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chemical engineering education

VOLUME 34

NUMBER 2

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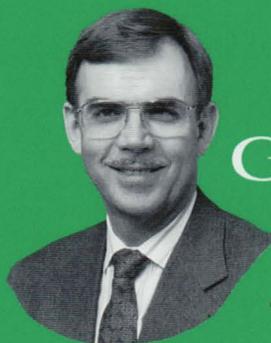


Chemical Engineering Division, American Society for Engineering Education

American Institute of Chemical Engineers

AWARD LECTURE- Part 2

Particle Dynamics in Fluidization and Fluid-Particle Systems: Teaching Examples, *Liang-Shih Fan*



G.V.(Rex) Reklaitis

of "Old Purdue"

- Toward Technical Understanding: Part 5. General Hierarchy Applied to Engineering Education (p.138)..... *Haile*
- Random Thoughts: The Scholarship of Teaching (p. 144) *Felder*
- Teaching PDE-Based Modeling to ChE Undergraduates: Overcoming Conceptual and Computational Barriers (p. 146) *Thompson*
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- Use of an Emission Analyzer to Demonstrate Basic Principles (p. 178)..... *Lodge*

...and chemical engineering at

UNIVERSITY OF ALBERTA

SPECIAL SECTION

THE FUTURE OF ENGINEERING EDUCATION

Part 3

Developing Critical Skills (p.108)
Woods, Felder, Rugarcia, Stice

Part 4

Learning How to Teach (p. 118)
Stice, Felder, Woods, Rugarcia



2000 ASEE Annual Conference

Chemical Engineering Division Program

June 18-21, 2000 • St. Louis, MO

Pre-Conference Workshop

"Modern ChE and ME Laboratory Instrumentation"
Sunday, June 18, 8:30 am to 4:15 pm
Coordinators:
Jim Henry and Charles Knight
Workshop Cost \$65

ChE Division Lectureship

Monday, June 19, 4:30-6:00 pm
Moderator Michael Cutlip
Washington University

Social Activities

ChE Division Reception
Monday, June 19, 6:30- 8:00 pm
Moderator Robert Ybarra
Washington University

ChE Division Awards Banquet

Tuesday, June 20, 6:30-8:00 pm
Moderator Michael Cutlip
Missouri Botanical Garden, Spink Pavillion
Guest Speaker Dr. Peter Raven,
Director of Missouri Botanical Garden
Cost: \$48

Technical Sessions

Session 2213, "ChE Instruction in the Future"

Tuesday, June 20, 8:30-10:15 am: Co-Moderators Kirk Schulz and Christopher Wiegstein
Paper 1: "Approaches or Learning and Learning Environments and Lecture Environments," Donald Woods, Andrew Hrymak, and Heather Wright

Paper 2: "Lectures or Electrons: Which Works Better for Chemical Engineering Fundamentals Class?" Billy Crynes, Connie and Barbara Greene

Paper 3: "An Inductive Approach to Teaching Heat and Mass Transfer," Robert Hesketh and Stephanie Farrell

Paper 4: "Expandable Polystyrene Batch Reactor Design: An Academic/Industrial Collaboration in Teaching Reaction Engineering," Robert Barat and Ronald Gabbard

Paper 5: "The Student Consultant: Enhancing Communication Skills in the Undergraduate Laboratory," Dennis Miller

Session 2313, "Instructional Technology: The Future of ChE Instruction?"

Tuesday, June 20, 10:30 am-12:00 pm: Co-Moderators Thomas Edgar and Scott Fogler

Paper 1: "Development of an Extended Campus Chemical Engineering Program," Jimmy Smart, William Murphy, G. Lineberry, and Bonita Lykins

Paper 2: "Molecular Simulation Via Web-Based Instruction," Peter Cummings, David Kofke, and Richard Rowley

Paper 3: "Analysis of Instructional Technology Usage in the Introductory Chemical Engineering Course," Richard Felder, Amy Michel, and Jan Genzer

Paper 4: "Information Technology and Chemical Engineering Education: Evolution or Revolution?" Thomas Edgar

Session 2513, "The Greening of the ChE Curriculum"

Tuesday, June 20, 2:30-4:15 pm: Co-Moderators Dennis Sourlas and Ashish Gupta

Paper 1: "Production of Clean Fuel: A Biochemical Experiment for Unit Operations Laboratory Developed Through Undergraduate Research Projects," Muthanna Al-Dahhan

Paper 2: "Minimizing the Environmental Impact of Chemical Manufacturing Processes," Joseph Shaeiwitz, Roger Schmitz, Mark McCready, Joan Brennecke, Mark Stadtherr, Richard Turton, and Wallace Whiting

Paper 3: "Development of an Elective Course on Pollution Prevention," Dennis Sourlas and Ashish Gupta

Session 2613, "Implementing Soft Skills Into ChE Curriculum"

Tuesday, June 20, 4:30-6:00 pm: Co-Moderators Douglas Ludlow and James Newell

Paper 1: "Integrating Soft Criteria into the Curriculum," W. Nicholas Delgass, Philip Wankat, and Frank Oreovicz

Paper 2: "Training in Multidisciplinarianism," Daina Briedis and R. Mark Worden

Paper 3: "An Industrial Internship Program to Enhance Student Learning and Marketability," Zenida Keil and Melanie Basantis

Paper 4: "An Investigation of the Communication Culture of an Introductory Chemical Engineering Class," Heather Cornell, Wade Kenny, and Kevin Myers

Paper 5: "The Business Meeting: An Alternative to the Classic Design Presentation," James Newell

Session 3313, "The Future of Engineering Education"

Wednesday, June 21, 10:30 am-12:00 pm: Plenary Session Moderator Dendy Sloan

Speakers: Donald Woods, "Intrinsic and Extrinsic Rewards of Teaching Excellence"; Richard Felder, "Teaching Methods That Work"; James Stice, "Learning How To Teach"; and Armando Rugarica, "A Vision for A New Century."

Session 3413, "ChE Laboratories in the Next Millennium"

Wednesday, June 21, 12:30-2:15 pm: Co-Moderators Richard Gilbert and Steve LeBlanc

Paper 1: "A Laboratory for Enhancing Process Control Courses Using Real-Time MATLAB/Simulink," Babu Joseph, Deepak Srinivasagupta, and Chao-Ming Ying

Paper 2: "A Fluidized Polymer Coating Experiment," C. Stewart Slater, Robert Hesketh, and Michael Carney

Paper 3: "Enhancement of Instrumentation and Process Control Studies at the Undergraduate Level," Rebecca Toghiani, Hossein Toghiani, Donald Hill, and Craig Wierenga

Paper 4: "Development of Unit Operations Fermentation Laboratory Experiment Using Industrial Collaboration," G. Dale Wesson, William Muth, Bryan Landen, and Egwu Kalu

Paper 5: "Introducing Freshmen to Drug Delivery," Stephanie Farrell and Robert Hesketh

Paper 6: "Incorporation of Graduate Facilities Into Undergraduate Unit Operations Laboratory," Muthanna Al-Dahhan

Session 3513, "ChE Education: How Do We Assess It?"

Wednesday, June 21, 2:30-4:15 pm: Co-Moderators Daina Briedis and Susan Montgomery

Paper 1: "Student Portfolios: Assessing Criteria 2000," Carolyne Garcia and Edgar Clausen

Paper 2: "The Process of Learning Chemical Engineering: What Works and What Doesn't," David Dibiasio, William Clark, Anthony Dixon, and Lisa Comparini

Paper 3: "Assessing Chemical Engineering Education As It Is Delivered," Joseph Shaeiwitz

Paper 4: "Principal Objects of Knowledge (POK's) in Colloquial Approach Environments," Pedro Arce

Session 3613, "ChE, Computers and the Next Millennium"

Wednesday, June 21, 4:30-6:00 pm: Co-Moderators Skip Rochefort and Valerie Young

Paper 1: "A Virtual Reality-Based Safety and Hazard Analysis Simulation," John Bell and Scott Fogler

Paper 2: "Combining High-Level Programming and Spreadsheets: An Alternative Route for Teaching Process Synthesis and Design," Jorge Gatica, Mauricio Colombo, and Marla Hern-ndez

Paper 3: "24x7: Lab Experiments Access on the Web All the Time," Jim Henry

Paper 4: "MATLAB Application in Reactor Design and Simulation," Charles Okonkwo and Gbikeloluwa Oguntimien

Paper 5: "Professional Simulation Packages as Effective Teaching Tools in Undergraduate ChE Curriculum," David Dixon, Jan Puszynski, and Larry Bauer

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Chemical Engineering Education

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CHEMICAL ENGINEERING EDUCATION (ISSN 0009-2479) is published quarterly by the Chemical Engineering Division, American Society for Engineering Education, and is edited at the University of Florida. Correspondence regarding editorial matter, circulation, and changes of address should be sent to CEE, Chemical Engineering Department, University of Florida, Gainesville, FL 32611-6005. Copyright © 2000 by the Chemical Engineering Division, American Society for Engineering Education. The statements and opinions expressed in this periodical are those of the writers and not necessarily those of the ChE Division, ASEE, which body assumes no responsibility for them. Defective copies replaced if notified within 120 days of publication. Write for information on subscription costs and for back copy costs and availability. POSTMASTER: Send address changes to CEE, Chemical Engineering Department, University of Florida, Gainesville, FL 32611-6005. Periodicals Postage Paid at Gainesville, Florida.

G. V. (Rex) Reklaitis

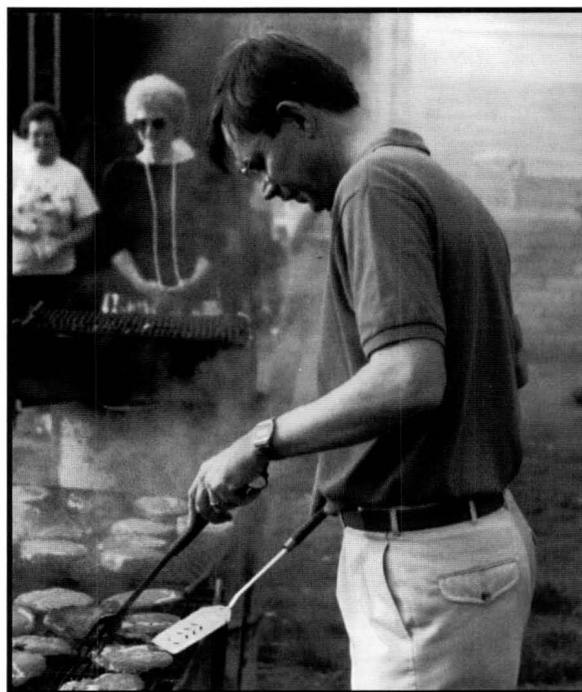
of
“Old
Purdue”

PHILLIP C. WANKAT, FRANK S. OREOVICZ
Purdue University • West Lafayette, IN 47907

Professor Rex Reklaitis' CV is impressive: Head at Purdue for twelve years, author or editor of six books and editor-in-chief of *Computers & Chemical Engineering*, with over 110 refereed publications and numerous seminar and conference presentations; involvement in the organization of 42 conferences and symposia; director of AIChE, past president and current trustee of CACHE; NSF postdoctoral fellow and Senior Fulbright Fellow; winner of the ASEE ChE Division lectureship award and ASEE ChE Division Corcoran award, Fellow of AIChE, winner of AIChE Computing in Chemical Engineering award; research advisor for 37 MS students and 28 PhD students, and involvement in grants for over five million dollars for research and over ten million dollars for the School of Chemical Engineering. Listening to this is enough to make any good Boilermaker sing *Hail, Hail to Old Purdue*.

But, what is Rex Reklaitis really like?

Out of the upheaval of World War II in Europe in 1942, the world gained one Reklaitis—Rex was born while his parents were traveling through German-occupied Poznan, Poland, on October 20—and lost another two years later when his father became a casualty of the war. From then on his uncles, and later his stepfather, filled that role as part of the extended family that helped mold Rex. They lived in Bavaria until moving to the United States when he was ten.

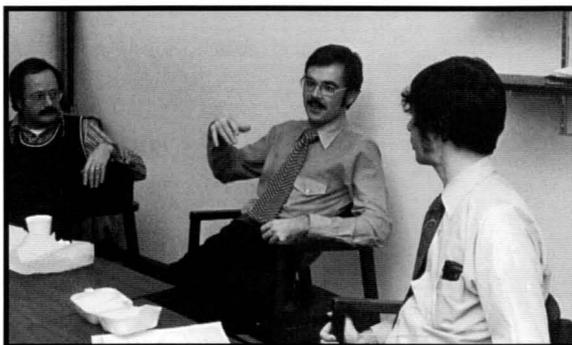


Professor-turned-chef grills 'em up at a departmental picnic.

Arriving in a new country at such a tender age, Rex was able to learn English much more quickly than is the experience of most adults—and without any trace of an accent. He was already bilingual in Lithuanian and German. Learning a third language also helped make him aware of the importance of grammar and structure in language, and before too long he was speaking as well as, if not better than, most native Americans. He and his mother became naturalized citizens in 1958. After graduating in 1961 from St. Rita high school in Chicago, he enrolled at the Illinois Institute of Technology [also alma mater of one author (FSO) and of the other author's father]. He graduated from IIT with a BS in chemical engineering in 1965. (Back then, graduating in four years was common.)

While growing up in Chicago, Rex became interested in classical music, especially opera, and learned to play

Rex with Ron Barile (left) and Lowell Koppel (right) at a faculty lunch in December of 1976. ►



Rex and Janine, hosts at a party in their home in 1994, sharing a smile with Ramki Ramkrishna and Linda Wang. ▼



Rex presents an award to Kristi Anseth (now a professor at the University of Colorado, Boulder) at the annual Razz banquet in 1991. ►



the mandolin and the clarinet—the love of music has remained with him through the years. He ran track and played tennis in high school, and his uncles introduced him to carpentry and sailing. Sailing and skiing (which he first did in high school on old-fashioned wooden skis) have remained his two major hobbies.

He met Janine when they were 15, but only she realized that it was a fateful meeting. He “awoke” when they later became reacquainted through student organizations at the end of their sophomore years in college. When Rex decided to go to graduate school at Stanford in 1965, Janine followed him and enrolled at the University of California-Berkeley. They were married on August 20, 1966.

Rex and Janine settled down in San Francisco and faced the daily routine of Rex taking the Southern Pacific to Palo Alto while Janine drove across the Bay Bridge to Berkeley. Commuting lost its charm after a while, so in 1968 Janine transferred to Stanford, and they moved to Palo Alto. Rex worked with Professor Doug Wilde at Stanford and also had significant interactions with Professors Andy Acrivos and David Mason. He took four years to earn his master’s degree and no time at all to earn his PhD, since both degrees were awarded in 1969.

(He claims that a secretary forgot to tell him to turn in a form to claim his master’s!)

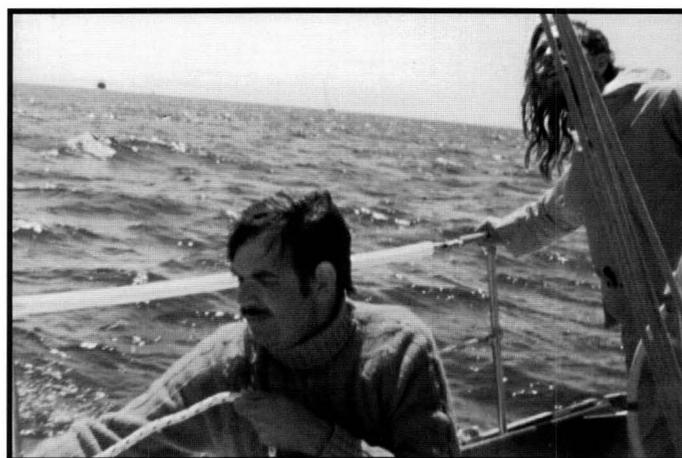
From 1969 to 1970, Rex was an NSF Postdoctoral Fellow at the Institut für Operations Research und Elektronisch Datenverarbeitung in Zurich, Switzerland. He worked with the Institute directors, Professors Künzi and Krelle on nonlinear optimization. Janine continued working on her PhD while they were in Switzerland.

In the summer of 1970, Rex started as an Assistant Professor at Purdue, a position he had accepted before starting his postdoctoral year in Switzerland. He and Janine settled in West Lafayette and Rex started the interesting and challenging life of an assistant professor while Janine finished her PhD (which she received from Stanford in 1972). She subsequently accepted a position as assistant professor of linguistics at the University of Illinois at Chicago, and once again the Reklaitis family became commuters as



Rex's first love—competing in the Chicago-to-Mackinac race, with his uncle aboard in 1979 (top photo, left) and again in 1980 in much rougher waters (bottom photo, left)...

...and his second love—skiing, here with Janine on the slopes in Breckenridge, Colorado, in 1999.



they moved to Crown Point, Indiana, which is essentially halfway between Chicago and Lafayette.

The eleven years in Crown Point were most productive for Rex. He drove the hour to Purdue three days a week on Interstate I-65, without a doubt one of the flattest and most boring highways east of the Mississippi. He survived the drive by listening to classical music and opera selections on the car stereo as he planned the day's events in the morning and processed them as he returned home in the evening. The other two days he spent working at home on his books and other research. With few interruptions at home he became very prolific, especially since he watches very little television and only occasionally sees a movie. Little did he know then that administrative duties would eventually reduce his research output.

Living near Lake Michigan also provided more time for sailing and put Rex and Janine close to the Chicago Lyric Opera. The family still purchases season tickets for the opera. Shakespeare forms another of his abiding interests.

Rex and Janine's oldest son, George, was born in 1974 and their youngest, Victor, in 1979. At Crown Point, Janine's grandmother and Rex's uncle lived with them and helped raise the two boys, giving the boys the experience and advantages of an extended family. The family moved back to West Lafayette in 1983.

At Purdue, Rex progressed steadily up the ladder, being promoted to associate professor in 1976 and full professor in 1980 while he was on sabbatical as a Senior Fulbright Lecturer at Vilnius State University and the Lithuanian Academy of Science in Vilnius, Lithuania (which was then an unwilling part of the USSR). Realizing Rex's special qualities, in 1985, Dean Henry Yang persuaded him to become the Assistant Dean of Engineering at Purdue.

In addition to his other duties, Rex was appointed as Interim Head of the School of Chemical Engineering in August of 1987 when Professor Ron Andres stepped down as Head. The School then prepared to start a new Purdue tradition—a long internal/external search for a new Head.

After a few weeks, though, it became evident to the chemical engineering professors on the committee that Rex was the ideal candidate. They were able to persuade the dean to forego the external search since it was clearly unnecessary. Thus, late in 1987, Rex officially became Head of the School of Chemical Engineering, an office he has since fulfilled with distinction.

Rex has been very successful in hiring outstanding new faculty and helping them obtain NSF CAREER and other prestigious grants. He has developed an active Industrial Advisory Council consisting of about twenty companies and frequently personally hosts the board members. The council is currently working with the faculty on five projects: continual renovation of equipment in the undergraduate laboratory, purchase of new research equipment, hosting young faculty at their research facilities, developing realistic design problems, and developing a survey of graduates and employers for an ABET outcomes assessment. After years of effort, Rex has also obtained approval from the administration to add a new wing to the chemical engineering building that will increase its space by sixty percent. This will allow for a much-needed increase in the size of the faculty. All chemical engineering has to do now is raise the money for this purpose!

Throughout all this time, Rex's teaching and research continued unabated. A dedicated teacher and educator who has taught many of the courses in the curriculum, he revised the introductory course in mass and energy balances at Purdue and developed new courses on "Optimization" and "Computer-Aided Process Design." His efforts on two of these courses resulted in two textbooks, *Introduction to Material and Energy Balances* (Wiley, 1983) and *Engineering Optimization*, with A. Ravindran and K. Ragsdell (Wiley, 1983). Both books have sold around 9500 copies—very respectable numbers. The second edition of the optimization book is currently being prepared.

Undergraduate students have always found Rex's office door open to them. He takes great care in teaching the senior



The Reklaitis family, at home for Christmas 1998.

design course, but despite his heavy schedule, enjoys morning meetings with student groups. He patiently pushes students to produce "just a little bit better" results. Then, during the spring semester he interviews most of the graduating seniors. These "exit interviews" provide very useful feedback to the school, and some of the ideas generated by them have been adopted. Rex has also been a strong advocate for student groups in chemical engineering. It is not unusual for the Reklaitis' to entertain up to 40 students from various groups in their home before Christmas vacation. Rex does his share by doing clean-up duty.

Working with a team assembled by Professor Bob Squires, Rex developed educational modules using videotape and computer simulations to give students a feel for complex processes. The modules were generously supported by industrial contributions, and the completed modules are being distributed by CACHE. Several articles on these modules have been published, the most famous of which, "Purdue-Industry Computer Simulation Modules: The Amoco Resid Hydrotreater Process" (*Chem. Eng. Ed.*, **32**, 98, 1991) by R.G. Squires, G.V. Reklaitis, N.C. Yeh, J.B. Mosby, I.A. Karimi, and P.K. Andersen, won the ASEE ChE Division Corcoran award for best paper that year. As a culmination of his interest in the use of computers in engineering education, Rex now serves on the editorial board for the journal *Computer Applications in Engineering Education*.

Rex's research in computer applications in chemical engineering and batch processing is well known. He developed, implemented, and demonstrated computer-aided methodology for the design, scheduling, and operation of batch processes. This research involved development of a modularly structured, dynamic/discrete process simulator that defined the structure of batch-processing networks and generated preliminary equipment sizes. In particular, his research highlighted the importance of intermediate storage and developed new scheduling algorithms for multiproduct plants.

Rex has coauthored well over 110 research papers and

Continued on page 153.

UNIVERSITY OF ALBERTA

Tradition and Innovation



Chemical & Materials Engineering Building

J. FRASER FORBES, SIEGHARD E. WANKE

University of Alberta • Edmonton, Alberta, Canada T6G 2G6

Chemical engineering has played a key role in the development of Canada's oil and gas and associated petrochemical industries, and chemical engineering at the University of Alberta (UofA) has been an integral part of the growth of the petrochemical industry in western Canada. The UofA is located in Edmonton, capital city of the Province of Alberta. The western part of the province is part of the majestic Canadian Rockies - The Continental Divide makes up a significant part of the western border between Alberta and British Columbia. The southeastern part of the province is part of the Canadian Prairies, while the north is part of Canada's extensive boreal forest. To the south, Alberta borders on Montana—Big Sky Country. Alberta also has a lot of "big sky"; there are more hours of sunshine per year than in any other part of Canada.

Oil and natural gas fields are found throughout the great sedimentary basin from the Alberta foothills in the west to the prairies in the east. Heavy oil and oil sand deposits, which contain more hydrocarbons than the Middle East, are located north and east of Edmonton. The discovery of oil in

the 1940s and the beginning of large-scale commercial development of the oil sands in the 1970s had major impacts on chemical engineering education in Alberta. The evolution and current state of the chemical engineering program, with some gazing into the future, make up the heart of this article.

