about the contrasts between their undergraduate educational experience and their impending BS-level working reality. For example, successful engineers (whether employed in sales, processing, design, management, or any other capacity) are often called upon to

- **Recognize problems that aren't apparent**  
(For example, being able to walk through a production floor and see opportunities for cost-savings, or recognize subtle ethical questions that others overlook.)
- **Define problems that are nebulous**  
(Problems in the real world rarely come numbered for easy reference.)
- **Choose solutions that are realistic**  
(A skill that doesn't necessarily mean limiting the range of possible solutions—often the most successful engineers are ones who recognize the practical possibilities of seemingly impractical approaches.)
- **Plan how to make solutions work**  
(A process that includes marshalling resources, motivating others, keeping people on task, recognizing potential

*pitfalls, and a complex combination of many other discrete social skills.)*

- **Convince others to follow**  
(This involves recognizing that the importance and urgency of a “problem” and the feasibility of a “solution” are directly proportional to the skill and clarity with which they are presented and defined.)
- **Cooperate in dealing with contingencies**  
(This involves realizing that exercising patience and understanding with one's group members generates the cooperative solidarity necessary for overcoming crises.)

Undergraduates should view themselves as continually striving to meet this positive ideal through the constant acquisition of constructive practical social skills.

## CONCLUSION

In summary, undergraduate engineering students likely confuse familiarity with what engineers produce with what professional engineers actually do on a daily basis. This confusion is reinforced through introductory engineering survey courses and an overall curriculum that emphasizes the built products and technical aspects of engineering over the social processes through which these products are generated. Although students are given an opportunity for direct exposure to engineering workplace realities through intern and co-op experiences, the aforementioned preconceptions are counterproductive to using these experiences in the context of developing genuine, conscious insight into the essential social aspects of engineering practice.

Engineering educators would benefit students by simply alerting them to the fact that the creative, challenging process of learning to “do” engineering will not end, but only begins, at graduation. Likewise, undergraduates would benefit from being presented with contextualized examples of the daily workplace realities of corporate engineering life. Taking a few moments to illustrate the social side of engineering practice, along with devoting some curricular effort to reinforcing these aspects of engineering work, would help motivate students to think about their professional futures in concrete terms and provide undergraduates with a constructive context for developing positive professional social skills. In the end, this would result in more reflexive, more effective engineering professionals.

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# AUTHOR GUIDELINES

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