HISTORY

The UofA opened for classes in 1908, about three years after the western part of the Northwest Territories of Canada became the Province of Alberta. The UofA campus is located on the south bank of the North Saskatchewan River, which flows through the center of Edmonton. The first Annual Calendar of the university described this site on the riverbank, 200 feet above the river, as a "beautiful wooded park, which lends itself splendidly to an architectural scheme suitable for university purposes." Today the campus is surrounded by the city of 700,000 inhabitants. Despite the tremendous growth of Edmonton, the river valley that runs through the center of the city is largely an undeveloped, beautiful park. As the city has grown, so has UofA. The

university's enrollment has grown from 45 students in 1908 to slightly over 30,000 in 1999.

Size of the chemical engineering classes has also grown from the first three graduates in 1928 (when chemical engineering was a special program in the Department of Chemistry) to between 65 and 70 Bachelor of Science degrees awarded annually for the last few years. Many other changes have occurred since 1928. In 1946, the department became one of the departments in the Faculty of Engineering, and in 1948, shortly after the discovery of a major oil field just south of Edmonton, it was renamed the Department of Chemical and Petroleum Engineering.

For the next 25 years, the department offered undergraduate and graduate programs in chemical and in petroleum engineering; it was also during this period that research began to be an increasingly important component of the department's activities. In 1973 the OPEC oil embargo precipitated an oil crisis, and the department again became the Department of Chemical Engineering when the petroleum engineering faculty members joined another department. In the late 1970s, a co-operative engineering program was introduced in which participants obtain 20 months of relevant industrial experience as part of the five-year undergraduate program. The majority of our chemical engineering undergraduate students are currently enrolled in the co-op program. The computer process control (CPC) program was introduced as an undergraduate elective stream in 1986 and the first students graduated from this unique program in 1989. (A more detailed history of our department can be found in Wanke^[1] and Mather.^[2])

The 1990s witnessed major changes. The department had 18 academic faculty members when the decade started, but by 1996 one-third of them had retired and been replaced and an additional two new positions had been created through expansion of the program. In addition, nine materials faculty joined the department, resulting in the first Department of Chemical and Materials Engineering in Canada. The influx of new staff brought with it excitement and new approaches to teaching and research in the department.

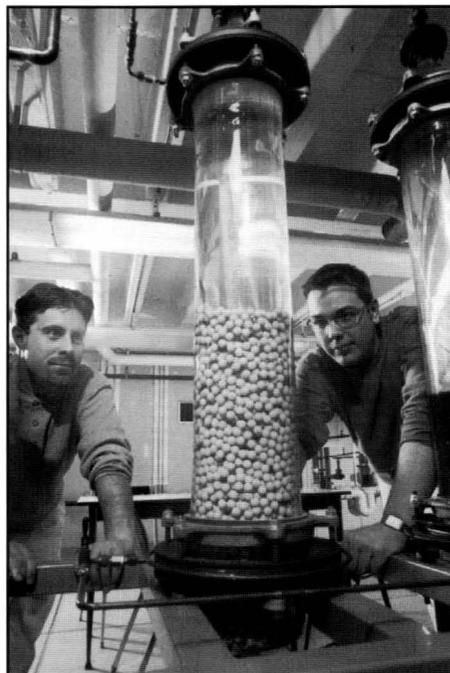
The changes and growth experienced in the 1990s were accompanied by significant growth in the numbers of undergraduate and graduate students. Each undergraduate engineering program has a quota in the sophomore year; the chemical engineering quota increased from 65 to 75 in 1996, to 90 in 1999, and will increase to 100 in 2001. About two-thirds of the chemical engineering

Application of surface-science principles to the process industries, and the development of mathematical and analytical tools for improved process performance and materials characterization, will be the focus of our research in the next decade.



◀ *Tina Barker in the departmental scanning electron microscopy laboratory.*

Undergraduate student and instructor next to fluidized bed column. ▶



sophomores completed their first year of engineering at the UofA; the remaining one-third are transfer students from junior colleges and transfers from other programs. A total of 299 undergraduate students are registered in chemical engineering in the 1999-2000 academic year. The number of graduate students has also increased significantly, from about 75 in 1996 to 110 in 1999; on the average, 40 to 45% of graduate students are PhD students and the remainder is enrolled in a variety of master's programs. The department also hosts a large number of postdoctoral fellows, research associates, and visiting faculty; currently 29 postdoctoral fellows, 22 research associates, and 5 visiting professors reside in the department.

The current academic staff consists of 24 chemical engineering and 10 materials engineering faculty; 16 of these 34 have been hired within the past five years, and there are four academic vacancies to be filled within the next three years. The department also employs 20 permanent support staff: three machinists and two electronics technicians who run the departmental machine and instrument shops and custom-build and repair equipment for undergraduate and research laboratories; two computing and network specialists who keep the computing, data acquisition, and network systems functioning; four laboratory technologists who assist with the undergraduate laboratories and operate special facilities such as the departmental scanning electron microscope; and the remaining support staff provide the clerical and administrative support necessary for smooth operation of the department.

The staff, graduate students, researchers, and some of the classrooms are housed in the Chemical and Materials Engineering Building. This 8-story, 184,000-ft² building was built in 1968, and currently over 80% of its space is occupied by the Department of Chemical and Materials Engineering, which will be the sole occupant of the building after an Electrical and Computer Engineering Research Facility is completed in 2001. Although the building is over thirty years old, it has been well maintained and the laboratory space is of excellent quality. Much of the large-scale separation equipment and high-pressure reactor facilities were constructed in the departmental machine and instrument shops. These two shops, along with the interfacing expertise of our computer staff, have contributed significantly to the success of our experimental research programs.

PROGRAMS

Teaching chemical engineering principles with applications to Alberta's industries is one of the main functions of

the department, and undergraduate students can choose from a variety of program and delivery options. Three degrees are offered: a BSc in Chemical Engineering, Chemical Engineering (Computer Process Control), and Materials Engineering—all of which can be completed in the traditional mode (eight academic semesters) or the co-operative education program (eight academic semesters plus twenty months of engineering work experience interspersed with the academic terms). Approximately one-third of the students are pursuing the regular route to their engineering degree and two-thirds are pursuing the co-operative route. All the programs are accredited by the Canadian Engineering Accreditation Board.

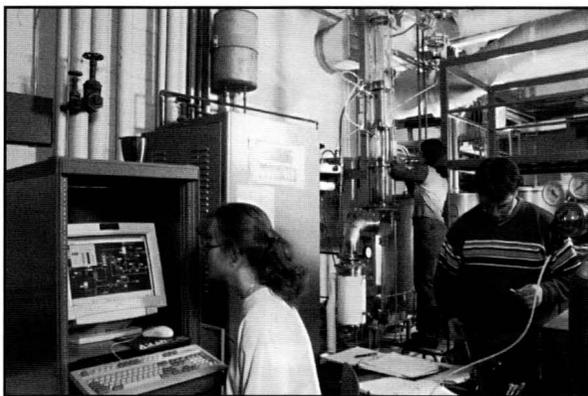
Undergraduate students usually enter the chemical engineering programs after a common first year of study, summarized in Table 1. First-year engineering students are placed in specific programs of study according to a quota for each program, based on their indicated preferences and grades. In March of each year, the first-year engineering students select three programs of study in which they are interested, ranking their choices in order of preference. Then, based on each student's

GPA and the quota for the various programs, the Faculty of Engineering assigns students to specific programs of study. The yearly entrance quotas for the chemical engineering programs currently total 90 students and will be expanding to 100 students within the next two years. Of the approximately 90 students per year that have been admitted to chemical engineering programs during the last several years, almost all have indicated chemical engineering as their "first" choice.

As shown in Table 2, the traditional chemical engineering program is similar to many programs across North America. The key exception is the emphasis placed on both chemical engineering laboratories and process design. The chemical engineering laboratories consist of three separate courses, which serve the dual purposes of providing the students with hands-on experience with pilot-scale chemical engineering processes (e.g., heat exchangers, distillation columns, fluidized bed systems, etc.) and report writing. The design stream includes courses in engineering economics and finance, as well as two single-semester process design courses. The engineering economics and first design course provide each student with a solid foundation to complete the second design course, which is project based. In this final design course, each student group, involving three or four students, chooses a separate design project drawn from local industries.

The CPC program is a blend of chemical engineering

Teaching chemical principles with applications to Alberta's industries is one of the main functions of the department, and undergraduate students can choose from a variety of program and delivery options.



▲ Undergraduate students doing the senior distillation laboratory.

fundamentals, specialty process-control courses, and components from electrical engineering and computing science. Wood^[3] provides a historical perspective on the program as well as details of the development and design of the program. In 1999, the CPC program was modified to create two streams: computing systems and signal processing. The two streams are defined by technical-elective packages. In the computing-systems stream, students take electrical engineering courses in digital logic and microprocessors, a second computing science course, and a further technical elective. In the signal-processing stream, students take an additional mathematics course in complex variable theory, the electrical engineering signal-processing course, a second computing science course, and a further technical elective. Thus, the CPC program uniquely positions students to fill a niche in the process industries.

At the graduate level, Master of Science (MSc), Master of Engineering (MEng), and Doctor of Philosophy (PhD) degrees in three disciplines (Chemical Engineering, Process Control, and Materials Engineering) are offered. The MSc and PhD degrees are research-based and require that a student take six graduate-level, single-semester courses for the MSc degree and nine graduate-level, single-semester courses for a PhD degree. Of these courses, three must be selected from a core program, with the remainder being chosen to suit the student's interests. Since these degrees are research-based, each student must also complete a thesis. At the PhD level, students must complete three written preliminary examinations taking three hours each (usually after the first eight months of the program) and a candidacy examination of the proposed research and the student's capability to pursue the proposed research. The MEng degree is course-based and requires completion of ten graduate-level, single-semester courses as well as a project. The MEng is considered to be a terminal degree and not a route to the PhD program.

Recently, at the graduate level, a number of joint degree programs have been evolving. The two programs currently in place are Chemical Engineering and Medical Sciences, and Chemical Engineering and Biological Sciences. Coursework includes core chemical engineering courses, courses taken from the "partner" discipline, and courses that match the student's interests. These joint degree programs are new to the UofA, but student interest is driving their development.

One of the strengths of the UofA programs is interaction with industry. This interaction occurs formally through some

▼ Dr. Suzanne Kresta and students in a problem-solving lab.



TABLE 1
Common
First-Year Engineering
Curriculum

Subject Area	Single Semester Course Equivalents
Chemistry	2
Physics	3
Mathematics	3
Computing	1
Humanities	1
Other	0.67

TABLE 2
Chemical Engineering Curricula
Beyond the First Year

Subject Area	ChE*	CPC**
Chemistry	2	1
Mathematics, Statistics, Numerical Methods	5	5
Thermodynamics	3	2
Transport Phenomena	4	4
Reactor Design and Analysis	1	1
Process Design, Analysis, and Economics	4	4
Chemical Engineering Laboratory	3	2
Process Control	1	4
Materials Science	1	1
Electrical Engineering Fundamentals	1	2
Technical Electives	4	4
Communications (oral and written)	1.67	1.67
Humanities	3	3
Other	0.67	0.67

* Chemical Engineering: figures given as single-semester course equivalents.

** Computer Process Control: figures given as single-semester course equivalents.

unique programs and research projects, and informally due to the diverse set of industries in the Edmonton area. The program that has the largest single impact on ensuring industrial interaction with the undergraduate students is the Stollery Executive-in-Residence program. It is used to bring practicing engineers from a variety of industries into the department to provide guidance to student groups working on their design projects; it usually requires a commitment of approximately two weeks of the practicing engineer's time, spread over an academic term. Further, the Stollery visitors usually bring design projects from their own companies with them. The visiting engineers are also invited to give special lectures in other courses, where they provide context for the course subject matter.

At the graduate level, a large and growing number of research projects enjoy the partnership of local companies. These often require graduate students to spend extended stretches of time in company labs or at plant sites. This trend toward industrial participation in the training of graduate students seems to be of interest to local industries and is expected to expand.

RESEARCH

The second main function of the department is research, which has focused on adding to the chemical engineering knowledge base and addressing problems of the process industries, with particular emphasis on Western Canadian industries. The oil and gas industries in Western Canada strongly influenced the areas of research in the department during the 1950s and 1960s. Establishment of world-scale petrochemical facilities in Alberta in the 1970s and 1980s influenced the direction of applied research, and the increasing importance of the synthetic crude production in the 1980s and 1990s opened up exciting new areas for application of chemical engineering fundamentals. Construction of modern pulp mills and newsprint facilities in the 1990s added another dimension to the department's applied research.

Funding for research comes from external sources: in the 1998-99 fiscal year, funding obtained by the academic staff, excluding central overhead charges, exceeded \$4.5 million (Cdn); about 65% of the funds came from federal and provincial government agencies, and the remaining 35% came from industry. Five of the main areas of chemical engineering research are briefly described below.

Catalytic Reaction Engineering • Catalysis and reaction engineering research has been done in the department since the 1950s when investigation of selective hydrocarbon oxidation and Claus catalysis were started. Claus catalysis for the conversion of hydrogen sulfide to elemental sulfur is still of great importance since most of Alberta's natural gas contains hydrogen sulfide. These studies not only resulted in significant improvements in sulfur recovery, but also resulted in the development of techniques (such as infrared methods) for examination of fundamental processes

occurring on the surfaces of heterogeneous catalysts. Understanding the behavior of these catalysts led to the application of hydrophobic supported metal catalysts, which are finding applications in new processes such as the production of hydrogen peroxide and for the removal of organic compounds from contaminated aqueous streams. These catalysts are also well suited for catalytic distillation for water-containing systems. Current catalytic reaction engineering projects include: catalysts for environmental applications (both liquid and air), development of catalytic distillation processes, heavy-oil upgrading catalysts, and olefin polymerization catalysts (Ziegler-Natta and single-site catalysts). Departmental facilities for catalytic studies include various catalyst characterization equipment (chemisorption and physisorption, x-ray diffraction, scanning electron and atomic force microscopies, and infrared spectroscopy) as well as numerous reactors, including a continuous high-pressure system for studying hydrocracking of bitumen and a reactor system for catalytic olefin polymerization in the gas phase.

Computer Process Control • With the establishment of the Data Acquisition and Control and Simulation (DACS) Centre in the department in 1968, research in computer process control became one of the main research areas in the department. Each one of the many workstations in the center today has much more computational power than the IBM 1800 housed in the original DACS Centre, but the general aim of today's research is the same as that of three decades ago (*i.e.*, development of techniques that allow computers to be used for improving the efficiency and reliability of industrial process operations). Research areas have broadened over the years from the more traditional process control and identification to include process monitoring and the application of multivariate statistics, controller-performance assessment, artificial intelligence, process-fault diagnosis, and process optimization. The size of the process-control research group has grown commensurate with the broadening of the research scope. The computer process-control research facilities include a network of computers (Unix workstations and personal computers) and experimental equipment, including pilot-scale reactors, distillation columns, and other small experiments.

Fluid Mechanics and Transport Phenomena • The study of multiphase flow and flow in porous media, with emphasis on oil pipe lines and crude oil reservoirs, were major topics of research in the department from the 1940s to the 1970s. In the 1970s and subsequent decades, research shifted to experimentation and modeling of complex flows with applications to the transport processes encountered in the processing of oil sands. The work included modeling of complex processes used in the extraction of bitumen from sand, as well as experimentation necessary to increase understanding of the chemistry and physics that govern the processes in the liberation of the bitumen from the surface of the sand and subsequent processing of the bitumen. Research in this area contributed significantly to the improvement of commercial processes for the economic production of synthetic crude from the Alberta oil sands. Syncrude Canada Ltd., the largest producer of synthetic crude (225,000 bbls per day in 1999) has recognized these major contributions and co-sponsors, with the Natural Science and Engineering Research Council of Canada) two industrial research chairs in the department. Research in this area is moving from the continuum to the molecular level. Current projects include measurement of interfacial properties of individual drops in emulsions, interactions between bitumen droplets using a microcollider appa-

ratus, and stabilization of bitumen-in-water emulsions by clays. Other active projects in this area include fluid dynamics aspects of pulp and paper processing and computational (CFD) and experimental studies in the area of mixing and separation equipment optimization.

Thermodynamics and Separation Technologies • Thermodynamics research, largely dealing with vapor-liquid equilibrium of systems related to oil and natural gas, started in the 1940s. It culminated in the 1970s with the publication of the Peng-Robinson equation of state. The separation research in these decades emphasized the measurement of data and modeling of systems used in the removal of hydrogen sulfide and carbon dioxide from natural gas. The process models developed for the sour-gas separation units and the vapor-liquid equilibrium data obtained for the amine-sour gas systems are still used today. In the 1980s, separation research shifted to improving the energy efficiency of packed and trayed columns. Fundamental work on factors affecting the efficiency of separation columns, including studies in interfacial properties, resulted in the development of column packings and column internals with improved efficiencies. These improvements are being used commercially. Current work is using the vastly increased power of computational fluid-dynamics (CFD) packages to model the influence of packing geometry on detailed flow patterns, with the aim of improving separation efficiencies. Distillation and packed towers, with one-foot diameters, are used to validate the CFD predictions. Research projects in thermodynamics today deal with the application of statistical rate theory to interfacial and membrane transport, experimental and molecular simulations of miscibility of polymer blends, and measurement of hydrocarbon solubility in polymers.

Advanced Materials • This is the most recent general area of research in the department. It started in the 1980s with an industrial-sponsored project on gas-phase olefin polymerization; the use of new catalysts to produce polyolefins with novel molecular architecture continues to be an active research area. Investigation into the thermorheological properties and microphase separation in block copolymers is ongoing. The preparation of magnetic microparticles with different surface functionalities is being studied; such particles have wide application in removal of contaminants from industrial effluents, carriers for drug delivery, and biological cell separation. The merger with materials engineering in 1996 brought many projects in advanced materials into our department, including surface modifications for improved wear resistance, preparation of electronic materials, and sintering of cemented tungsten carbide.

Other Research Activities • Academic staff participates in various formal interdisciplinary projects beside the chemical-materials projects; these include projects with the Departments of Biological Sciences, Chemistry, Civil and Environmental Engineering, Electrical and Computer Engineering, Mathematics, and Mechanical Engineering. Graduate students, who will receive double major degrees as described previously, are involved in several of these interdisciplinary projects. There are also joint research projects with other Canadian universities as well as with universities in China, Germany, Great Britain, New Zealand, Poland, Taiwan, and Thailand.

THE FUTURE

Chemical engineering continues to change, and the pro-

grams at the UofA are no exception. The huge increases in computing and networking systems will affect the delivery of undergraduate and graduate programs and influence theoretical, modeling, and experimental research. Increasingly powerful and reliable design packages will reduce the amount of instruction dealing with empirical information, *e.g.*, property and transport correlations. The efficiencies provided by improved software and computing systems will be used to include more instruction on interfacial and molecular processes (*e.g.*, molecular phenomena important in colloidal suspensions, emulsions, and adsorption).

This return to the fundamentals of chemical engineering and applied chemistry is needed if our students are to play a major role in the burgeoning oil-sands industry. The increased reliance in Canada on synthetic crude oil, up to 50% of Canada's oil use of 2010, will require chemical engineers with a sound knowledge base in interfacial science (*e.g.*, the molecular processes involved in removal of high molar mass hydrocarbons from sand, the processes involved in the economic removal of solids from "stable" colloidal solids in process water suspensions, and the removal of corrosive materials present in submicron suspensions or emulsions). The revised curriculum should also reflect the changes in process control tools available today (*e.g.*, dynamic process simulation software, computer-aided mathematics packages, robust-optimization packages, etc.).

The applied research in the department will continue to focus on the main industrial activity in Alberta; the oil-sands (synthetic crude oil) industry, the petrochemical industries, and the pulp-and-paper industry. These industries will continue to be the core of Alberta's process industry for many decades, and the problems to be solved will be a continuing challenge to the university. The increased capabilities of available analytical, instrumental, and computational tools will allow solution of previously intractable problems; however, the basic principles of science and mathematics are still applicable to these problems. Departmental research will concentrate on the application of fundamental science and mathematics to the solution of practical problems and the development of new tools and techniques to solve these problems. Application of surface-science principles to the process industries, and the development of mathematical and analytical tools for improved process performance and materials characterization, will be the focus of our research in the next decade.

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THE FUTURE OF ENGINEERING EDUCATION

Part 3. DEVELOPING CRITICAL SKILLS

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In the first paper in this series^[1] we proposed that our goals as engineering educators should include equipping our students with problem-solving, communication, teamwork, self-assessment, change management, and lifelong learning skills. These goals are consistent with ABET Engineering Criteria 2000,^[2] currently a consideration of great importance in the United States and (we predict) in other countries in the near future. In the second paper^[3] we described a variety of instructional methods that have been shown to improve student learning. In this paper we will consider the application of some of those methods to the development of the desired skills.

Process skills are “soft” skills used in the application of knowledge. The degree to which students develop these skills determines how they solve problems, write reports, function in teams, self-assess and do performance reviews of others, go about learning new knowledge, and manage stress when they have to cope with change. Many instructors intuitively believe that process skills are important, but most are unaware of the fundamental research that provides a foundation for developing the skills, so their efforts to help their students acquire the skills may consequently be less effective than they might wish.^[4,5]

Fostering the development of skills in students is challenging, to say the least. Process skills—which have to do with attitudes and values as much as knowledge—are particularly challenging in that they are hard to explicitly define, let alone to develop and assess. We might sense that a team is not working well, for example, but how do we make that intuitive judgment quantitative? How might we provide feedback that is helpful to the team members? How can we develop our students’ confidence in their teamwork skills?

Research done over the past 30 years offers answers to these questions. In this paper, we will suggest research-

backed methods that will help students to develop critical skills and the confidence to apply them. As was the case for the instructional methods discussed in Part 2,^[3] all of the suggestions given in this paper are relevant to engineering education, can be implemented within the context of the ordinary engineering classroom, use methods that most engineering professors feel comfortable with, are consistent with modern theories of learning, and have been tried and found effective by more than one educator.

Research suggests that the development of *any* skill is best facilitated by giving students practice and not by simply talking about or demonstrating what to do.^[4-6] The instructor’s

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role is primarily that of a coach, encouraging the students to achieve the target attitudes and skills and providing constructive feedback on their efforts. A number of approaches to process skill development have been formulated and proven to be effective in science and engineering education, including Guided Design,^[7-10] active/cooperative learning approaches,^[3,11-16] Thinking-Aloud Pairs Problem Solving (TAPPS),^[17-20] and the McMaster Problem Solving program.^[4,18-20]

EIGHT BASIC ACTIVITIES TO PROMOTE SKILL DEVELOPMENT

The following activities promote establishing an effective learning environment for process skill development:

1. *Identify the skills you want your students to develop, include them in the course syllabus and (if department faculty agree) the university catalog, and communicate their importance to the students.* If developing problem-solving and teamwork skills are among your objectives for a course, include “problem solving” and “teamwork” in the list of course topics in the syllabus and university catalog and allocate time for activities that will provide practice in them.^[7,21] Be sure the students understand the relevance of the skills to their professional success, and discuss the skills with the same level of seriousness and enthusiasm that you use when presenting the technical content of the course.

2. *Use research, not personal intuition, to identify the target skills, and share the research with the students.* Table 1 summarizes evidence-based target problem-solving skills. A more complete compilation of novice versus expert evidence is given by Woods,^[22] with more recent evidence also available.^[23,24] Target skills have also been identified for communication,^[25-28] teamwork,^[11,16,29-36] assessment (including self-assessment),^[29,37,38] lifelong learning,^[4,39-47] and change management.^[4,48-52]

3. *Make explicit the implicit behavior associated with successful application of the skills.* Much processing takes place subconsciously in the head of a skilled practitioner. When asked “How do you do that?” the reply is often “I don’t know; it just happens.” Our task is to take the skill and behavior apart, discover what is really important (based on research), and communicate it to the students in easily digestible chunks. Illustrative objectives and assessment methods for most skills can be downloaded

TABLE 1
Some Evidence-Based Components of Expert Problem Solving^a

Problem solving is the process used to effectively and efficiently obtain the best value of an “unknown” or the best decision for a given set of constraints when the method of solution is not obvious.^b

Evidence-based targets	Progress toward internalizing these targets				
	20%	40%	60%	80%	100%
1. Describe your thoughts aloud as you solve problems.					
2. Occasionally pause and <i>reflect</i> about the process and what you have done.					
3. Do not expect your methods for solving problems to work equally well for others. ^c					
4. Write things down to help overcome the storage limitations of short-term memory (where problem solving takes place).					
5. Focus on accuracy and not on speed.					
6. Interact with others. ^c					
7. Spend time reading the problem statement. ^d					
8. Spend up to half the available time defining the problem. ^c					
9. When defining problems, patiently build up a clear picture in your mind of the different parts of the problem and the significance of each part. ^f					
10. Use different tactics when solving exercises and problems. ^g					
11. Use an evidence-based systematic strategy (such as read, define the <i>stated</i> problem, explore to identify the <i>real</i> problem, plan, do it, and look back). Be flexible in your application of the strategy.					
12. Monitor your thought processes about once per minute while solving problems.					

^a (© by Donald R. Woods, 1998). Some of the items in this table are derived from material in References 22–24.

^b This process is in contrast to exercise solving, wherein the solution methods are quickly apparent because similar problems have been solved in the past.

^c An important target for team problem solving.

^d Successful problem solvers may spend up to three times longer than unsuccessful ones in reading problem statements.

^e Most mistakes made by unsuccessful problem solvers are made in the definition stage.

^f The problem that is solved is not the problem written in the textbook. Instead, it is your mental interpretation of that problem.

^g Some tactics that are ineffective in solving problems include (1) trying to find an equation that includes precisely all the variables given in the problem statement, instead of trying to understand the fundamentals needed to solve the problem; (2) trying to use solutions from past problems even when they don’t apply, and (3) trial and error.

from the World Wide Web.^[7,51]

4. *Provide extensive practice in the application of the skills, using carefully structured activities, and provide prompt constructive feedback on the students' efforts using*

There is a temptation for instructors to select their own terminology for problem-solving strategies in their courses. This temptation should be resisted. . . . being exposed to different problem-solving terminology in different courses is a source of confusion to students.

evidence-based targets. People acquire skills most effectively through practice and feedback. No matter how many times students may see a skill demonstrated, they rarely master it until they attempt it and receive guidance in how to improve their performance after each attempt.

5. *Encourage monitoring.* Monitoring is the metacognitive process of keeping track of, regulating, and controlling a mental process, considering past, present and planned mental actions. As students are working, ask them to pause periodically and write responses to questions that force them to deepen their problem-solving approach and improve their understanding. For example,

- ▶ Why am I doing this?
- ▶ What really is the problem?
- ▶ What are the constraints?
- ▶ If I was unsuccessful, what did I learn?
- ▶ Am I finished with this stage?
- ▶ What options do I have? Which is most likely to succeed?
- ▶ Can I write down these ideas?
- ▶ Can I use charts, graphs or equations to represent the ideas?
- ▶ If I had a value of, how would that help me in solving the problem?
- ▶ Can I check this result?
- ▶ Have I spent enough time defining the problem?
- ▶ What other kinds of problems can I solve now that I have solved this one correctly?

Schoenfeld^[52] has shown the importance of monitoring in the development of problem-solving skills.

6. *Encourage reflection.* Reflection is the metacognitive process of thinking about past actions. For each problem the students solve, each communication they write or team task they accomplish, periodically ask them to write reflections

on how they approached the task. For example, Kimbell, *et al.*,^[23] report that occasionally asking students to stop the problem-solving process and describe what they are doing improves the problem solving and the quality of the product. For example, students may be asked to respond to questions such as "What did you do?" and "What did you learn about problem solving?" Schon,^[53] Chamberlain,^[54] Brookfield,^[55] and Woods and Sheardown^[56] also highlight the importance of reflecting.

7. *Grade the process, not just the product.* For some assignments, grade *only* the problem-solving process, the team process, or the prewriting process. Grade the reflections, using the target skills (*e.g.*, those listed in Table 1) as the criteria. Some specific examples are available for problem solving^[57] and teamwork.^[35]

8. *Use a standard assessment and feedback form.* Departmental instructors should decide on criteria, and the same assessment and feedback forms should be used across the curriculum.

DEVELOPING PROBLEM-SOLVING SKILLS

In addition to the eight basic activities,

- *Use a standard research-based problem-solving strategy across several (and ideally, all) courses in an instructional program.* There is a temptation for instructors to select their own terminology for problem-solving strategies in their courses. This temptation should be resisted. Only a few of more than 150 published strategies are based on research, and being exposed to different problem-solving terminology in different courses is a source of confusion to students. Select an evidence-based strategy such as the six-stage McMaster Problem Solving Strategy: Engage, Define the Stated Problem, Explore, Plan, Do It, and Look Back.^[58]

- *Solve some problems in depth.* If you would normally work through four problems in a given period of time, take the same amount of time to solve just one problem and hand out illustrative solutions for the other three. Enrich the experience for the students when you work out the problem: for example, purposely make wrong assumptions so that they eventually realize that "this is not working out." Take time to explore questions like "What went wrong?" "What have we learned?" "Now what?" Ask the students to carry out some of the problem-solving tasks, individually or in small groups. Anonymously display on transparencies students' attempts to carry out specific steps such as identifying the system, defining the problem, drawing a diagram, and creating symbols for unknowns.

- *Help students make connections between the problem statement, the identification of required technical knowledge, and the problem solution.* For example, "We have just solved problem 5.6. Identify the key words in the problem

statement that helped you to identify the information needed to solve the problem. Which key words helped you identify the required simplifying assumptions?" Explicitly making such connections helps build problem-solving expertise.^[21,59]

Writing Skills

In addition to the eight basic activities, *give assignments that require writing*. Long essays are not required: single paragraphs can be effective at facilitating the development of writing skills and do not impose a heavy grading burden on the instructor. Brent and Felder^[60] offer suggestions for brief writing assignments that address a variety of different instructional objectives. In-class writing exercises are particularly valuable in that they provide snapshots of what the students actually do. Students can often be observed following a typical pattern of unsuccessful writing: they sit with pen poised, staring at the paper and waiting for inspiration to strike. Encourage them to brainstorm ideas about the topic and about the target audience and to try to find a match between the audience needs and the topic. Suggest that they free-write without critiquing themselves and then discard sections that don't work.

Teamwork Skills

Many instructors seem to believe that simply giving three or four students something to do together—a laboratory experiment, for example, or a process design project—should somehow enable all of them to develop the skills of leadership, time management, communication, and conflict resolution that characterize high-performance teams. Unfortunately, it is not that easy. What often happens under such circumstances is that one or two students do most or all of the work and all students get the same grade. This promotes a great deal of resentment of both the slackers and the instructor. It does not promote development of teamwork skills.

If promoting teamwork skills is an objective, use a structured approach to teamwork such as *cooperative learning*^[11,13,15] in addition to the basic eight activities. The team assignments should be structured to assure positive interdependence (that is, if anyone on the team does not fulfill his or her responsibilities, everyone is penalized in some manner), individual accountability for all the work done on the project, face-to-face interaction (at least part of the time), development and appropriate use of interpersonal skills, and regular self-assessment of team functioning.

Part 2 of this series^[3] offered suggestions for meeting the defining criteria of cooperative learning and for overcoming the resistance that some students initially feel toward the approach. The following procedures help make students aware of several of the requisites of good team functioning:

- *Assign a chairperson/coordinator for every meeting.*

Research has shown that groups function better if a designated chairperson coordinates arrangements. The chair's tasks are to schedule meetings, to make sure that all team members know what they are supposed to do prior to each meeting, and to keep everyone on task. Research also shows that the chair's role differs from the role of leader^[33]—someone who holds greater decision-making authority than the other team members—although serving as chairperson helps develop leadership skills. (We do not recommend including

Many instructors seem to believe that simply giving three or four students something to do together—a laboratory experiment, for example, or a process design project—should somehow enable all of them to develop the skills of leadership, time management, communication, and conflict resolution that characterize high-performance teams. Unfortunately, it is not that easy.

the role of leader in team activities.) Require the chairperson to prepare and circulate an agenda ahead of time and ask the group to give written feedback to the chair at the end of each meeting. The chairperson can use this input to reflect on his/her skill and to set targets for improvement.

- *Have the group hold a "norms" meeting soon after they are formed.* Ask the teams to hold a meeting at which they decide on group behavior norms, reaching consensus on specified questions such as "What is the role of the coordinator?" "How will we handle missed meetings and lateness?" "How will we make decisions?" "How will we deal with team members who repeatedly fail to meet their responsibilities?" "How will we deal with conflicts that develop in the group?" The teams should summarize their norms on a sheet of paper, sign it, and turn a copy in to the instructor. Several weeks later, the instructor might return the copy and ask them to reflect on how well they are meeting the norms. A checklist of 17 items that should be addressed in establishing norms is available.^[7]

- *Ask students to complete inventories such as the Myers-Briggs Type Indicator,^[61] FIRO B,^[31,62] Johnson's conflict inventory,^[63] or the Index of Learning Styles.^[64]* Suggest that team members share their results and discuss the implications, making sure they are aware that the most effective groups include people with different styles. Although differences might lead to apparent conflict, they can be used to bring a synergy to group activities that might otherwise be unattainable.

- Incorporate formal team-building exercises as part of

your implementation of cooperative learning.^[16]

Self-Assessment Skills

In addition to the basic eight activities,

• *Have the students write resumes.* Although workshop activities can develop self-assessment skills, a concrete activity such as writing a resume is an excellent way to put the skill to practical use.

• *Include self-assessment as part of what you do to help develop any other skill.* Combine writing, reflection, and self-assessment by requiring students to submit their analysis of evidence of skill mastery gathered from classwork and other applications of the skills. Examples of such reports are available on-line.^[7] Data show that self-assessment tends to correlate with external assessments of skill mastery.^[7,51,65]

Lifelong Learning Skills and Problem-Based Learning

The learning process may be broken down into the following tasks:^[66]

- Sense problem or need
- Identify learning issues
- Create learning goals and assessment criteria
- Select resources
- Carry out the learning activities
- Design a process to assess the learning
- Do the assessment
- Reflect on the learning process

In traditional instruction, the student is responsible only for the fifth of these tasks (learning activities), the last task (reflection) is usually omitted, and the instructor takes responsibility for the remaining tasks. *Lifelong learners*, on the other hand, take some responsibility for performing all of the tasks themselves.

One approach is to focus one of the eight tasks on lifelong learning. For example, cooperative groups could be asked to “identify the learning issues” in a problem. Another more ambitious option is to *convert “reporting back” to “teaching.”* When students have completed an independent study or a research project, they typically report back by giving a speech. The class listens with varying degrees of interest. The dynamics change if the student *teaches* the material to a small group. The audience listens intently and asks questions, because now each of them is expected to *learn* the material being presented. The student speaker becomes the teacher. He/she learns and applies the ideas offered in Part 2 of this series^[3] and receives the benefits of those that will be presented subsequently in Part 4 (how to train the teachers).

Perhaps the most ambitious option for promoting the

development of skills in most of the tasks is called *problem-based learning* (PBL).^[47,66,67] Problems and projects can be incorporated into a course in a variety of ways. At one extreme is the traditional approach in which problems are given at the end of each text chapter and homework is assigned after the professor has lectured on the subject. The role of the problems is to help students deepen their understanding of previously-acquired knowledge. In contrast, when PBL is used, the problem is posed *before* the students have acquired the knowledge needed to solve it. This inductive ordering simulates the research environment: the students begin with a problem and then proceed to figure out what they need to know, create hypotheses, read the literature and/or search the Web, talk to experts with related knowledge, acquire critical information through modeling, experimenting and discovering, and finally solve the problem. The approach may be applied in any educational setting including lecture classes, laboratory courses, and design courses.^[68]

Once a problem has been posed, different instructional methods may be used to facilitate the subsequent learning process—lecturing, instructor-facilitated discussion,^[51] guided decision-making,^[8–10] or cooperative learning.^[3,11,13–16] As part of the problem-solving process, student groups can be assigned to complete any of the learning tasks listed above, either in or out of class. In the latter case, three approaches can be adopted to help the groups stay on track and to monitor their progress: (1) give the groups written feedback after each task, (2) assign a tutor or teaching assistant to each group, or (3) create fully autonomous, self-assessed “tutorless” groups.

Guided decision-making^[8–10] is a model for the first option. The instructor anticipates how groups might handle each learning task and creates written feedback to guide the process. This approach was designed to allow one instructor to manage many groups at a time. It has been used successfully in the teaching of engineering design at the University of West Virginia^[68] and of pharmacy at Purdue University.^[69] Option #2—assigning a tutor to each group of four to seven students—has been used extensively in the health sciences.^[43,46]

Option #3 is used when a tutor cannot be provided for each group (a common situation in engineering) and/or when the goal is to move students away from dependence on the instructor toward independence and interdependence. Each group is trained and empowered with process skills (described previously in this paper); the groups monitor and self-assess their work; and the instructor establishes conditions to aid the groups in self-management.^[7,70] The instructor should select a technical topic that would normally be “lectured” on for about three weeks, and use PBL to address it instead. The instructor’s role is to create the environment, monitor the students’ progress, and help them reflect on the

lifelong learning skills they are developing. Illustrative student reflections and self-assessments are available,^[7] as are more examples of how to move gradually into a full PBL model.^[51] This approach has been used successfully in engineering, science, and pharmacy education.^[4,71-73]

Extensive evaluation of small-group, self-directed, self-assessed, interdependent (cooperative) problem-based learning has been reported for medical schools.^[44-46] National Board Medical Examination scores earned by students in such programs were compared with scores earned by students in conventional programs. The experimental group scored lower on the exams testing basic science, while the opposite result was observed for the exams testing medical problem solving. The differences were statistically significant. The students who participated in a PBL program exhibited a greater tendency to adopt a deep (as opposed to surface or rote) approach to learning,^[74-77] a greater mastery of interpersonal and lifelong learning skills, and greater satisfaction with the learning experience. Positive program evaluations of the McMaster Problem Solving program in engineering^[4] and of the Guided Decision-Making Model^[10] have also been reported; however, the role of PBL in attaining these outcomes could not be easily determined because the programs studied involved multifaceted skill development efforts.

Change-Management Skills

People inevitably encounter unexpected and stressful changes in their lives, but successful people are able to cope with the changes in such a way that they emerge with renewed or even greater strength in performance, self-confidence, and interpersonal relationships, even if they initially experience losses in these domains. Stressful changes that students might experience include leaving home for the first time, being exposed to unaccustomed intellectual challenges, being thrust into a student-centered learning environment in which the instructor can no longer be counted on to supply all required knowledge, and making the transition from an academic world to the professional world.

Perry's Model of Intellectual Development^[40,67,78,79] (or an equivalent model such as King and Kitchener's *Model of Reflective Judgment*^[80]) provides a good framework for helping students cope with the expectations of the new learning

environment. According to William Perry, a Harvard psychologist, college students progress through some or (in rare cases) all of the following stages of development.

- Level 2 (Dualism). Every point of view is either right or wrong. All knowledge is known and obtainable from instructors and texts, and the student's task is to absorb what the instructor presents and demonstrate having done so by repeating it back. Confusion occurs if the text and the instructor do not agree. Dualists want facts and formulas and don't like theories or abstract models, open-ended questions, or active or cooperative learning.

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- Level 3 (Multiplicity). Most information is known, but there are some fuzzy areas with questions that have no answers yet but eventually will. The instructor's dual role is to convey the known answers and to teach students how to obtain the others. Students start using supporting evidence to resolve issues rather than relying completely on what authorities say, but they count preconceptions and prejudices as acceptable evidence, and once they have reached a solution they have little inclination to examine alternatives. Open-ended questions and cooperative learning are still resented, especially if they have too much of an effect on grades.

- Level 4 (Transition to relativism). Some knowledge is known but some is not and probably never will be. Students feel that almost everything is a matter of opinion and that their answers are as good as the instructor's. The instructor's task is to present known information and to serve as a role model that can be discounted. Independent thought is valued, even if it is not substantiated by evidence, and good grades should be given to students who think for themselves, even if they are wrong.

- Level 5 (Relativism). Knowledge and values depend on context and individual perspective rather than being externally and objectively based, as Level 2-4 students believe them to be. Using real evidence to reach and support conclusions becomes habitual and not just something professors want them to do. Different knowledge is needed and different answers are correct in different contexts; there is no absolute truth. The student's task is to identify the context and to choose the best answers for that context, with the instructor serving as a resource. Students at this level are comfortable with corrective feedback.

In contrast, when PBL is used, the problem is posed before the students have acquired the knowledge needed to solve it. This inductive ordering simulates the research environment: the students begin with a problem and then proceed to figure out what they need to know, create hypotheses, read the literature and/or search the Web, talk to experts with related knowledge, acquire critical information through modeling, experimenting and discovering, and finally solve the problem.

TABLE 2: Reflection on and Self-Rating of Skill Development Strategies

Reflection: _____				

	<i>Already Do this</i>	<i>Should Work</i>	<i>Might Work</i>	<i>Not My Style</i>
<i>Problem solving skill</i>				
Value the skill: make it an explicit outcome of your course	0	0	0	0
Hand out research evidence for the skill	0	0	0	0
Make implicit behavior explicit: list goals and criteria	0	0	0	0
Use student reflection and monitoring	0	0	0	0
Grade (mark) the problem-solving process	0	0	0	0
Use standard assessment and feedback forms	0	0	0	0
Solve some problems in depth	0	0	0	0
Use a common strategy for problem solving	0	0	0	0
Other _____	0	0	0	0
<i>Communication skill</i>				
Value the skill: make it an explicit outcome of your course	0	0	0	0
Hand out research evidence for the skill	0	0	0	0
Make implicit behavior explicit: list goals and criteria	0	0	0	0
Use student reflection and monitoring	0	0	0	0
Grade the communication process	0	0	0	0
Use standard assessment and feedback forms	0	0	0	0
Require in-class writing	0	0	0	0
Other _____	0	0	0	0
<i>Team skill</i>				
Value the skill: make it an explicit outcome of your course	0	0	0	0
Hand out research evidence for the skill	0	0	0	0
Make implicit behavior explicit: list goals and criteria	0	0	0	0
Use student reflection and monitoring	0	0	0	0
Grade the teamwork process	0	0	0	0
Use standard assessment and feedback forms	0	0	0	0
Assign a chairperson for every meeting	0	0	0	0
Start with a "norms" meeting	0	0	0	0
Other _____	0	0	0	0
<i>Self-assessment skill</i>				
Value the skill: make it an explicit outcome of your course	0	0	0	0
Hand out research evidence for the skill	0	0	0	0
Make implicit behavior explicit: list goals and criteria	0	0	0	0
Use student reflection and monitoring	0	0	0	0
Grade the self-assessment process	0	0	0	0
Use standard assessment and feedback forms	0	0	0	0
Require resumé writing	0	0	0	0
Other _____	0	0	0	0
<i>Lifelong learning skill</i>				
Value the skill: make it an explicit outcome of your course	0	0	0	0
Hand out research evidence for the skill	0	0	0	0
Make implicit behavior explicit: list goals and criteria	0	0	0	0
Use student reflection and monitoring	0	0	0	0
Grade the process	0	0	0	0
Use standard assessment and feedback forms	0	0	0	0
Use structured cooperative learning groups	0	0	0	0
Use guided decision-making	0	0	0	0
Use small group, self-directed, self-assessed PBL	0	0	0	0
Other _____	0	0	0	0
<i>Change management skill</i>				
Value the skill: make it an explicit outcome of your course	0	0	0	0
Hand out research evidence for the skill	0	0	0	0
Make implicit behavior explicit: list goals and criteria	0	0	0	0
Use student reflection and monitoring	0	0	0	0
Use the grieving-process model	0	0	0	0
Use the Perry inventory to guide students	0	0	0	0
List new opportunities afforded by the change	0	0	0	0
Run a change management workshop	0	0	0	0
Other _____	0	0	0	0

Special Feature Section

- Higher levels (6–9) involve the development of commitment to an internally-based system of values. Most entering college students can be found on Levels 2 or 3, and relatively few attain Level 5 by the time they graduate.

Students being asked to function at a level higher than their current level are likely to be under a great deal of stress, especially if the two levels are not adjacent. Their reactions to this stress account for much of the resistance and occasional hostility instructors often encounter when they begin to use student-centered teaching methods like cooperative and problem-based learning.^[66,81] If students learn strategies for managing the stress associated with the transition to student-centered instruction, they may be better able to deal with the stressful professional and personal situations they will inevitably encounter later in their lives.

Strong justification for helping students learn to cope with change is the all-too-common situation wherein a well-intentioned faculty member hears about problem-based or cooperative learning and simply launches students into it, with little or no explanation or preparation. The outcomes of such experiments often include student anger and frustration, petitions to the department head, and terrible student ratings. One can hardly blame instructors in this situation for going back to more conventional teaching, to the ultimate detriment of their students. When students are helped to prepare for change, it may not eliminate their unhappiness about it but they are likely to tolerate it long enough to begin to see the benefits.

The first six of the eight basic activities described previously apply to the development of change-management skills. In addition,

- *In class or in your office, tell students about the stages of reaction to stressful change.* People who find themselves in highly stressful situations may go through some or all of the stages that have been associated with the grieving process: shock, denial, strong emotions, resistance and withdrawal, acceptance, struggle, better understanding, and integration.^[66,81] Students undergoing this process may find it helpful to know how the process works, and more to the point, that it eventually ends. You might also take a few minutes to elaborate on how the students can use the same stage model to help them manage other stressful situations such as death of a friend or relation or the loss of a job. Doing so is another way to demonstrate concern about their careers and lives beyond the confines of the classroom, which is one of the hallmarks of effective teaching.^[3]

- When using student-centered instruction, acknowledge to the students that it may be stressful to some of them but make it clear that you are doing it for good reasons. If possible, get them to come up with benefits themselves. For example,

In this course we will be using extensive cooperative learning, following the rules and procedures in the syllabus that we just outlined. Hundreds of research studies have shown that this approach leads to some real benefits for students. Form groups of three and make a list of what those benefits might be. Then I'll tell you what the research shows and we'll see how many of them you get."

- Run a workshop on the management of change.^[4,7]

SUMMARY

- Transmitting knowledge is the easiest part of teaching; far more challenging is the task of equipping students with the critical skills they will need to succeed as professionals and responsible members of society. The following strategies have been recommended to help achieve this goal:

1. *Identify the skills you wish your students to develop and communicate their importance to the students.*
2. *Use research, not personal intuition, to identify the target skills. Share some of the research with the students.*
3. *Make explicit the implicit behavior associated with successful application of the skills.*
4. *Provide extensive practice in the application of the skills, using carefully structured activities. Provide prompt constructive feedback on the students' efforts.*
5. *Encourage monitoring.*
6. *Encourage reflection.*
7. *Grade the process, not just the product.*
8. *Use a standard assessment and feedback form.*

Additional suggestions have also been given that apply specifically to the development of problem-solving, writing, teamwork, self-assessment, lifelong learning, and change-management skills.

IF YOU GET ONE IDEA FROM THIS PAPER

Focusing lectures, assignments, and tests entirely on technical course content and expecting students to develop critical process skills automatically is an ineffective strategy. Instructors who wish to help students develop problem-solving, communication, teamwork, self-assessment, and other process skills should explicitly identify their target skills and adopt proven instructional strategies that promote those skills. We suggest that you reflect on the strategies listed in Table 2 and rate their potential applicability to your teaching.

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THE FUTURE OF ENGINEERING EDUCATION

Part 4. LEARNING HOW TO TEACH

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In the next few years a large number of college teachers will retire to enjoy their golden years far from the sound of class bells, the demands of lectures, exams, grades, research, and committee work, and all the other joys and vexations of their busy lives as educators. Hired in the expansionist 1950's and 1960's, they have fought the good fight and have found satisfaction in their work, their colleagues, and their students. Their departure is watched with interest by the young PhDs who would like to have their jobs. It will be the biggest turnover in faculty since the University of Bologna was founded a thousand years ago!

And what of the qualifications of these hordes of would-be teachers? Do they know anything about course design, learning psychology, classroom dynamics, student learning styles, testing, grading, analysis, synthesis, cooperative learning, problem-based learning, leading discussions...? Do they know anything about teaching? You can bet they probably know very little, but know not that they know not. Teaching? "Why, I'll just teach the way I was taught. By the way, can I borrow your lecture notes?"

Then there are the in-betweeners, who have been teaching for three to fifteen years. Obtaining funding for their research is the biggest roadblock on their path to tenure.^[1] They spend inordinate amounts of time writing grant proposals and keeping their research programs together in the face of ever-shrinking funding pools. "It's ridiculous—the two-inch thick proposal has to be so detailed that I almost have to do the research before I can write it," one grumbles in frustration. When they aren't writing proposals and cultivating funding agencies, they visit companies to forge connections that may lead to industrial support. If they venture into the education literature to try to see what they might do

more effectively in the classroom, they soon encounter a language that's foreign to them, with terms like *epistemology*, *Bloom's taxonomy*, *Jungian typologies*, and *Perry levels*. Deciding that they don't have time to decipher all that gibberish, they give up and just go on lecturing.

Still other faculty members may have given up on the chase for research funds to focus on teaching, concentrating on writing clear sets of notes and designing and preparing good overhead transparencies. They may try some experiments in the classroom such as putting students in teams to work on problems, but find that their ratings drop, and decide to "Forget that!" They subsequently focus on playing it safe—avoiding rocking the educational boat—because student ratings are their bread and butter.

Many of the problems faced by these diverse souls—the wannabe faculty members in PhD or postdoctoral programs, the new or well-established professors who suspect there are more effective ways to do things but don't exactly know how, and those who have little time to spare from their never-ending quest for research dollars—stem from a single cause. With rare exceptions, no one teaches college teachers to teach! They receive training as researchers, join faculties, and enter their classrooms without so much as five seconds of instruction on what to do there. A few of them seem to have an innate ability to motivate students and facilitate learning and high-level skill development and some acquire this ability through years of experience. Many never acquire it, however, and in the absence of any pedagogical training, they teach the way their teachers (who also never received any training) taught them. This is a questionable way to run a profession, but it's been done this way for centuries.

The first paper in this series^[2] established the need to

change the traditional way of delivering engineering education in order to respond to rapidly changing conditions in technology and society, and the second two papers^[3,4] explained some of the education jargon and offered ideas for improving teaching effectiveness and personal satisfaction with teaching. We now come to the question of how engineering faculty members can best learn their craft and continue to keep up with emerging developments in educational methods. In this paper, we will describe a variety of faculty preparation programs and offer suggestions for self-study.

GRADUATE COURSES ON TEACHING

Every skilled craft provides formal instruction and/or mentorship for its new practitioners...except college teaching, which expects its newcomers to learn everything themselves by trial-and-error. While there is something to be said for trial-and-error learning, requiring it for a craft as complex as teaching is absurd. If the learning occurs at all, it normally takes years, and the ones who pay the penalty for the errors are not the ones who make them.

Much of the knowledge and many of the skills college teachers need to be effective can be taught. Good courses on college teaching are offered on a few—perhaps several dozen—campuses, but our applause at their existence should be somewhat restrained. Why don't we see such courses at every college that offers the doctoral degree? What happened to good old academic entrepreneurship? A change is long overdue.

Graduate courses on teaching offer several benefits:

- ▶ Teaching Assistants (TAs) support their graduate studies by providing formal or informal instruction to undergraduates in lecture and lab courses. The students whom the TAs are assisting deserve good teaching, which is what they (and their parents and, for public universities, the state legislature) think they are paying tuition to get. If we can improve the skills of the TAs by as little as five percent in a teaching course, the cost of the course would be a bargain. There is no way a teaching course could fail to lead to at least that much improvement.
- ▶ A well-designed teaching course gives students considering academic careers a much better picture of the profession than they could ever get in the normal course of a graduate program. Their career decisions are much better informed after they take the course, and if they eventually take teaching positions their professional learning curves could be shortened by years. Moreover, if the course is taught well, some students leaning toward industrial careers might be motivated to go into teaching, helping to meet the challenge of filling all the faculty vacancies predicted to occur in the coming decade.
- ▶ Students who take teaching courses receive training in effective presentation, teamwork, assessment of learning, time management, dealing with student-related problems, and other important topics that are not part of normal

graduate training outside schools of education. The resulting knowledge and skills are useful and marketable, whether the graduate joins a faculty or goes into an industrial or government career.

There are several reasons why such courses are not commonplace, their benefits notwithstanding. First, most faculty do not see a need for courses on teaching, believing that the knowledge and skills required to teach effectively can just as well be picked up on the job. (If they think about some of their colleagues or their own teachers, they will quickly see the fallacy of this reasoning. We never see our own shortcomings in our mental telescope, of course.) In addition,

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many dissertation advisors actively discourage their graduate students from taking courses that are not required to pass the qualifying exams and take time away from research. Finally, most engineering faculty do not feel prepared by their own education or experience to teach courses on teaching. This fact in itself is a criticism of our system, which allows us to practice in a profession whose skills we are not equipped to pass on to others.

The time has come to change the way we think about preparation for college teaching. In the first three papers in this series, we proposed viewing undergraduate education less as amassing of information and more as learning how to think, how to create, and how to develop the motivation and skill to be a lifelong learner and problem solver. In this paper, we argue that a graduate education should be viewed in a similar way. Learning how to do research is an important component of a PhD program, but it should be exactly that—a component. All engineering PhDs do not go into research as soon as they graduate, and very few of those who do spend their entire careers there. They may become design engineers, middle and upper-level corporate managers, consulting engineers, faculty members, department heads, deans, provosts, and chancellors, and a wide variety of other things that do not involve research. Part of our responsibility to our graduate students is to equip them with some of the communication and interpersonal skills they will need to succeed in those positions. Providing training in teaching is a good step in this direction. Following are some examples of how it might be done.

Since 1972, Jim Stice has offered a course at the Univer-

sity of Texas at Austin on improving teaching skills.^[5] The following topics are covered in a typical one-semester offering:

1. *Introduction and overview (1 period)*
2. *The Kolb Learning Style Inventory (2 periods)*
3. *The Myers-Briggs Type Indicator (2 periods)*
4. *Instructional design (1 period)*
5. *Writing instructional objectives (2 periods)*
6. *Production of overhead transparencies (1 period)*
7. *Microteaching: short videotaped presentations by class members (4 to 5 periods for a class of about 15)*
8. *Testing and grading (3 periods)*
9. *Student characteristics (1 period)*
10. *Teaching by lecture (1 period)*
11. *Teaching by discussion (1 period)*
12. *Learning theory (2 periods)*
13. *Microteaching II (4 to 5 periods)*
14. *Theories of Jean Piaget (1 period)*
15. *Individualized instruction (2 periods)*
16. *Teaching problem solving: analytical thinking (3 periods)*
17. *Teaching problem solving: creativity (1 period)*
18. *Where the teaching jobs are (1 period)*
19. *Summary of the course; evaluation (1 period)*

Stice suggests that anyone who has the interest and several years of teaching experience can teach such a course. Those who feel apprehensive about the first few offerings can team up with someone from the College of Education—which is what Stice did—or the Instructional Development Center. Teaching the course will provide a real learning experience for the instructors (as teaching courses always does). After a few semesters the engineering professor should be able to go it on his/her own, although if the course is going well there is a lot to be said for continuing to present as a team. The prime recommendation is to keep the class small—say, below 15—primarily because the microteaching exercises (topics 7 and 13) take too long when the class size increases.

Since the early 1980s, Phil Wankat and Frank Oreovicz have offered a 2- to 3-credit course on college teaching in the School of Engineering at Purdue University.^[6] Their general outline follows:

Part I. Methods and procedures

1. *What works*
2. *Efficiency and effectiveness*
3. *Taxonomy and objectives*
4. *ABET and accreditation*
5. *Problem solving and creativity*
6. *Obtaining an academic position*
7. *Teaching methods: lecture, cooperative groups, discussion, teaching with technology, mastery and Personalized System of Instruction (PSI), laboratories, design*
8. *Graduate mentoring*

9. *Testing and grading, cheating and discipline*
10. *Evaluation of teaching*

Part II. The student

1. *Piaget, Jung, and Perry*
2. *How people learn*
3. *Motivation*

Part III. Redesign of engineering education

1. *Web page project*
2. *Case study: ideal graduate program*
3. *Project: ideal undergraduate program*

At McMaster University, North Carolina State University, and other campuses, the campus Instructional Development Center offers courses to graduate students thinking about going into teaching and to interested faculty. Attendance by engineering graduate students is generally low unless someone in the school of engineering vigorously champions the courses and encourages graduate students to attend them.

WORKSHOPS AND SEMINARS

Workshops and seminars lasting anywhere from an hour to a week are far more common than academic courses as vehicles for teaching about teaching. These programs may be external to any campus (e.g., professional society conference workshops), campus-wide, engineering-specific, or departmental.

The National Science Foundation sponsors the *Engineering Education Scholars Programs (EESP)*,^[7] week-long summer workshops at Carnegie Mellon University, Stanford University, and the University of Wisconsin that examine all facets of academic careers. The EESPs are for engineering graduate students and relatively new faculty members, with 30-40 applicants accepted for each offering. Nationally known engineering educators give presentations, and the program at Carnegie Mellon University uses the excellent book by Davidson and Ambrose^[8] as a required text. Table 1 summarizes the topical outlines of recent offerings. In the summer of 1999, the University of Wisconsin presented the *Science and Engineering Education Scholars Program* to new faculty members and graduate students in science.

The *National Effective Teaching Institute [NETI]* is a three-day workshop given to faculty members in engineering and engineering technology under the auspices of the American Society for Engineering Education (ASEE), with some funding from industry.^[9,10] Beginning in 1991, the NETI has been given every year immediately preceding the annual ASEE Meeting in June. The topics include learning styles and teaching styles, planning a course (including writing instructional objectives) and getting it off to a good start, effective lecturing, active and cooperative learning, testing and grading, helping students develop problem-solving and critical and creative thinking skills, dealing with student problems

and problem students, and managing the stresses associated with academic careers. Deans of engineering and engineering technology are invited every January to nominate up to two of their faculty members to attend the NETI. Nominations are accepted on a first-come-first-served basis, and the enrollment is closed at 50. Since 1991, 472 faculty members from 157 different institutions have participated.

One-day and half-day workshops on education-related topics are generally offered before, during, or after the annual ASEE meeting in June^[11] and the Frontiers in Education (FIE) Conference in October or November.^[12] Educational workshops are also offered by the American Institute of Chemical Engineers, the Mexican Institute of Chemical Engineers, and other professional societies. Every five years

the Chemical Engineering Division of the ASEE sponsors a week-long “summer school” for chemical engineering faculty that offers a rich set of workshops on effective teaching in general and on teaching specific topics.

The Educational Research and Methods Division of the ASEE has compiled a list of its members who present workshops on campuses around the country.^[13] The list includes workshop topics and fees.

Many universities offer workshops and seminars on different aspects of academic careers or specifically on teaching. Some are open to all faculty members and some are designed specifically for new faculty members and/or graduate students. The paragraphs that follow describe several programs of this type.

At the University of Texas, a unique approach for new faculty is the three-day Summer Seminar, initiated in August 1980 by Jim Stice and his colleagues in the campus-wide Center for Teaching Effectiveness.^[14,15] All new hires are invited to attend by their department chairs and the Provost. The presenters—all UT faculty members and administrators (including the president)—discuss a variety of topics, including learning and teaching styles, instructional objectives, writing a syllabus, testing and grading, student characteristics, important university rules and regulations, research activities and resources, and what to do on the first day/week of class. Attendance ranges from 60 to 90 each year. Participants have reported that when they arrived at the seminar they felt like strangers, and by the end they felt they were members of the academic community. The seminar wasn’t really planned with this result in mind—it was a real bonus! The unsolicited remarks of one participant are worthy of etching in marble: “After 30 years I am changing my career. I never expected to be a college teacher, and I’ve been worried about what in the world to do with my students. I didn’t know what to expect from them, I didn’t know what they expected from me, and I had no idea how to conduct a class. Lately I’ve had stomach problems, and I haven’t had a good night’s sleep in three weeks. Then I came to your seminar, and now I know what I’m going to do, and I have some ideas about how to do it—and I’m sleep-

TABLE 1
Engineering Education Scholars Program Workshops*

	<i>University of Wisconsin-Madison</i>	<i>Carnegie Mellon University</i>	<i>Stanford University</i>
Sunday	Get acquainted	Prior knowledge assessment; introductions; challenge of change	Goals; problem-based learning activity; activity; Why am I a professor? academic roles—teaching, research, administration
Monday	Goals; retention; options for teaching; improving teaching; collaborative learning	Goals; retention; understanding student needs; diversity; processes in learning	Trends in engineering education; how students learn—diversity and learning styles; NSF programs
Tuesday	Academic careers; finding mentors; seeking tenure; writing grant proposals; climbing the academic ladder; departmental tours	Systematic course design; problem-based learning; balancing teaching, research, and administration; assessment of learning; active learning; accounting for student workloads	Lecturing; problem-based learning; instructional technology
Wednesday	Course design; assessing student performance	Course design; mentoring and supervising graduate students; videotape participant presentations with feedback	Videotape participant presentations with feedback; course design
Thursday	Innovative teaching options (overview and parallel workshops); panel—young faculty reflect from the trenches	Getting research funding; NSF programs; the future of engineering education; instructional technology	Balance in an academic career; stress and time management; getting tenure; networking and staying current
Friday	NSF programs; participant exchange of materials developed; activity—participants share materials	Ethics; workshop evaluation	Participant presentations; workshop evaluation; celebration
Saturday	Diversity; workshop evaluation		

* This table shows workshop outlines for one recent year; the programs at each institution vary from year to year. All programs also include “open” times, which might be free times, planned social events, concerts, banquets, or sports events.

ing like a baby again. I am very much in your debt.”

It is worth noting that the new faculty members who attended the Summer Seminar from 1980 through 1984 received an extra week's salary. This stipend was a powerful incentive to participate. Many said something like, “I came for the money—and I'm glad I did!” In 1985 the prices of oil and beef went down the drain, and the economy of the State of Texas suffered to an extent that the University was no longer able to provide the extra salary money. Attendance at later Summer Seminars suffered, but by this time the administrators had heard a lot of positive things from those of their faculty who had attended, and so the Seminar's good reputation was established. It is still held each summer, and department chairs and deans still recommend that their new people attend.

Several years after the inception of the Summer Seminar, members of the regular faculty began to ask if they could attend it. This was not felt to be a good idea, so instead a second program called the Seminar for Experienced Faculty was initiated at a more sophisticated level.^[16] It was held in January during the week before registration for the spring semester, and also lasted three days. The first year the number of participants was modest, but those attending were very enthusiastic. In the third year, 170 experienced faculty members attended.

At North Carolina State University, three-day faculty workshops have been offered annually in the College of Engineering since 1986 by Richard Felder and faculty colleagues. The workshop content is similar to that described previously for the National Effective Teaching Institute. Felder, *et al.*,^[17] describe the workshop and offer tips for getting engineering faculty to attend such workshops and making them effective. The suggestions include having both engineering expertise and pedagogical expertise on the presenting staff (sometimes the same individuals can fill both roles but this situation is rare), emphasizing practical applications and putting learning theory and research in a supporting role, and drawing examples primarily from engineering courses.

At the Universidad Iberoamericana in Puebla, Mexico, an eight-hour teaching workshop is presented to all beginning professors, the School of Engineering offers workshops on teaching development in a yearly summer program, and the Department of Teaching Development offers courses and workshops for Mexican and Latin American institutions. A series of seven seminars on academic careers given to chemi-

cal engineering students at Carnegie Mellon University is described by Ko.^[18]

MENTORSHIPS

In most skilled professions, novices are mentored by experienced practitioners who provide guidance and constructive feedback on the novices' initial efforts. This process can cut years off the learning curve normally required for unmentored novices to reach an acceptable level of effectiveness at a skilled profession. Doctors, psychologists, lawyers, pre-college teachers, and practitioners of every type of craft are routinely inducted into their professions with the aid of such guidance. As noted previously, the only skilled profession that does not routinely provide mentoring is college teaching.

Felder^[19] describes a mentoring program in the Chemical Engineering Department at North Carolina State University where each new faculty member is assigned a research mentor and a teaching mentor. The teaching mentor—who should be an excellent teacher with a desire to serve in that capacity—and the new professor co-teach a course in the latter's first semester. The mentor initially takes most of the responsibility for planning lectures, class activities, assignments, tests, and conducting classes; the mentee observes and takes notes; and the two discuss the class at a weekly debriefing meeting. As the semester progresses, the mentee gradually takes more responsibility for the instruction and the mentor becomes more of an observer, refraining from intervening in class if the mentee gets into difficulty and troubleshooting the problem at the next debriefing. Next semester, the mentee teaches a course and the mentor functions only as an occasional observer in class and consultant at periodic (but not necessarily weekly) debriefings. The mentor also makes an effort to introduce the mentee to faculty colleagues with related interests, both locally and at professional conferences. After the first year, the formal mentorship terminates and the mentee joins the normal teaching rotation.

A similar mentoring approach called *peer counseling* was pioneered by Roger Beck of the University of Alberta and has spread to campuses throughout Canada. Still another approach to teaching improvement involves partnerships in which two faculty colleagues visit each other's classrooms and offer feedback and suggestions.^[20,21]

Some institutions have programs wherein faculty members provide mentoring in teaching to graduate students con-

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templating academic careers. The University of Colorado has an advanced TA requirement for all PhD students that is typically fulfilled in the third year of graduate study.^[22] Typically, the student prepares and presents several videotaped lectures, prepares and grades homework and test questions, holds office hours, and teaches a recitation section if one is offered for the course, and the instructor provides feedback and guidance at weekly meetings. In the “Preparing the Professoriate” program at North Carolina State University, a faculty mentor and graduate student mentee may work together on a course (as at Colorado) or on a classroom research study.^[23,24]

An important requirement for a mentorship program is for department heads and deans to recognize that effective mentoring takes a certain amount of skill and a great deal of time. Several hours of mentor training should be provided by campus instructional development staff or experienced mentors, and all mentors should be compensated in some manner for their efforts.

NETWORKING

The most common—and arguably the most effective—way for new members of a professional organization to learn the ropes and adapt to the local culture is informal networking with experienced colleagues. Unfortunately, many new faculty members are introverted and wait in their offices for their more experienced colleagues to come to them. It does not always happen, and it is least likely to happen to women and minority faculty in engineering, who may have the greatest need for such support.

In *The New Faculty Member*,^[25] Robert Boice reports on studies he has conducted of the early careers of many professors. Boice found that about 13% of his subjects were “quick starters” who reached high levels of research productivity and teaching effectiveness in their first 1-2 years on faculties, as opposed to the 4-5 years required by most new faculty members. Prominent among the factors that differentiated quick starters from their more numerous counterparts was that the quick starters spent between two and four hours per week networking with faculty colleagues—going to lunch or for a cup of coffee with them or visiting them in their offices—and talking about research and teaching. Boice strongly recommends that new faculty members force themselves to engage in such activities and that department administrators and senior faculty members frequently initiate conversations with new colleagues in their first year.

Other vehicles for teaching-related networking are campus *learning communities*,^[26,27] in which groups of faculty members meet periodically to talk about teaching-related topics or to read and discuss selected references on teaching, and meetings of professional societies like the American Society for Engineering Education. Other organizations that

sponsor conferences on teaching and learning include the American Educational Research Association, International Society for Exploring Teaching Alternatives, National Science Teacher’s Association, and the Canadian organization called Society for Teaching and Learning in Higher Education. Woods and Ormerod^[28] offer additional ideas about networking and its importance.

CONSULTATIONS WITH CAMPUS TEACHING EXPERTS

Analyzing a videotape of a lecture with the help of a teaching consultant is an effective (albeit sometimes humbling) first step toward teaching improvement. The Clinic to Improve University Teaching of the University of Massachusetts developed the following structured approach to classroom videotaping that can be implemented either with a consultant or alone.^[29] Before the class, make a list of six questions you have about your lecturing and write down your guesses at the answers. Have the class videotaped and ask the class members to complete a traditional student evaluation form. Complete the same form yourself twice—once based on how you felt the class went and once based on how you guess the students rated the experience. Then watch a replay of the videotape and analyze it in the context of your six questions. Compare the student evaluations with your two sets of responses and identify five strengths and two areas to work on. This process works best if you go through the process with a consultant, but it is still useful if you do it alone. Much can be learned even without the videotaping.

RESOURCES FOR SELF-STUDY

Books ■ McKeachie’s *Teaching Tips*^[30] is probably the best known general reference on college teaching. Now in its 10th edition, it offers suggestions on every aspect of teaching and cites research supporting the suggestions. An excellent reference that applies specifically to technical disciplines is Wankat and Oreovicz’s *Teaching Engineering*,^[31] which recently became available on the World Wide Web; other books discuss the attributes of effective college teaching and teachers irrespective of discipline.^[32-39] Some references survey the theory and practice of the instructional models discussed in References 3 and 4 that have repeatedly been shown to promote learning and skill development. Johnson, *et al.*,^[40] do this for cooperative learning, and Woods^[41] does it for problem-based learning. For Mexican and Latin American educators, Rugarcia’s book, *La Formación de Ingenieros*,^[42] is recommended.

Several references are written specifically for faculty members new to the profession, including books by Davidson and Ambrose,^[8] Schoenfeld and Magnan,^[43] Whicker, *et al.*,^[44] Gmelch,^[45] and the previously mentioned work of Boice^[25] on the characteristics of “quick starters.” The last reference may be particularly useful to department heads and senior

faculty members serving as mentors to their junior colleagues.

Assessment of learning is becoming an increasingly important topic in engineering education as the day approaches when the outcomes-based Engineering Criteria 2000 becomes the accreditation standard for all U.S. engineering departments.^[46] Besides the usual midterm and final examinations, classroom assessment techniques (CATs) can be used to monitor what students are learning and what confuses them. Angelo and Cross^[47] describe a variety of CATs that can be used to assess learning and student attitudes, and Boud^[48] offers ideas for helping students to self-assess their own learning.

Journals and Newsletters ■

ASEE Prism is the news journal and *The Journal of Engineering Education* (JEE) the research journal of the American Society for Engineering Education. *Prism* contains Washington updates, feature articles on current issues and recent developments in engineering education, and a column on teaching methods written by Wankat and Oreovicz, the authors of *Teaching Engineering*.^[31] *JEE* contains articles on instructional methods and programs as well as reviews of recent books of interest to engineering professors. Both journals come with membership in the ASEE.

Other journals containing useful articles for college teachers include *The Journal of College Science Teaching*, *College Teaching*, *Change*, *Journal on Excellence in College Teaching*, the *AAHE Bulletin* (published by the American Association for Higher Education), and *Studies in Higher Education*. Several education journals such as *Chemical Engineering Education* and, in Spanish, *Educación Química* and *Revista del IMIQ*, focus on issues related to specific branches of engineering.

Newsletters that offer teaching tips and summaries of recent books include *The Teaching Professor*,^[49] *The National Teaching and Learning Forum*,^[50] and *Cooperative Learning and College Teaching*.^[51]

Electronic and Videotape Resources ■ A substantial and rapidly growing collection of resources for instructors can be found on the World Wide Web. Table 2 lists sites particularly relevant to engineering education. The sites contain class materials (including multimedia resources), teaching and assessment guides, handouts for students, and links to still more sites.

A growing number of listservers provide rich opportunities for interaction with colleagues seeking to improve their teaching. Table 3 lists several of them.

TABLE 2
Useful Web Sites for Engineering Educators

<u>Site</u>	<u>Comments</u>
World Lecture Hall < www.utexas.edu/world/lecture/index.html >	Lecture notes and multimedia resources for courses in many fields, including engineering.
NEEDS—National Engineering Education Delivery System < www.needs.org >	Multimedia resources for a vast collection of topics.
Resources in Engineering and Science Education (Richard Felder's Web site) < www2.ncsu.edu/effective_teaching/ >	Articles, "Random Thoughts" columns from <i>Chemical Engineering Education</i> , student handouts, software tutorials.
Deliberations on Teaching and Learning in Higher Education (London Guildhall University) < www.lgu.ac.uk/deliberations/ >	Material on collaborative learning, assessment of learning and teaching, and engineering education.
Collaborative Learning Website (National Institute of Science Education) < www.wcer.wisc.edu/nise/CL1/CL/clhome.asp >	Practical suggestions, anecdotes, research citations, and an extensive annotated bibliography on cooperative learning.
Field-Tested Learning Assessment Guide (National Institute of Science Education) < www.wcer.wisc.edu/nise/CL1/flag/flaghome.asp >	Techniques, resources, and references on assessment of learning in science, mathematics, engineering, and technology.
Computer-Based Teaching and Learning Links (University of Newcastle) < http://lorien.ncl.ac.uk/ming/Resources/cal/CAL.htm >	Large collection of links to sites that deal with applied and theoretical aspects of instructional technology.
Taking Your Course On-Line (North Carolina State University) < www2.ncsu.edu/ncsu/ccedu/online/ >	Suggestions and resources for course delivery via the World Wide Web and other electronic media.
Problem-Based Learning and the McMaster Problem-Solving Program (McMaster University) < http://chemeng.mcmaster.ca/innov1.htm >	Techniques and instructional resources for both programs.
For Your Consideration (University of North Carolina) < www.unc.edu/depts/ctl/fyc.html >	Short monographs on topics such as active learning, writing to learn, teaching large lecture classes, and assessment of teaching and learning.
Mount Allison University Teaching and Learning Page < http://aci.mta.ca/MtATeach/ >	Listings of education-related conferences and links to other sites sorted by topic (collaborative learning, learning styles, technology, etc.).
Links to a Better Education < http://w3.nai.net/~bobsalsa/linkstoa.htm >	Handouts for students on learning and problem-solving skills, taking tests, critical thinking, technical writing, time management, teamwork, learning styles, creativity, and many other topics.
University of Guelph < www.tss.uoguelph.ca/trc.html >	Suggestions, on-line assessment tools, and links to sites that deal with learning styles, teaching portfolios, copyright laws, and course design
University of Technology, Sydney (Australia) < http://www.cti.usu.edu.au/pb.html >	Survival guide for new teachers, evaluating teaching and courses, teaching portfolios.

The National Technological University regularly offers seminars on education-related topics over satellite links to campuses around the country, and also makes available videotapes of past programs.^[52] Some topics that have been presented include cooperative learning (Karl Smith and Richard Felder), programs for minorities (Ray Landis), learning styles (Felder), and women in engineering (Eleanor Baum).

The University of Technology at Sydney makes available excellent videotapes on four topics—"Lectures," "Tutorials," "Practicals," and "Assessment"—and a support text called *Survival Guide for New Teachers*.^[53] The University of Victoria offers a series of "Critical Incident Videotapes," brief scenarios of typical class problems that provide focal points for discussion.^[54] For example, the ten critical incidents on Tape 1 include one that deals with a student at one level of intellectual development trying to write an essay that calls for thinking at a higher level, and another that involves students complaining to the instructor that the class lacks structure. Woods has produced a videotape on self-directed learning that can be obtained by request.^[55] Margarita Sanchez of the Instituto Tecnológico y Estudios Superiores de Monterrey (ITESM) offers satellite-linked courses on problem solving.

A MODEL ENGINEERING FACULTY DEVELOPMENT PROGRAM

Beginning in 2001, engineering departments seeking accreditation will have to show that they are equipping their graduates with a specified array of skills and that they have established a program to assess the levels of these skills and remedy any deficiencies revealed by the assessment.^[46] Qualitative changes in the content and delivery of engineering courses along the lines outlined in the first and second papers of this series will be required to attain the desired learning outcomes. To implement these changes, most engineering professors will have to be educated in the new instructional methods, as opposed to the relative few who have been motivated to learn about them in the past.

A model engineering faculty development program is being developed by the Southeastern University and College Coalition for Engineering Education (SUCCEED) and implemented at the eight Coalition campuses.^[26] The core of the program is a broad variety of learning opportunities and resources for faculty members and graduate students. Opportunities may include courses on teaching, workshops and seminars, mentorships and partnerships, learning communities, and individual consulting with instructional develop-

ment personnel. Some of these programs are open to all faculty members and others are designed specifically for faculty members in their first two years of teaching. Programs for graduate students include courses on teaching, workshops and seminars, and mentorships. Some of the graduate student programs are designed for teaching assistants and others for students contemplating academic careers. Resources for self-study are also provided as part of the program, including books, journals, videotapes, and guides to useful Web sites. Program facilitators should collectively have expertise in both pedagogy and engineering.

An essential component of a successful faculty development program is strong institutional support. An adequate budget is of course a necessary condition. Beyond that, academic administrators should convey a clear expectation that the faculty will be good teachers, good teaching

TABLE 3
Education-Related Listservers

<i>Organization or Theme</i>	<i>Information</i>	<i>E-mail Address</i>
Alternative and collaborative learning		<L-aclrng@psuvm.psu.edu>
Alternative learning approaches		<altlearn@sjuvm.stjohns.edu>
Association for Higher Education		aahegit@list.cren.net <LISTPROC@list.cren.net>
Adult education network		aednet@pulsar.acast.nova.edu
Ass'n. for the Study of Higher Education		<ashe-L@listserv.american.edu>
Problem solving and creativity, learning	The approach of Tony Buzan to learning, memory, and creativity	<listserv@sjuvm.stjohns.edu>
Cooperative Learning		<CL_news@iubm.ucs.indiana.edu> CL@jaring.my <LISTSERVER@jaring.my> "Subscribe CL firstname lastname"
Learning Styles		<edstyle@sjuvm.stjohns.edu>
Higher Education Processes		<heproc-L@listserv.american.edu>
Problem-based Learning		<imsacpbl-L@imsa.edu>
	PBL-LIST. Monash University, Australia	<LISTSERV@eng.monash.edu.au> "SUB PBL-LIST yfname ylname"
Center for Faculty Development	University of Arizona	<lnasst@listserv.arizona.edu>
Exploring the way we educate		<newedu-L@uhccvm.uhcc.hawaii.edu>
Prof. and Organizational Development		<pod@lists.acs.ohio-state.edu>
Society for Teaching and Learning in Higher Education (Canada)		stlhe-L@unb.ca <listserv@unb.ca> "sub STLHE-L yfname ylname"
Continuous Quality Improvement		CQI-L@mr.net <listserv@mr.net>

will be rewarded in tangible ways, and inadequate teaching will be penalized. We will return to this point in the last paper in this series.

SUMMARY

Few engineering schools explicitly prepare their graduate students to teach, and new professors consequently join faculties equipped with a PhD in their discipline but no background in pedagogy. Also, most colleges and universities have few criteria to screen prospective candidates for their teaching ability; much of the emphasis in hiring is on perceived potential as a researcher. Candidates often give seminars on their research, and if they can give a passable performance and can answer a few questions without complete intellectual collapse, then their teaching skills are judged "good enough." As time passes, some of those hired become good teachers by instinct and others learn their craft by years of trial-and-error effort, but some never rise above mediocrity or worse.

Teaching is a complex craft, but the skills required to do it effectively can be taught. In this paper we have outlined the elements of an effective engineering faculty development program. To recapitulate, we advocate a program that includes a subset of teaching improvement workshops, courses, seminars, mentorships and partnerships, learning communities and consultation with campus teaching experts. Graduate courses in college teaching should be provided for those students who think they might be interested in academic careers. The faculty development coordinator should maintain resources for self-study, including books, journals, multimedia resources and guides to useful Web sites. Such a program should enable a far greater percentage of new faculty hires to become highly effective in 1-2 years—*i.e.*, to become what Robert Boice has termed "quick starters"—instead of the 4-5 years required by most of the new faculty members Boice studied.

Table 4 invites reflections on the options for teaching improvement presented in this paper.

IF YOU GET ONE IDEA FROM THIS PAPER

We have described many options for new instructors to learn the craft of teaching, including courses, workshops and seminars on teaching, professional society conferences, mentorships, and working with teaching consultants. Faculty members should take advantage of as many of these opportunities as possible rather than relying on trial-and-error for mastering the craft of teaching.

ACKNOWLEDGEMENTS

We thank Chris Knapper, Queen's University,

TABLE 4
Reflection and Self-Rating

	Rate the ideas			
	Already do	Would work	Might work	Not my style
Draw on others				
Take a course on effective teaching	0	0	0	0
Attend workshops on teaching	0	0	0	0
Ask for a mentor	0	0	0	0
Partner with a colleague to improve teaching	0	0	0	0
Work with a teaching consultant	0	0	0	0
Be videotaped in class	0	0	0	0
Other _____	0	0	0	0
Self study				
Read books about effective teaching	0	0	0	0
Read articles in education journals	0	0	0	0
Watch videotapes about effective teaching	0	0	0	0
Browse education-related Web sites	0	0	0	0
Other _____	0	0	0	0
Keep up to date				
Join the American Society for Engineering Education	0	0	0	0
Read at least one education journal each month	0	0	0	0
Subscribe to an education-related listserv	0	0	0	0
Attend an education conference	0	0	0	0
Other _____	0	0	0	0
Pass on your knowledge				
Give a workshop or seminar on effective teaching	0	0	0	0
Serve as a mentor to a new instructor or graduate student	0	0	0	0
Give a conference presentation and/or write a paper about a teaching method you have tried.	0	0	0	0
Teach a course on effective teaching	0	0	0	0

Kingston; Alan Blizzard and Dale Roy, McMaster University; Susan Ambrose, Carnegie Mellon University; Rich Noble, University of Colorado; and Phil Wankat, Purdue University, for their comments and suggestions.

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Chemical Engineering Division, ASEE
1999 Union Carbide Award Lecture

PARTICLE DYNAMICS IN FLUIDIZATION AND FLUID-PARTICLE SYSTEMS

Part 2. Teaching Examples*

LIANG-SHIH FAN

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In Part 1 of this lecture, I discussed the general educational issues concerning particle technology, with specific emphasis on fluidization and fluid-particle systems. In this part I will discuss some pertinent materials pertaining to fluidization and fluid-particle systems that could readily be integrated into existing required chemical engineering course materials. These materials, each introduced to students for a specific purpose, cover both gas-solid and gas-liquid-solid fluidization systems. In addition, I will discuss relevant commercial codes that are available for students to learn about the computation of fluid-particle systems. Some representative results marking the state-of-the-art efforts in computational fluid dynamics of fluidization will also be given.

L.-S. Fan is Distinguished University Professor and Chairman of the Department of Chemical Engineering at The Ohio State University. His expertise is in fluidization and multiphase flow, powder technology, and particulates reaction engineering. Professor Fan is the U.S. editor of *Powder Technology* and a consulting editor of the *AIChE Journal* and the *International Journal of Multiphase Flow*. He has authored or co-authored three books, including *Principles of Gas-Solid Flows* (with Chao Zhu; Cambridge University Press, 1998).

Professor Fan is the principal inventor (with R. Agnihotri) of a patented process, "OSCAR," for flue gas cleaning in coal combustion and is the Project Director for the OSCAR commercial demonstration, funded at \$8.5 million as Ohio Clean Coal Technology, currently taking place at Ohio McCracken power plant on The Ohio State University campus.

He has served as thesis advisor for two BS, twenty-nine MS, and forty-two PhD students at Ohio State, and is a Fellow of the American Association for the Advancement of Science and the AIChE.

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SAMPLE SUBJECTS OF PERTINENCE TO CHEMICAL ENGINEERS

It is ideal to encompass both the two-phase and three-phase systems in the teaching of fluidization as these two systems behave significantly differently. Salient subjects concerning gas-solid fluidization and gas-liquid-solid fluidization are given below.

Flow surrounding a bubble, two-phase theory, and flow segregation • introduced so students will be familiar with the use of proper assumptions for developing theories that capture the dominant behavior features.

Gas-solid fluidization phenomena are strongly dependent on the physical properties of the solid particles employed. Therefore, it would be appropriate to introduce the classification of fluidized particles to the student. Particles are classified into four groups (*i.e.*, Groups A, B, C, and D) based on their fluidization behavior. This classification, known as Geldart's classification,^[1] is shown in Figure 1, where particles are classified in terms of the density difference between the particles and the gas, $(\rho_p - \rho)$, and the average particle diameter, d_p . Figure 1 was obtained empirically and has been widely adopted in the fundamental research and design of gas-solid fluidized beds. Group C comprises small cohesive particles ($d_p < 20 \mu\text{m}$). Group A particles, with a typical size range of 30 to 100 μm , are readily fluidized. For Group B particle fluidization, there exists no maximum stable bubble size. Group D comprises coarse particles ($d_p > 1 \text{mm}$), which are commonly

processed by spouting.

We would then demonstrate to the student the rise of a bubble or slug in a dense gas-solid suspension using a simple known experiment that involves placing fine particles (FCC, Group A particles) in a sealed

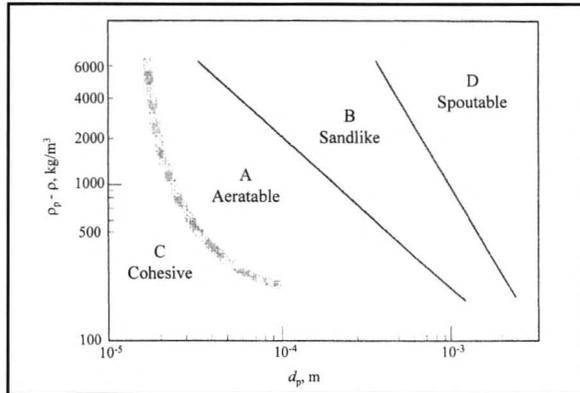


Figure 1. Geldart's classification of fluidized particles.^[1]

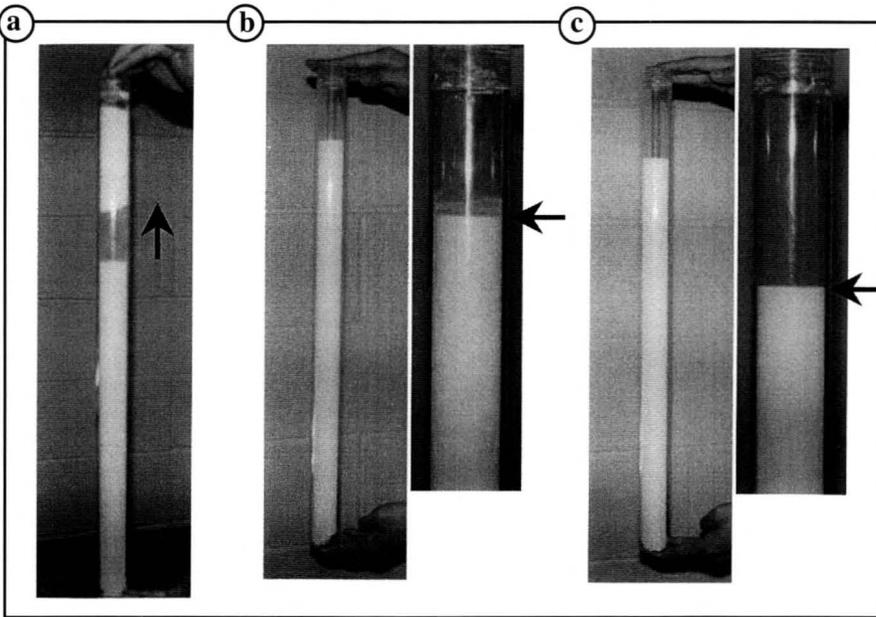


Figure 2. Simple fluidization experiments: (a) slugging regime, (b) particulate fluidization regime, and (c) packed-bed regime.

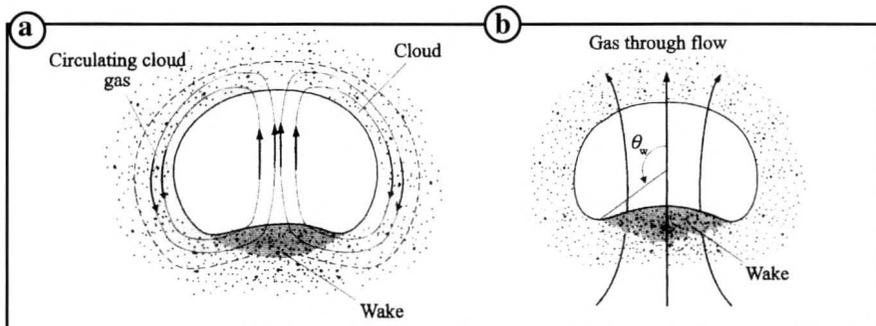


Figure 3. Bubble configurations and gas-flow patterns around a bubble in gas-solid fluidized beds. (a) Fast bubble (clouded bubble) $U_b > U_{mf} / \alpha_{mf}$; (b) Slow bubble (cloudless bubble) $U_b < U_{mf} / \alpha_{mf}$.

tube. The tube is 58 cm long and 87% full of particles. As shown in Figure 2, when the tube is flipped upside down a slug rises in the tube (Figure 2a). When the slug exits to the top of the tube, it leaves behind a dense particle bed (Figure 2b) that has a height higher than the packed condition of the particles (Figure 2c). The physical implication from comparing Figures 2b and 2c is that a bed of fine particles can be expanded by gas to an extended height without the formation of bubbles. This would lead to a discussion of the onset of bubbling.

Bubbles are formed as a result of the inherent instability of gas-solid systems. The instability of a gas-solid fluidized bed is characterized by fast growth in local voidage in response to a system perturbation. Because of the instability in the bed, the local voidage usually grows rapidly into a shape resembling a bubble. Although it is not always true, the initiation of the instability is usually perceived as the onset of bubbling, which marks the transition from particulate fluidization to bubbling fluidization. The theoretical explanation of the physical origin and prediction of the onset of the instability of gas-solid fluidized beds has been attempted.^[2] Efforts

have focused on the primary forces behind the stability among interparticle contact forces, particle-fluid interaction forces, and particle-particle interaction via particle velocity fluctuation.

Fluidization of fine particles (Group A particles) without the formation of bubbles is known to be in the particulate fluidization regime. For large and/or heavy particles (*i.e.*, Group B or D particles), particulate fluidization does not exist. That is, the onset of bubbling coincides with that of minimum fluidization of the packed bed.

Most bubbles in gas-solid fluidized beds are of spherical cap or ellipsoidal cap shape. Configurations of two basic types of bubbles, fast bubble (clouded bubble) and slow bubble (cloudless bubble)^[3] are schematically depicted in Figure 3. The cloud is the region established by the gas that circulates in a closed loop between the bubble and its surroundings. The cloud phase can be visualized with the aid of a color tracer gas bubble. For example, when a dark brown NO_2 bubble is injected into the bed (see Figure 4), the light brown color surrounding the bubble represents the cloud region.^[4] When the bubble-rise velocity is higher than the interstitial-gas velocity, a "clouded" bubble forms in which the circulatory flow of gas takes place between the bubble and the cloud, as shown in Figure 3a. The cloud size decreases as the bubble-rise velocity increases. As the

bubble-rise velocity becomes significantly higher than the interstitial-gas velocity (*i.e.*, U_{mf} / α_{mf}), the cloud size becomes so thin that most of the gas circulates inside the bubble. When the interstitial-gas velocity is greater than the bubble-rise velocity, it yields a “cloudless” bubble in which the emulsion phase gas flows through the bubble phase, as shown in Figure 3b. This gas through-flow in the bubble is also known as invisible bubble flow, which is distinguishable from visible bubble flow. Bubbles in Group D particle fluidized beds are typically characterized by cloudless bubbles.

To describe the complex particle and gas flows around the bubble in the fluidized beds described above, we introduce the model of Davidson and Harrison^[5] because of its fundamental importance and relative simplicity. The model employs the following key assumptions:

1. The bubble is solids-free and spherical, and has a constant internal pressure.
2. The emulsion phase is a pseudocontinuum, an incompressible and inviscid single fluid with an apparent density of $\rho_p(1 - \alpha_{mf}) + \rho\alpha_{mf}$.

With these assumptions, the velocity and pressure distributions of the “fluid” in a uniform potential flow field around a bubble, as portrayed in Figure 5, can be given as^[5]

$$\begin{aligned} U_{pf} &= -U_{b\infty} \left(1 - \frac{R_b^3}{r^3} \right) \cos \theta \\ V_{pf} &= U_{b\infty} \left(1 + \frac{R_b^3}{2r^3} \right) \sin \theta \end{aligned} \quad (1)$$

and

$$P_{pf} = P_{pf}|_{z=0} + \left(\frac{\partial p_{pf}}{\partial z} \right)_{\infty} \left(r - \frac{R_b^3}{r^2} \right) \cos \theta \quad (2)$$

where the subscripts “pf” and “∞” represent the pseudofluid and the undisturbed conditions, respectively, $U_{b\infty}$ is the rise velocity of an isolated bubble, and R_b is the bubble radius. The pressure far away from the rising bubble in a fluidized bed can be approximated at minimum fluidization. Thus, Eq. (2) becomes

$$P_{pf} = P_{pf}|_{z=0} - (\rho_p - \rho)(1 - \alpha_{mf})g \left(r - \frac{R_b^3}{r^2} \right) \cos \theta \quad (3)$$

Figure 6 shows a good comparison between the measured dynamic pressure and the calculated results based on Eq. (3). The profile indicates that there is a local high-pressure region near the bubble nose and a local low-pressure region around the bubble base, *i.e.*, the wake region. The low pressure in the wake region promotes pressure-induced bubble coalescence in the bed.

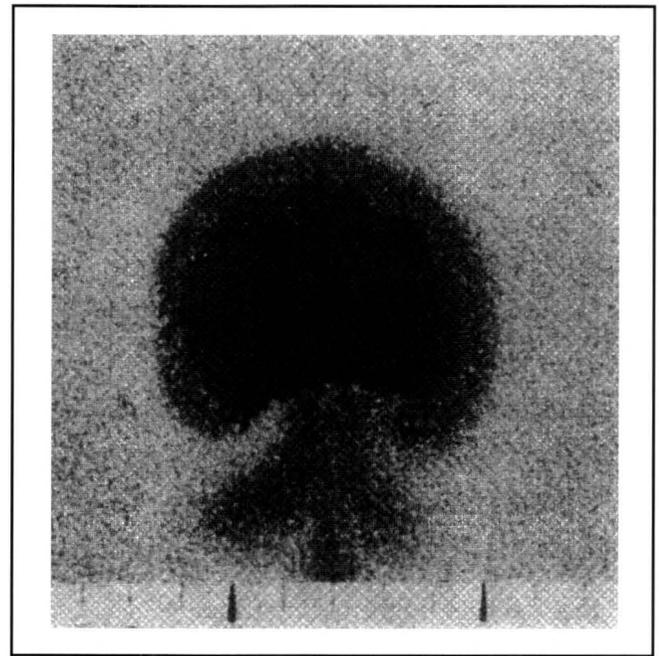


Figure 4. An NO₂ bubble rising in a two-dimensional ballotini bed showing the cloud region of the bubble (from Rowe,^[4] reproduced with permission).

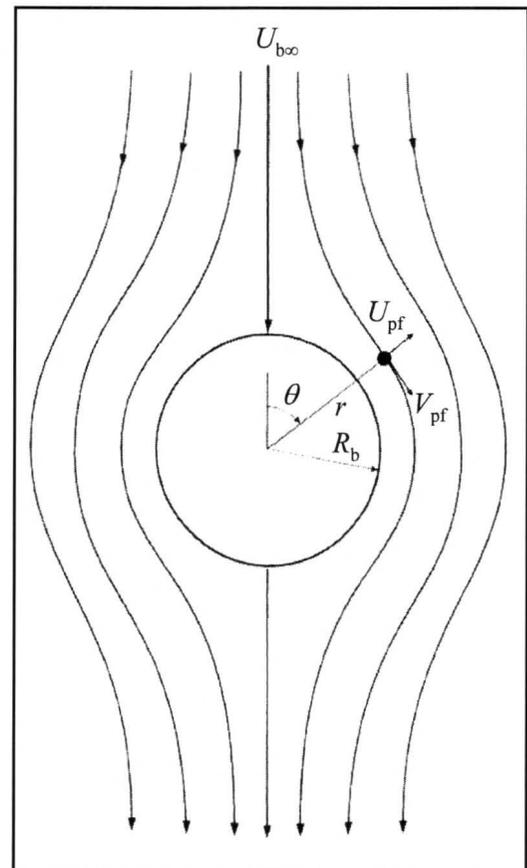


Figure 5. Potential flow around a spherical bubble in a two-dimensional projection (from Davidson and Harrison^[5]).

The macroscopic behavior of a fluidized bed can be described using the two-phase theory of fluidization.^[9] This theory considers the bed to be divided into two phases, *i.e.*, the bubble phase and the emulsion phase, as shown in Figure 7, with a corresponding division of superficial gas flow in the bed to each of the two phases, *i.e.*, U_{em} to the emulsion phase and $\alpha_b U_{bb}$ to the bubble phase, where α_b is the volume fraction of bubbles in the bed, and U_{bb} is the average bubble-rise velocity in the bed. Many analyses of transport phenomena of a bubbling fluidized bed are made based on this simple two-phase theory. The two-phase theory concept is also extended to describe the macroscopic flow behavior of high-velocity fluidization in which the core-annular flow structure prevails in the column. In fluidization, particle collisions and particle-turbulence interaction yield a dense, wavy, clustering solids layer in the wall region and dilute solids in the core region. The core region and wall region can be treated as two interpenetrating phases in the analysis of this flow behavior.

Phenomena of bubble wake dynamics in liquid-solid suspensions • introduced so students will understand the importance of identification of the governing factors underlying complex phenomena

A large number of liquid-solid fluidized beds are operated in the presence of gas bubbles. In both reactive and non-reactive systems, gas bubbles play an essential role in determining the behavior or performance of the bed. For example, gas bubbles are usually a source of reactant gas species whose transport phenomena often depend on the fluid flow around the bubble; gas bubbles induce intimate liquid/solids mixing; and in a three-phase fluidized bed, gas bubbles are responsible for solids entrainment to the free-board and bed contraction. It has been specifically recognized that the bubble wake located immediately underneath the bubble base is the dominating factor contributing to bed performance. It is, thus, of primary importance for students to understand the fluid dynamic behavior of the bubble wake and its interaction with the bubbles so that they will be vested with sound, fundamental knowledge in their efforts toward modeling, simulation, and design of such particulate reactor systems.

In the following, the bubble wake structure in a liquid-solid suspension^[10] is introduced, followed by experimental evidence highlighting the important role of the bubble wake in process systems.

■ **Bubble Wake Structure** • Figure 8a shows a photograph of a relatively large two-dimensional nitrogen bubble rising through a water-774 μm glass bead fluidized bed at $Re_b (=bU_b/\nu, \text{ based on bubble breadth, } b)$ of 8150. The schematic diagram shown in Figure 8b indicates two regions: the primary wake region includes two vortices—on the right-hand side is well-established circulatory motion, and on the left-hand side the vortex is just forming. Outside the primary wake region, there exists a slightly deformed, large vortex that is isolated by streams of external flow across the wake from right to left. As seen in the figure, the solids concentra-

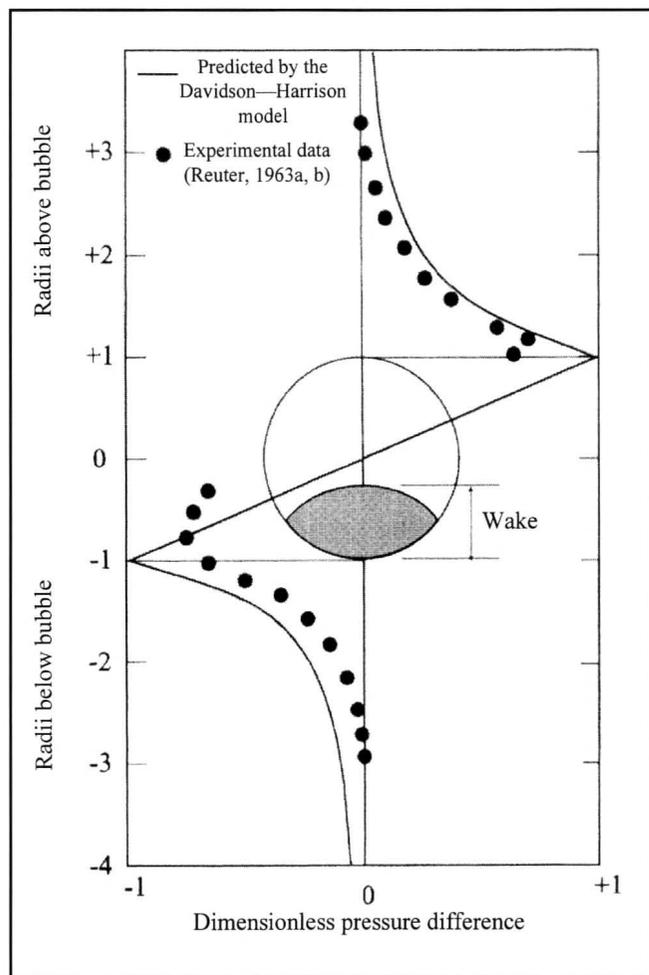


Figure 6. Pressure distribution in the vicinity of a rising three-dimensional bubble with a comparison of the experimental data by Reuter^[6,7] and the Davidson-Harrison model prediction (from Stewart^[8]).

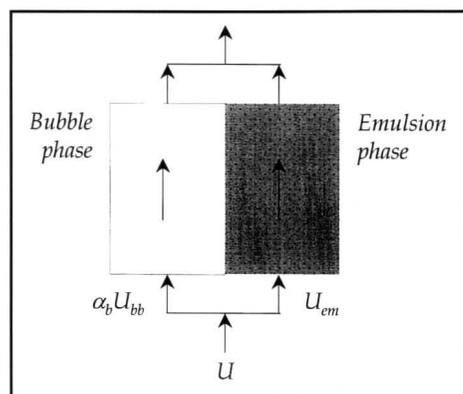


Figure 7. Gas flow distribution in the bed based on the two-phase theory.

tion varies within the wake; lower solids concentration regions were observed immediately beneath the bubble base and around the vortex center, while higher concentration regions occurred around the vortices and especially in the regions where the two vortices interact.

■ Bed Contraction • When gas is introduced to a liquid-solid fluidized bed of small particles (see Figure 9a), contraction instead of expansion of the bed occurs (Figure 9b). An increasing gas flow rate causes further contraction up to a critical gas-flow rate beyond which the bed expands (Figure 9c).^[12] Considerable research has been conducted to study the unique bed-expansion characteristics in three-phase fluidization and showed that bed contraction can be attributed to the behavior of the bubble wake. Phenomenologically, bed-contraction phenomena could be explained by the presence of a solids-containing wake, which allows some liquid flow to bypass the liquid-solid fluidized region at a higher velocity. This bypass of liquid reduces the liquid velocity in the liquid-solid fluidized region, thus contributing to the bed contraction. Further increase in the gas velocity increases the gas holdup (or gas volume fraction) in the bed, leading to the bed expansion.

■ Bubble Coalescence • An important clue to the mechanism of bubble coalescence can be obtained through observation of rise patterns of successive bubbles. Figure 10 presents photographs representing the bubble-rise paths observed in two-dimensional water-fluidized bed of 460- μm glass beads (Figure 10a) and 1.5-mm acetate particles (Fig-

ure 10b) at a given bubble formation frequency f_b . As shown in the figure, the alternate shedding of the bubble wake yields a series of vortices that establish a staggered, snake-like liquid flow pattern downstream relative to the bubble; the central regions of the shed vortices appear as bright spots. The staggered liquid stream emanating from the leading bubble enhances the zigzag motion of the trailing bubble regardless of particle properties.

The figure demonstrates a bubble-pairing process for two different conditions. In Figure 10a, three bubbles initially rise with equal bubble spacing. As time elapses, the first and second bubbles are paired, with the second bubble being profoundly elongated. These two bubbles eventually collide.

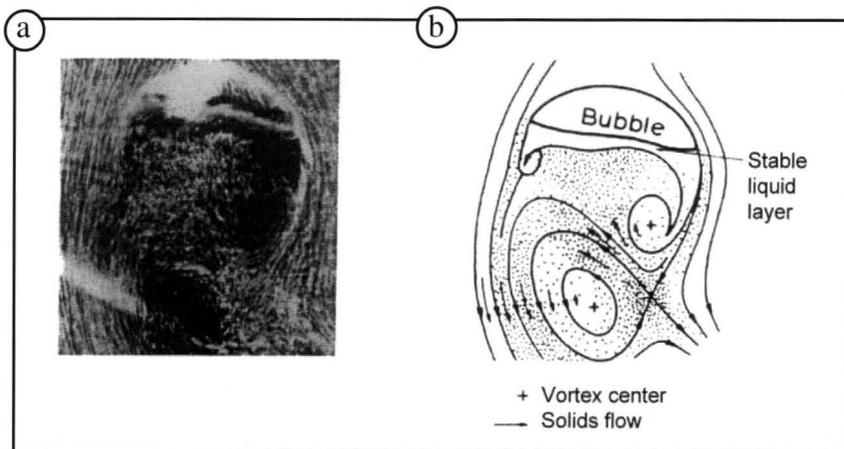


Figure 8. Bubble wake phenomena in a liquid-solid fluidized bed (from Tsuchiya and Fan,^[11] reproduced with permission).

a) Photograph of a circular-cap bubble and its wake in a water-774 μm glass bead fluidized bed.

b) Schematic interpretation of the wake flow.

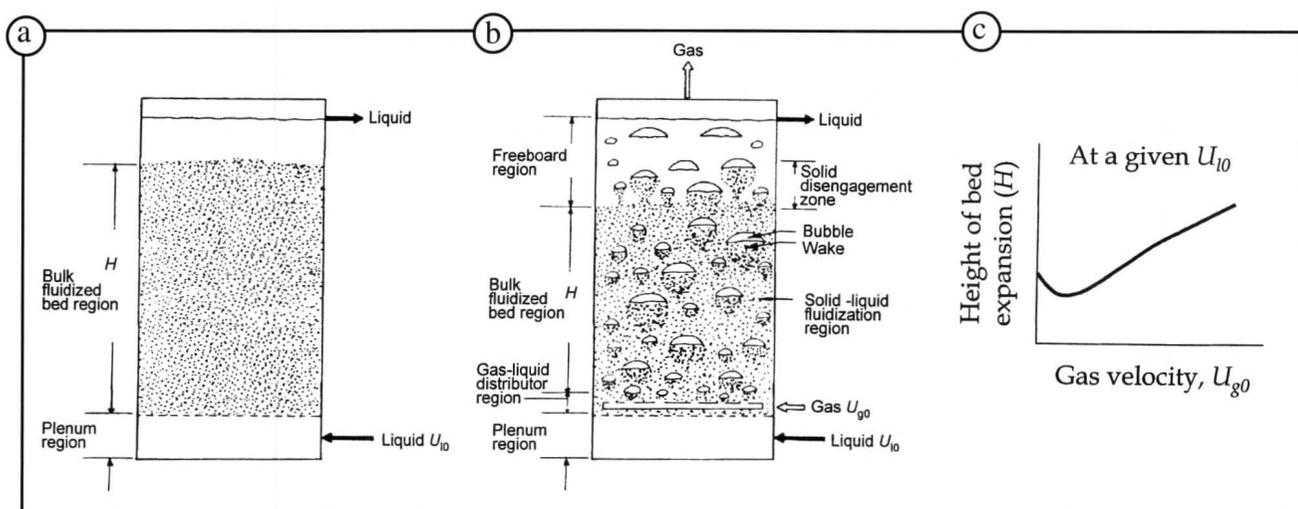


Figure 9. Bed contraction phenomena in gas-liquid-solid fluidization.

a) Liquid-solid fluidized bed at U_{10} .

b) Gas-liquid-solid fluidized bed at U_{10} and small U_{g0} .

c) Variation of height of bed expansion with gas velocity in a gas-liquid-solid fluidized bed.

A typical “catching up” process is shown in Figure 10b and demonstrates the acceleration of the trailing bubble toward a leading bubble due to the presence of the wake of the leading bubble, which results in bubble pairing and the eventual collision of the pair.

■ **Particle Entrainment** • The primary wake of a rising bubble and the resulting drift of particles above the upper free surface of a two-dimensional liquid-solid fluidized bed of calcium alginate particles are observed as shown in Figure 11 (next page) (inverse funnel shape). In the photograph, the extent (effective height) of particle carryover through the drift appears to be as significant as that via the bubble wake. The particles carried above the surface are discharged from the wake via wake shedding and are then settled down along with the drift particles as a result of gravitational force. As the freeboard region of a three-phase fluidized bed is based primarily on the particle disengagement behavior from the bubble wake, understanding the wake-shedding behavior allows an accurate design of the freeboard region of a three-phase fluidized bed.

■ **Precipitation of Calcium Carbonate** • Figure 12 (next page) shows a CO₂ bubble and its wake after injection of 100

bubbles. It is observed that at the early stage of carbonation, the bubble wake is clearly visible as a smoky region, revealing the formation of fine CaCO₃ particles. The smoky region is observed in the primary wake, which rises at the same speed as the rising bubble. More fine particles are produced in the wake region than in the bulk region. After injecting 100 bubbles, large “fluffy” aggregates are formed in the bulk region, and the wake region can be distinguished from the particle or aggregate size behind the bubble, as can be seen in the figure. The fluffy aggregates are of loosely packed particles that are easily broken down into smaller fragments by the vortical motion in the bubble wake. Significant changes in the morphology of the fine crystals and in the size distribution of the agglomerates that occur in the wake were observed only during the early stages of the reaction.

■ **Gas-Liquid Mass Transfer** • The mass transfer of gas bubbles is strongly influenced by the bubble- and wake-flow behavior. The solute is carried by the flow on the roof of the bubble along the boundary of the wake and is separated into two regions—within the primary wake region by the wake vortex and outside the wake region by the shedding vortex. The solute that flows into the wake is carried back to the bubble base. The shed vortex carrying the solute generates an external concentration vortex and eventually diffuses into the bulk flow. In addition to the convective diffusion by the liquid-solid flow, there is slow molecular diffusion of solute from the vortex sheet into the vortex center in the wake and from the wake surface into the bulk flow, but these contributions are negligible compared to convective diffusion.

The variations of the mass transfer patterns around bubbles with respect to time are given in Figure 13 (next page). It shows the circular-cap ozone-oxygen bubble and its wake rising in a starch-iodine-water, 0.46-mm glass-bead fluidized bed. As the bubble begins to rise, the reacted ozone molecules are carried from the edge of the bubble by the vortex sheet, and the wake underneath the circular-cap bubble is gradually saturated with ozone molecules. It can be seen that the shape of the bubble plus the wake is approximately circular. The zigzag trail behind the bubble is formed in the bulk of the liquid phase as a result of the vortex shedding. It is interesting to note that there is no trace of ozone molecules on the surface of the bubble roof since the reacted molecules are swept by the liquid flow. As a consequence, the convective diffusion induced by potential flow plays an important role in the mass-transfer mechanism on the bubble roof. As the bubble rises further, the wake (filled completely with gas molecules) starts to shed vortices. As shown in the figure, alternate sheddings are observed in low bed expansion conditions of the liquid-solid fluidized media. The shed vortices elongate their shape and the gas molecules begin to diffuse out from the center of the vortices into the bulk liquid by molecular diffusion, especially in the case of high bed expansion.

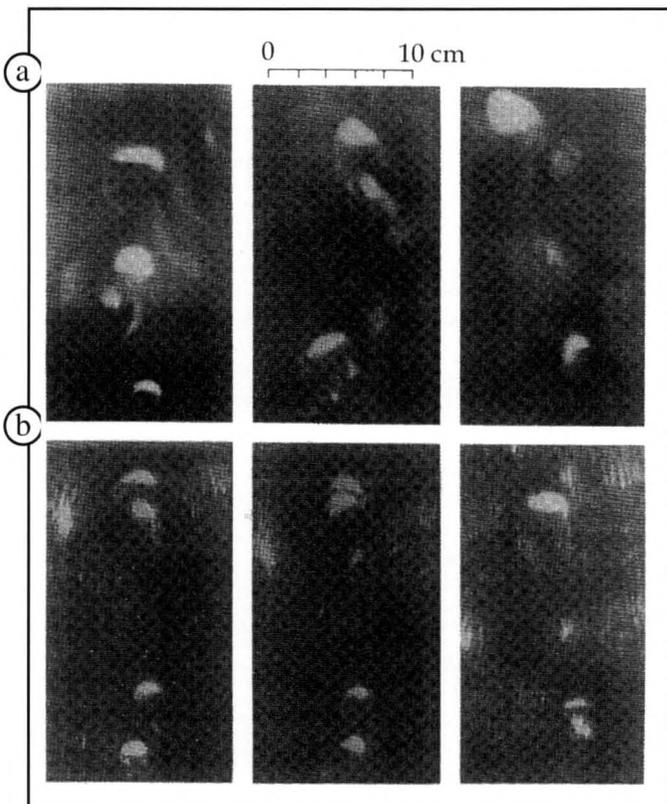
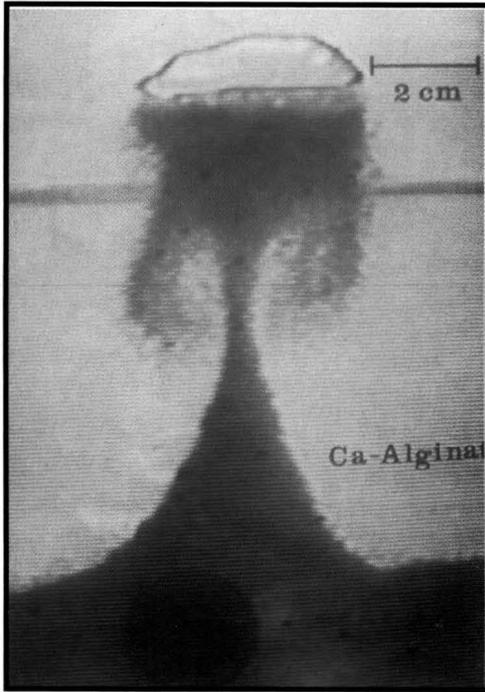


Figure 10. Bubble pairing followed by bubble collision for successive bubbles in two-dimensional water-solid fluidized beds (from Tsuchiya, et al.,^[13] reproduced with permission).

a) GB460: $b=2.8$ cm; $f_b=3.1$ s⁻¹; $Re_b=9180$

b) AT1500: $b=2.0$ cm; $f_b=3.0$ s⁻¹; $Re_b=4040$

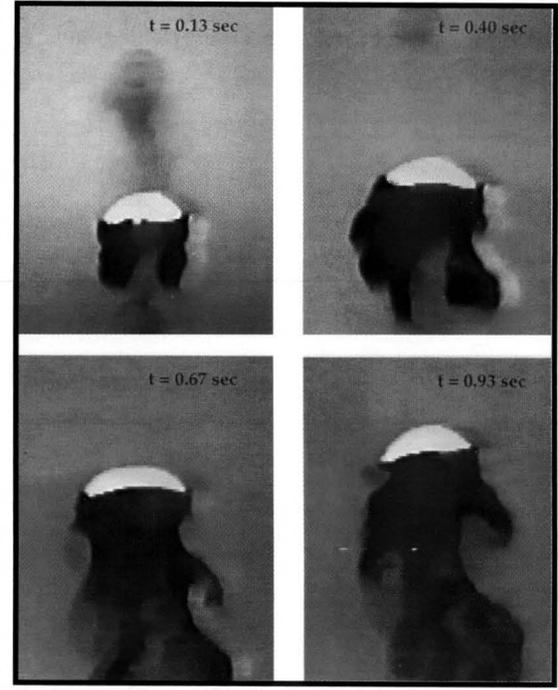


◀ **Figure 11.**

Entrainment of particles by bubble wake and drift induced by a rising bubble (from Tsuchiya, et al.^[14] reproduced with permission of the American Institute of Chemical Engineers, © 1992 AIChE).

Figure 12. ▶

Precipitation of CaCO_3 particles from a rising CO_2 bubble (from Tsutsumi, et al.^[15] reproduced with permission).

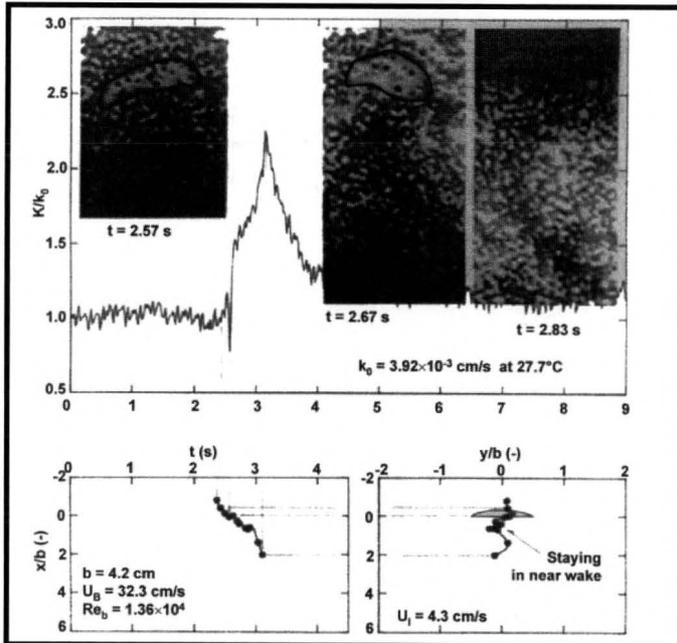


▲ **Figure 13.**

O_3 bubble rising in a KI-starch solution and 0.46-mm glass-bead fluidized bed.

▼ **Figure 15.**

Simulation results of bubble formation in a gas-solid fluidized bed using Fluent.



◀ **Figure 14.**

Instantaneous local liquid-solid mass transfer coefficients in the wake region and the effects of vortices on the primary wake (from Arters, et al.^[16] reproduced with permission).

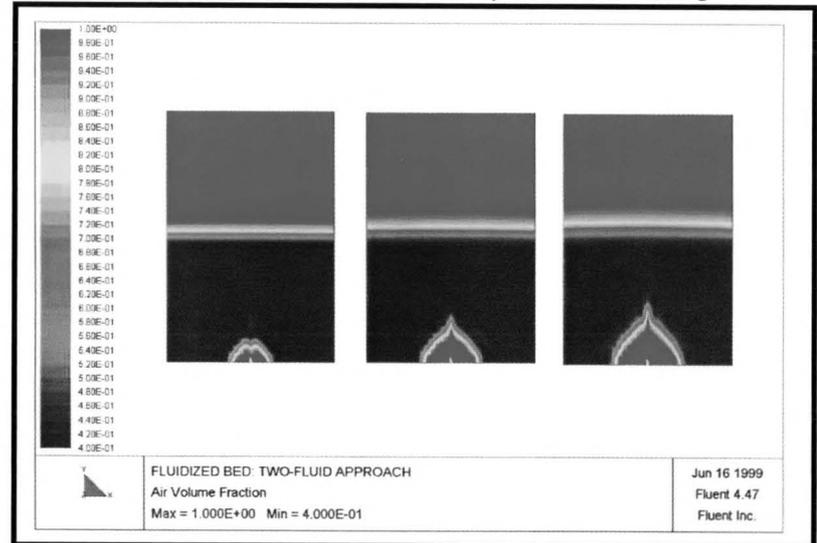
x - vertical downward distance from the bubble base

y - horizontal right-hand distance from the center of the bubble base

b - bubble breadth

U_B - absolute bubble rise velocity

Re_b - bubble Reynolds number based on the bubble breadth



■ **Liquid-Solid Mass Transfer** • Mass transfer from the liquid to the surface of the solid, and hence the reaction rate, are governed, apart from the activity of the solid, by the local flow patterns of the liquid relative to the solid. Due to the unique flow structures associated with the liquid in the wake and the presence of solid particles in this region, it is of interest to examine the interaction between a solid particle and a bubble wake and its effect on liquid-solid mass transfer. The instantaneous value of the mass transfer coefficient, k , for a single particle in a two-dimensional liquid-solid fluidized bed, subjected to the disturbance of a single rising gas bubble, can be measured by an electrochemical method using tethered particles. The method measures the limiting current and thereby allows evaluation of k . Visualization techniques can be employed to track the particle in relation to the bubble and bubble wake. Synchronization of the mass-transfer data acquisition with the video record allows a history of the local mass transfer to be analyzed.^[16]

Figure 14 shows the liquid-solid mass-transfer behavior interactions of a particle with the bubble and the primary wake. The axes in the figures are linked such that information regarding the mass transfer coefficient, event time, and particle position with respect to dimensionless bubble coordinates can be cross-referenced. The mass transfer coefficient is expressed in terms of k/k_0 , where k_0 is the liquid-solid mass transfer coefficient under liquid-solid fluidization conditions at the same liquid velocity. The most salient feature is that the interaction of the particle with the wake region produces substantial increases in the mass transfer coefficient. It can be seen in the figure that a twofold increase in mass transfer results when a particle traveling directly underneath and along with the bubble is ejected from the primary wake through the cross flow. The free shear layer formed at the bubble edge is also found to produce significant increases in mass transfer. Lesser increases are seen when the particle is exposed to a shear layer not strong enough to pull the particle into the flow.

COMPUTATIONAL FLUID DYNAMICS OF PARTICULATE SYSTEMS

Computation is an area of great importance. Students should be kept abreast of the current approach in computation for particulate systems. In the following, a general background on the basic methods of particulate flow computation is introduced and is followed by an example of a state-of-the-art computational problem that my research group is tackling.

General Background • The computational fluid dynamics approach has provided considerable insight into the dynamic behavior of multiphase systems. The Euler-Euler,^[17] Euler-Lagrange,^[18] and direct^[19] numerical simulations are three widely used approaches for particulate-system computation. In the Euler-Euler method, the individual phases are treated as pseudo-continuous fluids, each being governed by

the conservation laws expressed in terms of volume/time or ensemble-averaged properties. The conservation equations are closed by constitutive relations that could be obtained from empirical relationships, or theories. The dynamic motion of solid particles, especially for collision-dominated shear flows of solid particles, is often simulated using kinetic theory^[20] in which theoretical analogies between the gas molecule and solid particles are applied. In the Lagrangian approach, the discrete particles are treated as a group of point masses with their position, velocity, and other quantities being tracked based on the motion equation of individual particles. The dispersed phase can exchange momentum, mass, and energy with the fluid phase. In the dispersed phase, particle-particle collision dynamics characterize the particle-particle interactions. In direct numerical simulation, the fluid flow could be solved by using finite difference/volume/element discretization of the Navier-Stokes equations, or the lattice-Boltzmann, or Lagrangian multiplier method. Direct numerical simulations require no empirical constitutive equations and could provide detailed information about flow surrounding individual particles.

The Euler-Euler and Euler-Lagrange approaches have been incorporated in many commercial software packages. Fluent (by Fluent, Inc.), CFX (by AEA Technology), Flow3D (by Flow Science, Inc.), and CFDLIB (by Los Alamos National Lab) are some of the common packages used in academia and industry for chemical process applications. The results for a simulation of the bubble formation process in a gas-solid fluidized bed using Fluent 4.47 are shown in Figure 15. In this example, the Euler-Euler two-fluid approach is used to solve the gas and solid flow in a fluidized bed. The rectangular domain is 0.4 m wide by 0.6 m high and is filled halfway with a fluidized bed. The particle diameter used is 0.5 mm with a density of 2610 kg/m³. Air is used as the gas phase, which has a density of 2.3 kg/m³ and a viscosity of 1.7 x 10⁻⁵ kg/m-s. Initially, the bed has a uniform vertical air flow of 0.284 m/s introduced from the lower boundary. When a simulation is started, a vertical air jet is injected from the lower center of the fluidized bed. The orifice width of the air jet is 0.03 m. The bubble size is seen to increase significantly with time. Similar results were presented earlier by Sinclair^[21] using Fluent 4.32.

Examples of State-Of-The-Art Computation • My research group has been engaged in computation code development for simulation of the gas-liquid-solid fluidization systems.^[22] The discrete-phase approach is employed with the volume-averaged method, the discrete-particle method (DPM), and the volume-of-fluid method (VOF) used to account for the flow of liquid, solid, and gas phases, respectively. A bubble-induced force model (BIF), a continuum surface force model (CSF), and Newton's third law are applied to account for the couplings of particle-bubble (gas), gas-liquid, and particle-liquid interactions, respectively. A

close-distance interaction model (CDI) is included in the particle-particle collision analysis, which considers the liquid interstitial effects between colliding particles. The following presents representative results for a single bubble rising and particle entrainment by a single bubble in a liquid-solid fluidized bed under ambient conditions and multi-bubbles rising in a liquid-solid fluidized bed under high-pressure conditions.

The behavior of a single bubble rising in a liquid-solid fluidized bed suspension under ambient conditions is simulated in Figure 16. One thousand particles with a density of $2,500 \text{ kg/m}^3$ and a diameter of 1.0 mm are used as the solid phase. An aqueous glycerin solution (80 wt%) is used as the liquid phase. The superficial liquid velocity is 5 mm/s , yielding a solids holdup of 0.44 . It can be seen that the bubble is of spherical-cap shape rising rectilinearly. Also shown in the figure are photographs of a single bubble rising in a liquid-solid fluidized bed obtained experimentally under the same operating conditions as those of the simulation. As shown in the figure, the simulated and experimental results of the bubble-rise velocity and the bubble shape generally agree.

Figure 17 shows the simulated results of particle entrainment by a bubble from the bed

Figure 16.

Simulation and experimental results of a single bubble rising in a liquid-solid fluidized bed.

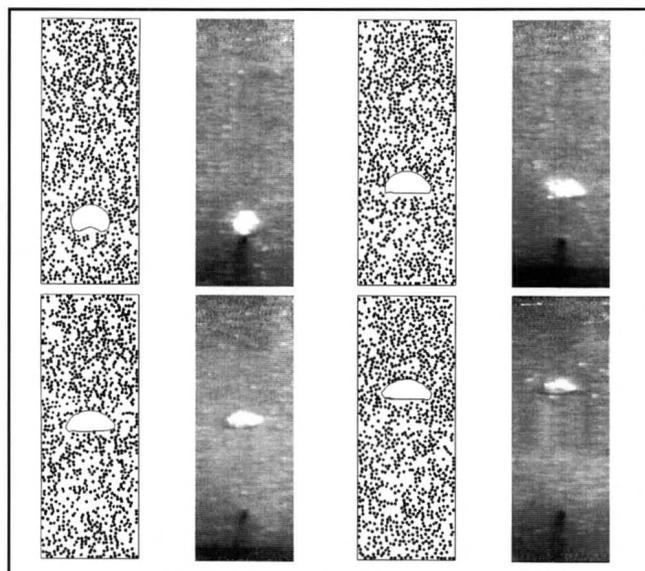


Figure 17.

Simulation results of a bubble emerging from the surface of a liquid-solid fluidized bed.

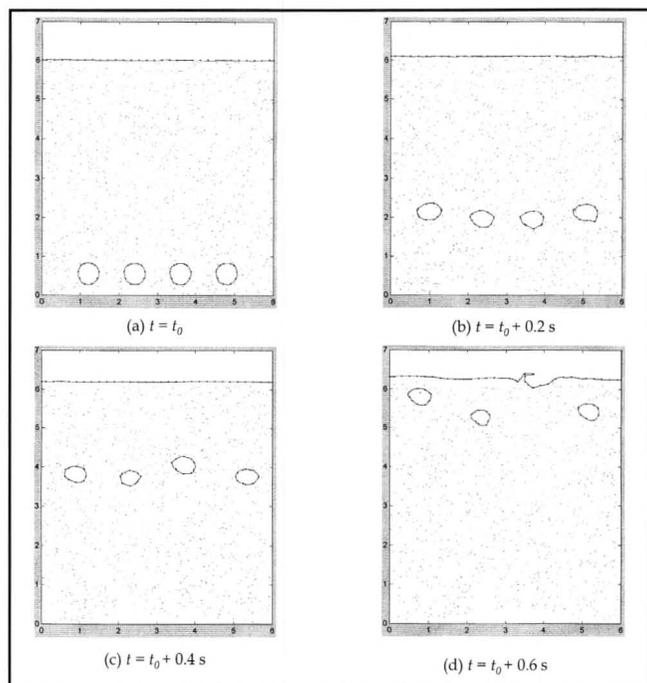
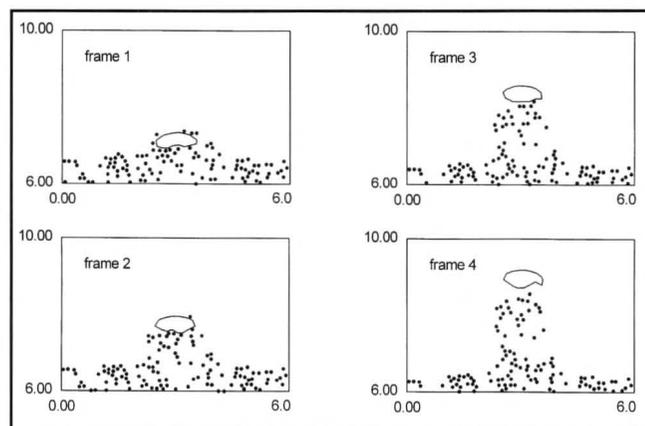


Figure 18. Simulation results of multi-bubble rising in a liquid-solid fluidized bed at a pressure of 17.3 MPa ($\epsilon_s=0.17$; $d_p=0.5 \text{ mm}$; $\rho_p=1,500 \text{ kg/m}^3$; $d_b=4.0 \text{ mm}$).

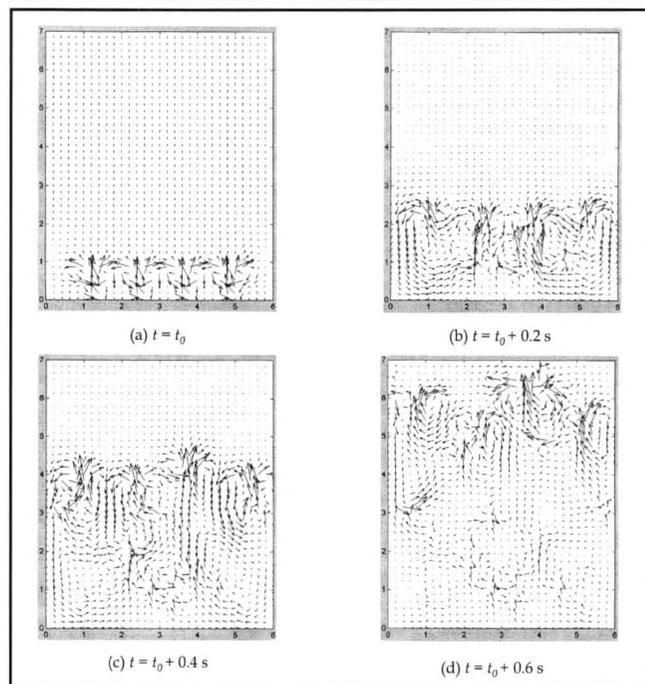


Figure 19. Simulated velocity vector fields of fluids for the conditions given in Figure 18.

surface. As seen in the figure, particles are drawn from the upper surface of the suspension into the freeboard of the bed through the wake behind the bubble; and particle-containing vortices are shed from the wake in the freeboard, consistent with the experimental observation shown in Figure 11. Figure 18 shows the rising of four bubbles in a liquid-solid fluidized bed with a solids holdup ϵ_s of 0.17 and a pressure of 17.3 MPa. The corresponding velocity vector fields of fluids are shown in Figure 19. As can be seen from the figure, the four bubbles are not rising at the same velocity even though their initial conditions are the same. Clearly, complex interactions among gas bubbles, liquid, and solid particles result in nonuniformity of the flow field shown in Figure 19, yielding uneven rise characteristics of the bubbles.

CONCLUDING REMARKS

I would like to conclude my lecture with the following thoughts:

- *Multiphase fluidization is a subject of importance to chemical engineering education as it encompasses the fundamental physics that govern multiphase fluid and particle mechanics and their interactions. Furthermore, interest in the subject is heightened because of its significant industrial applications.*
- *For gas-solid fluidization, topics of most relevance include, for low-velocity fluidization, particle and bubble dynamics, bed stability, bubble-phase and emulsion-phase interaction, and two-phase theory. For high-velocity gas-solid fluidization, the core topics are particle segregation and clustering. For gas-liquid-solid fluidization, the bubble-wake dynamics is key to the fundamental characterization of transport phenomena. In gas-solid or gas-liquid-solid fluidization, the particle property, which is an important operating variable, affects the fluidization regimes and their transitions.*
- *The computational fluid dynamics approach has provided a viable means for flow system and chemical reactor characterization. Although available commercial codes may not always yield accurate predictions, the familiarity of students with these computational tools would fortify their capability of understanding complex multiphase fluidization systems.*

ACKNOWLEDGMENTS

This lecture is dedicated to the memory of Professor Shao-Lee Soo of the University of Illinois, Urbana. I benefited from Prof. John Davidson's lecture on fluidization seven years ago when I was on sabbatical at Cambridge University, in which he demonstrated the simple slug-rising device that I duplicated, shown in Figure 2. I am indebted to Prof. Jack Zakin and my research group members, Dr. Jianping Zhang, Mr. D.-J. Lee, Mr. Brian McLain, Mr. Will Peng, and Mr. Guoqiang Yang, who have provided constructive

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TOWARD TECHNICAL UNDERSTANDING

Part 5. General Hierarchy Applied to Engineering Education*

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In the first papers in this series, I presented a *special* hierarchy of technical understandings^[1-3] based on my experience in trying to help students learn and informed by our current knowledge of the structure and function of the human brain. In the previous paper,^[4] I showed how the special hierarchy is related to a more *general* hierarchy developed by Donald^[5] and, independently, by Egan.^[6] In discussing the general hierarchy, I adopted Egan's nomenclature, which identifies five levels of human understandings: somatic, mythic, romantic, philosophic, and ironic. Each level corresponds to a specific mode for getting thoughts out of the mind and into forms by which they can be dissected, analyzed, and reassembled. To recapitulate, the somatic level includes tactile learning, mythic corresponds to oral learning, romantic involves graphics and written learning, philosophic refers to learning by formal reasoning, and the ironic level encompasses exceptions, limitations, and learning by modeling.

It is the philosophic level that encompasses the basic cognitive skills required of engineers; these include use of formal logic, mathematical reasoning, critical thinking, and problem solving. But the special and general hierarchical models are both integrative; that is, progression to a higher level requires the individual to master skills and reorganize knowledge gained at lower levels. Consequently, students cannot develop facility with philosophic activities until they have mastered lower-level cognitive skills.

In this paper we illustrate how the five cognitive levels can be used to guide teaching and learning activities appropriate for engineering students. To do so, we apply each level to

the concept of energy. As noted previously,^[4] energy is already a highly abstract concept characteristic of those employed at a philosophic level of understanding; however, the word energy is common in daily discourse and, therefore, it is familiar to students. Nevertheless, freshman and sophomore engineering students generally have only vague notions of the concept, and often confuse energy with force and pressure. For these reasons, energy is a good concept for showing how the hierarchy could be applied.

We emphasize that the suggestions here are fragmentary and superficial; they are intended only to offer a flavor of the kinds of activities that could be pursued. Note that our goals are not so much to *develop*, say, somatic and mythic modes of technical understanding, but rather to *appeal* to such modes for understanding a particular concept.

SOMATIC UNDERSTANDING

At the most basic level, our objectives are to help students obtain a "physical feel" for kinds and quantities of energy. For example, we might have students try to increase the temperature of water in a bowl by using a hand-driven egg beater. Or we might have them manually compress air in a piston-cylinder device, such as a large medical syringe. To test whether energy is extensive, students could measure the time required for a 500-watt microwave oven to bring a cup of water to boil; then they could repeat the heating using two cups.

More elaborately, we could invert a bicycle, attach a friction-driven electric generator to the rear wheel, and run an

* Part 1, "Brain Structure and Function," *CEE*, **31**(3), 152 (1997); Part 2, "Elementary Levels," *CEE*, **31**(4), 214 (1997); Part 3, "Advanced Levels," *CEE*, **32**(1), 30 (1998); Part 4, "A General Hierarchy Based on the Evolution of Cognition," *CEE*, **34**(1), 48 (2000).

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electric circuit from the generator to a light bulb.^[7] Students would then be asked to keep the bulb burning by cranking the pedals by hand. If we add a voltmeter and ammeter to the circuit, students could determine the amount of power they generate. Such exercises need be only semi-quantitative, for the intent is to help students connect physical effort to measurable changes in temperature, volume, and current flow.

At the most basic somatic level, students confront physical situations and devices; at a higher level, we try to appeal to their somatic experiences without further direct contact. Such attempts might take the form of simple questions requiring modest computations. For example, if the cost of electricity is \$0.1 per kilowatt-hour, how much does it cost to burn a 100-watt light bulb for one hour? The energy density of a typical gasoline is about 45 MJ/kg; if your car gets 25 mpg, estimate the amount of energy (kJ) your car uses per mile. The energy density of ethanol is 30 MJ/kg; estimate the amount of energy (kJ) in a 750-ml bottle of white wine that is 12% alcohol by volume.^[8] The key here is to contrive questions that make contact with situations that are familiar to students, else the somatic advantage is lost.

MYTHIC UNDERSTANDING

An important binary alternative that is fundamental to any study of energy is this: Does energy come in only one form, or are there many forms? If there are many, can we convert among them? Can the students cite examples of conversions in both directions between two forms? For example, electric motors convert electrical energy to mechanical, while electric generators convert mechanical energy to electrical. Similarly, solar cells convert radiant energy to electrical, while light bulbs convert electrical energy to radiant.

Are some conversions between energy forms easier than others? Do some conversions occur naturally? Are some conversions undesirable so that we seek to prevent or restrict them? Are some forms primarily for energy storage? These can lead to such questions as: What common devices are used to store energy? What is the defining characteristic of a machine? Is there a distinction between a motor and an engine?

One way to exercise the oral and narrative components of mythic understanding is to discuss with students old misconceptions about energy and forms of energy. Examples include the ancient idea that fire is an element, or, in an updated version, that heat is a thing (“caloric”) that is con-

served. Other common misconceptions surround the distinctions between quantity of heat and the intensity of heat; thus, it is a difference in intensity (temperature), not quantity, that drives heat transfer. More subtle confusions are attached to the possibilities of changing temperature without heat transfer and transferring heat without a temperature difference.

As another exercise of the oral component, each student could be asked to give a three-minute presentation on the origin, etymology, and historical significance of one piece of energy-related jargon. Appropriate words could include energy itself, horsepower, Btu, watt, Joule, kinetic, potential, efficiency, and friction.

ROMANTIC UNDERSTANDING

To identify the principal features on the energy landscape, we can have students list various forms of energy: kinetic, potential, chemical, nuclear, radiant, electrical, magnetic, heat, work, etc. Can these be distributed among certain categories? Students should also list kinds of molecular energies: kinetic, potential from intermolecular forces, electronic, and nuclear.

To exercise the narrative component of romantic understanding, students could be asked to contrive a chain of conversions; for example, living plants convert radiant energy to chemical, people eat plants to convert chemical energy to other forms of chemical energy, human muscles convert

the stored chemical energy to mechanic energy, the muscles might crank a hand generator that converts mechanical energy to electrical, and the generator might be wired to a light, which converts electrical energy back to radiant.

To identify extremes, we would offer students numerical examples of situations involving large amounts of energy: the potential energy behind the Hoover Dam, the energy required to launch a Saturn V rocket, the energy consumed by all automobiles in the U.S. in one year. At the other extreme, we might cite the energy required by one light-emitting diode (LED), the amount to depress one key on a keyboard, or the amount used by a hummingbird during five minutes of flight.^[8]

To appeal to human interests and motivations, we could start by working out an estimate of the energy—hence, man-years of effort—required to construct one of the Great Pyramids of Egypt.^[9] Then we could note that the desire to replace man-power with machine-power motivated the in

... the special and general hierarchical models are both integrative; that is, progression to a higher level requires the individual to master skills and reorganize knowledge gained at lower levels. Consequently, students cannot develop facility with philosophic activities until they have mastered lower-level cognitive skills.

dustrial revolution. This leads to a description of socio-economic conditions prevailing in Europe in the early 1800s, and, in particular, to a discussion of Joule's careful, systematic, extended, experimental studies of the relations between heat and work. We could describe Joule's paddle-wheel experiments, which illustrated the equivalence of heat and work and led to an identification of internal energy. We would emphasize that these crucial experiments discredited the caloric theory of heat and laid the foundations for articulation of the principal of conservation of energy.

Another instructive story is that of the Haber-Bosch process for the catalytic formation of ammonia from its elements under high temperatures and pressures. That process was first used to make nitric acid for explosives and thereby enhanced Germany's ability to prosecute World War I, but after WWII, it made possible large-scale production of fertilizers that sustain the world's growing populations. Thus, we have an example of the common dilemma of technology being used and misused. But in the context of energy usage, this story illustrates one way in which technologies evolve: the fundamentals of the Haber-Bosch process are unchanged, but improvements have reduced the energy costs of the process by more than an order of magnitude—from 380 MJ/kg of NH_3 in 1930 to 35 MJ/kg in 1990.^[8] Many important

chemicals have histories that can be exploited to appeal to students' romantic understandings; another example is the story of the Leblanc soda process, nicely told by Cook.^[10]

Still another aspect of romantic understanding is embedded in the graphical representations of physical objects and processes—plots, schematic diagrams, and flowsheets. An effective initial exposure to these tools is to confront students with objects and have them create schematics: cooling cycles in refrigerators or room air conditioners, the cooling-water cycle on an automotive engine, the steam cycle at a power generating plant, the water lines through their houses

or apartments, etc. The educational advantage here comes when students can see and touch objects, and they attempt to represent relations among those objects abstractly on paper.

PHILOSOPHIC UNDERSTANDING

At the philosophic level, our first goal is to find those unifying generalizations that connect the things and concepts encountered at the somatic, mythic, and romantic levels: the stories, the devices and equipment, the many concepts, the transformations among concepts, the extremes, etc. The cognitive hierarchy guides us in how this is to be done. We emphasize that we do not, at this point, confront students with the answer—the generalized energy balance. Rather, we proceed systematically from concrete situation to abstract generalization, following the left leg in Figure 1. Our second goal is to help students develop the ability to use the generalized energy balance, which is represented by the right leg in the Figure. Thus, our pedagogical goal is distinct from the practical one.

We might start a philosophic discussion of energy with equations that define individual energy forms, such as mechanical work, electrical work, and changes in kinetic and potential energies. Then students would exercise those definitions by applying them to relatively simple situations: a) estimate the speed of a crescent

wrench as it hits the ground after a free fall from the top of a 30-foot distillation tower; b) estimate the work performed by an adiabatic air compressor; c) estimate the heat required to raise the temperature of 1 kg of water from 20°C to 100°C.

(a) Concrete Situation • To start the progression on the left in Figure 1, we choose one of the concrete situations that the students have already encountered; a possibility is the compression of a gas in an insulated piston-cylinder apparatus. Many choices are legitimate here, so long as the one chosen arises from a situation for which students have strong visual images.

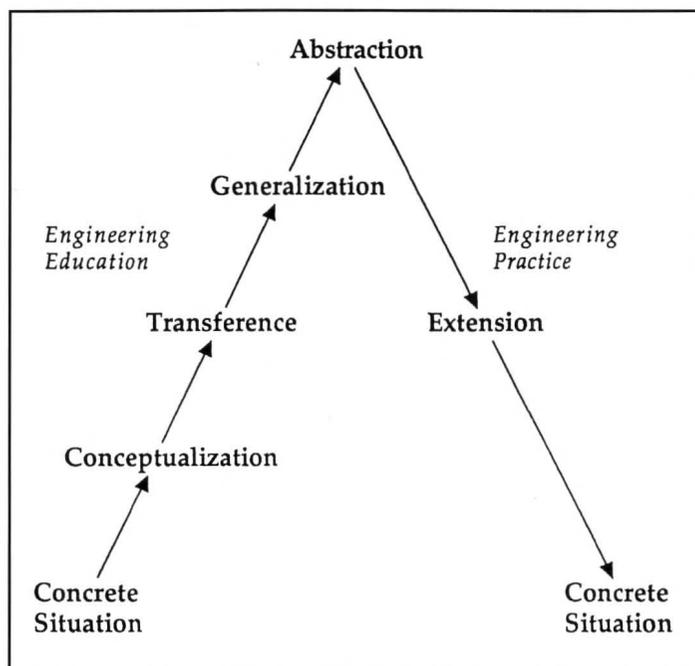


Figure 1. Understandings of abstractions develop in a bottom-up strategy from concrete situations to abstract concepts; thus, in helping students learn new concepts, we should start with concrete and specific examples and move toward abstract generalizations. We apply abstractions in a top-down fashion, however, from abstract notion to concrete situation. Thus, in helping students learn to solve problems, we should teach them to identify the generalized concept that applies and then to proceed deductively to their particular situation.

(b) Conceptualization • We now lead the students to identify the concept associated with the concrete example. We ask, what is it we, as engineers, are likely to want to know about the compression? Presumably, the amount of effort required. That effort is conceptualized by a particular form of energy—the work; here it is adiabatic work, because the apparatus is insulated. Note that because of the groundwork laid by the earlier somatic, mythic, and romantic exercises, the students should be able to participate actively in this discussion. Inversely, if those lower-level understandings have been ignored and instruction starts here at the philosophic level, then many students will be immediately overwhelmed. Once students have recognized work as the appropriate concept, we then have them calculate values for the adiabatic work under various sets of parameters applied to the piston-cylinder device.

(c) Transference • At this stage we want students to apply the concept of adiabatic work to situations other than the piston-cylinder apparatus. For example, we could pose problems involving adiabatic compressors, adiabatic turbines, and adiabatic pumps. The objective is for students to recognize that all such problems belong to the same conceptual class.

(d) Generalization • Now we come to the difficult stage at which we generalize away from the special case of adiabatic work processes. Thus, we first relax the adiabatic constraint and consider workfree heat transfer situations; then we introduce processes involving both work and heat transfer. We emphasize the extent to which these situations are conceptually the same as, but practically different than, the adiabatic work processes considered earlier. Then we consider steady-flow processes, with the introduction of flow work and the possibilities of changes in kinetic and potential energy. Finally, we end with a completely abstract consequence: the general energy balance, which applies to any process. This establishes the important connection among the various forms of energy; that is, this step relates the principal features of the energy landscape as identified at the romantic level.

Our second goal is to help students learn how to use the general energy balance; our strategy is now top-down, as on the right in Figure 1. Thus, we want students to appreciate that *any* situation they encounter is a special case, but we attack that special case by starting with the completely general energy balance and identifying the assumptions that are appropriate to the situation at hand. Thus, we would exercise the general energy balance applied to such situations as adiabatic processes on closed systems, to workfree processes on closed systems, and to steady-state processes on open systems. The latter would include illustrations of the special forms known as the mechanical energy balance and Bernoulli's equation. The concrete applications would include heat duties for heat exchangers, sizing of pumps, turbines, and compressors, analyses for thermal efficiencies,

etc. These kinds of activities are addressed in modern textbooks and many current learning strategies, so they need little attention here.

IRONIC UNDERSTANDING

To develop ironic understanding of energy, we would revisit the assumptions and limitations that pertain to the equations used at the philosophic level. For example, most calculations of mechanical work can be done only for idealized processes in which the driving forces are differential. For real processes, in which the driving forces are finite, we need an efficiency, obtained either from measurement or by estimation. To calculate changes in internal energy and enthalpy, we often need an equation of state that models the PVT behavior of the working fluids. Many texts restrict such calculations to the ideal-gas model, but students must be introduced to more realistic models, and they must be instructed in the engineering task of selecting a model that is appropriate to their problem. Thus we must confront issues associated with model processes and model substances. For example, we may be able to perform an exact analytic calculation of the required heat duty for a heat exchanger design, under the presumptions of particular model processes and model substances. However, such exact calculations are still approximate to the degree that the assumed models fail to represent the real situation. Students often have difficulty in reconciling how an approximate answer can be obtained from an exact calculation.

NONLINEAR INSTRUCTION

For purposes of clarity, the suggestions in the foregoing sections were presented in a linear progression that builds from somatic to ironic. In practice, however, instructors of college students need not—indeed, should not—proceed in such a linear fashion. Of course, somatic activities should generally be performed well before philosophic activities, but this does not mean we should avoid somatic and mythic digressions in an otherwise largely philosophic lecture. For example, continuing with energy as the focal point, the listing of types of energy (romantic) could be done as soon as students acknowledge that energy comes in many forms (response to the mythic binary). Calculation of the velocity of the falling crescent wrench (philosophic) could be embellished with the observation that the answer is independent of mass, so the velocity would be the same for a manhole cover or a pocket watch; this harks back to the tale of Galileo and the Leaning Tower of Pisa (a romantic reference). The discussion could be further extended by noting that the terminal velocity is independent of mass only when the air resistance is negligible; thus, we have done a model calculation that yields an approximate answer (ironic).

It is appropriate and beneficial to include somatic, mythic, and romantic allusions in a largely philosophic presentation;

One of an instructor's goals is to find the level of understanding at which students are balanced between perplexity and confidence; at that point of creative tension, teaching is most effective and learning most rapid.

however, the inverse procedure is counterproductive and should be avoided. That is, we accomplish little when we introduce abstract generalizations (such as the generalized energy balance) and models (such as Raoult's law) before somatic, mythic, and romantic contexts have been established for those generalizations and models.

At this point, kind Reader, you might indulge in the following reflective exercise. Pick a course you have taught recently; can you identify the cognitive level at which you did most of the teaching? For example, if most of the instruction took the form of anecdotes based on your industrial experience, then you were functioning at the mythic level with appeals to the somatic. If the instruction depended heavily on students reading the text, technical reports, research journals, and on their making and interpreting plots, schematic diagrams, and flowsheets, then you were working at the romantic level. If the instruction emphasized derivations, problem solving, and calculations, then you were at the philosophic level. If the instruction involved liberal doses of all of these, plus efforts to sensitize students to the uses and limitations of models, then you were teaching at the ironic level.

Any of these approaches may be right or wrong, effective or not, depending on the situation—that is, depending on what your students needed at the time. So now ask yourself, why did you choose to instruct at the level you did? Was the choice made implicitly for your own convenience and comfort, or was it made explicitly to address the needs of the students? What was the outcome of your work? If the students were generally frustrated, then your teaching level failed to match their needs. If the students were generally happy, comfortable, and secure, then your efforts probably were limited to reinforcing their current levels of understanding. If the students were apprehensive but stimulated, then they were probably growing toward higher levels. (If only the reality were as simple and clear-cut as these idealized comments imply.)

COMMENTS

As an individual grows through levels of understanding, lower-level understandings are not lost or displaced; rather, they are reorganized and subsumed into high levels. Nevertheless, there is a loss associated with each transition;^[6] for example, the admonition to “be objective” means to strip away mythic and romantic associations, such as emotion and anecdotal evidence, and reason logically.^[5] But if the basic somatic and mythic understandings are not lost, what is? Part of the process of solidifying understandings at one level

includes the creating of mental scaffolding that will support the transition to the next level.^[3] Once the transition is complete, the scaffolding collapses. But some people become attached to the scaffolding and experience a sense of loss when it collapses. Such is the nature of mental growth.

How much understanding does an individual need at one level before he can move to the next? The answer must be that it depends on the individual and the extent of his earlier experience with understandings at that level. For example, we conjecture that an individual who has developed somatic understandings of some concepts will find it easier to develop somatic understandings of other concepts. The situation must be much like the learning of a foreign language (or a computer language), which is made easier if the individual has already learned another. In higher education, we appeal to somatic, mythic, and romantic modes of thinking to solidify the foundations for philosophic and ironic understandings. Successful generalization (concrete to abstract) and extension (abstract to concrete) depend on facility with manipulating objects and concepts at somatic and mythic levels.

To illustrate let us consider the value of somatic thinking. Marvin Minsky^[11] asks why we insist on thingifying abstractions. It can only be because thingifications help our thinking. Thus, we think about energy as a thing, even though most forms of energy are abstract mathematical functions and are not objects at all. We do this so we can draw fruitful analogies between energy and mass: mass can flow into and out of systems, so can the energy-thing; mass is conserved, so is the energy-thing; mass is a resource whose use incurs cost, so is the energy-thing. The power of such analogies is so well accepted that we take it for granted. But our familiarity with such analogies must not blind us to the significance of the achievement nor to the difficulty students have in accepting such analogies and using them.

In recent years, engineering educators have renewed emphasis on the development of oral (mythic) and written (romantic) communication skills. But, according to the cognitive hierarchy, these skills are valuable not merely for communication; rather, they are important because they support subsequent development of understandings at the philosophic level. Further, the hierarchy asserts that oral skills develop before written skills; this reverses the order employed at many institutions, where oral skills are addressed late in curricula and after written skills have been exercised.

Students come to us at many different levels of understanding, and our obligation is to help them grow to higher

levels. It may be that many people in our society cannot become philosophic thinkers in any mathematical sense. Such people cannot become engineers, and their talents should be developed and applied in other ways. Further, some people can function at the philosophic level, but they may be more *effective* at some other level. These people can fulfill important and even creative roles in engineering; however, they cannot make informed judgments about the best use of their talents until they have acquired some skill in philosophic thinking.

Good teaching meets students at their current levels of understanding and attempts to push them to higher levels. This requires that instructors be able to cross readily among levels of understanding: this is an attribute of the ironic thinker. An obvious general rule-of-thumb is: If the student seems perplexed or confused, the instructor should push the discussion to a lower level of understanding. Equally important, but often overlooked, is the inverse: If students seem confident and secure, then the instructor should push the discussion to a higher level of understanding. One of an instructor's goals is to find the level of understanding at which students are balanced between perplexity and confidence; at that point of creative tension, teaching is most effective and learning most rapid. This goal is relatively easy to achieve for a single student (a graduate student), but exceedingly difficult to achieve for a group of heterogeneous talents and personalities (an undergraduate class).

Between, say, 1950 and about 1990, engineering education developed along ever-increasing theoretical, mathematical, and abstract lines; that is, engineering education came to be practiced almost completely at the philosophic level. Such is the natural progression that mirrors cognitive evolution. But in recent years we have come to realize that solely philosophic modes of instruction fail to help today's students. The typical reaction has been to dilute philosophic instruction in various ways. For example, some chemical engineering departments have reduced the philosophic content of the curriculum by removing physical chemistry, quantum mechanics, transport phenomena, or computer programming. In the courses that remain, the philosophic content has, perhaps, been diluted by over-emphasis on "practical" applications and flowsheet design. But too much attention to applications produces a catalog of special cases, when the objective should be development of organizing principles that generalize across individual situations. Further, today's flowsheet design tends to be accomplished with the aid of process-simulation programs; but without sufficient command of philosophic and ironic thinking, students can only allow such exercises to devolve to syntheses of black boxes, with issues of engineering judgment relegated to default settings of the software. Such dilutions of philosophic instruction actually make matters worse:^[6] not only do they

fail to develop philosophic thinking, but they also leave students with confused and useless somatic, mythic, and romantic understandings of technical material.

Rather than dilute the philosophic content of engineering curricula, we should be moving in the other direction. As a rough generalization, our goals might be to use early engineering courses to solidify understandings at the somatic, mythic, and romantic levels. But though the levels would be emphasized, higher modes would not be neglected; some foreshadowing of philosophic and ironic thinking must also be done. Then, once students begin the transition to philosophic thinking, the curriculum should develop that thinking by being *more* abstract and theoretical, not less. This is the direction of growth for individuals, cultures, and even engineering.

Finally, we ask, is there any level of understanding beyond ironic? I think the only proper answer is, we don't know. Donald notes that each level of understanding incorporates a particular mechanism for off-line processing—for getting thoughts out of the mind so they can be more readily manipulated, dissected, and reassembled.^[5] At the somatic level, the off-line processor is the human body; at the mythic level, it is speech; at the romantic level, it is graphics and writing; at the level of (technical) philosophic and ironic thinking, it is mathematics and written chains of logic. So the question is, can we find another mechanism for out-of-mind processing? Can the computer fulfill this role? I think we can only wait and see.

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Random Thoughts . . .

THE SCHOLARSHIP OF TEACHING

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In his landmark 1990 monograph, *Scholarship Reconsidered*,^[1] Ernest Boyer observed that the work of the professoriate involves four different functions: *discovery* (advancement of the frontier of knowledge in a discipline), *integration* (putting research discoveries in broader contexts, making connections across disciplines), *application* (applying the outcomes of discovery and integration to socially consequential problems), and *teaching* (helping students to acquire specified knowledge and develop specified skills and attitudes). Boyer argued that these four activities are equally vital to the academic mission and that the academy should therefore recognize and reward scholarship equally in each of them.

The scholarship of discovery—frontier research—is what most faculty members think of as academic scholarship, and while the scholarship of integration and the scholarship of application may not occupy the same honored position in the faculty incentive and reward system, most professors would at least agree that they exist in principle. It's a different story with the scholarship of teaching. Administrators and faculty members traditionally put teaching and scholarship in non-overlapping categories: some argue that “scholarship of teaching” is a contradiction in terms, and many who concede its theoretical possibility question whether it can be validly assessed.

What is the scholarship of teaching?

According to Boyer, the elements that define teaching as a scholarly activity are mastery of the subject being taught, knowledge of pedagogical methods that have been proven effective at promoting learning and skill development, and commitment to continuing personal growth as an educator. To this list might be added involvement in educational research and development—designing, implementing, assessing, and disseminating innovative instructional methods and materials.

Research in education-related disciplines has a long-established tradition. When done right, it adheres to the same standards of scholarship that characterize good engineering

research. These standards have not been routinely observed in engineering education, however, and until relatively recently most of the literature has consisted of variations on the theme, “We tried this method and liked it and so did the students.”

This situation has begun to change in the past decade, largely due to the efforts of the National Science Foundation Division of Undergraduate Education and the Engineering Education Coalitions, and a growing percentage of the engineering professoriate is now engaging in serious educational research and development. It is no longer enough to say that everyone liked a method and the students performed well when it was used. The NSF project monitor and the *Journal of Engineering Education* reviewers will inevitably respond with questions such as “What learning objectives were you trying to achieve?” “How well were those objectives met?” and “How do you know—what were your assessment measures, your control populations, your statistical analysis procedures, your evaluation criteria?”

How should the scholarship of teaching be assessed?

Boyer proposes making the scholarship of teaching a legitimate basis for awarding tenure and promotion to faculty members who choose to make education a major focus of their careers. (Not all faculty members should be expected to do so.) This proposal—which has predictably encountered considerable skepticism and some outright hostility from administrators and professors—will gain widespread acceptance only if criteria for evaluating the scholarship of teaching are established and generally agreed-upon. I propose that the evaluation should consist of answering three questions:

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1. *To what extent did the teaching qualify as a scholarly activity?* Answering this question requires evaluating the faculty member's subject knowledge, pedagogical knowledge, commitment to growth as an educator, and involvement in educational research and development.

2. *How effective was the teaching?* How well has the faculty member's teaching motivated students to learn and promoted their acquisition of desired knowledge, skills, and attitudes?

3. *How effective was the educational research and development?* How well were the faculty member's educational innovations designed, implemented, assessed and evaluated, and disseminated? What has been their impact on engineering education?

The data that can be used to answer these questions fall into four categories: *archival data* (lists of courses developed and taught, representative instructional materials and student products; numbers of undergraduate and graduate students advised and faculty colleagues mentored; disciplinary and education-related conferences and workshops attended; journals subscribed to; conference presentations, seminars, and workshops given; articles, books, and courseware published); *learning outcomes assessment data* (test results, evaluations of written and oral project reports

and other student products, student self-assessments); *subjective evaluations by others* (student end-of-course ratings, retrospective student and alumni ratings, peer ratings, awards and recognition received, reference letters); and *self-assessment data* (statement of teaching philosophy and goals, self-evaluation of progress toward achieving the goals). A subset of these items gathered into a teaching portfolio provides a sound basis for assessing the scholarship of teaching.”

Glassick, *et al.*,^[2] suggest the following standards for evaluating educational innovations:

- *Clear goals:* Is the basis of the work clearly stated, the questions addressed important, and the objectives realistic and achievable?
- *Adequate preparation:* Does the scholar display an understanding of existing scholarship in the field and the skills needed to assemble the necessary resources and do the work?
- *Appropriate methods:* Were the methods used appropriate for the goals, applied effectively, and suitably modified when necessary?
- *Significant results:* Were the goals achieved? Did the work contribute significantly to the field?
- *Effective presentation:* Was the work presented effectively and with integrity in appropriate forums?
- *Reflective critique:* Does the scholar critically evaluate his or her own work,

bringing an appropriate breadth of evidence to the critique and using the critique to improve the quality of future work?

Faculty members doing educational research that meets these standards are clearly contributing to the scholarly mission of the university. They merit advancement up the faculty ladder—tenure, promotion, and merit raises—no less than faculty members who meet institutional standards for disciplinary research.

Table 1 contains a matrix that may be used to custom-design a process for assessing the components of the scholarship of teaching.

Continued on page 152.

TABLE 1
Assessment of the Scholarship of Teaching

	Subject Knowledge	Pedagogical Knowledge	Commitment to Personal Growth	Innovation and Dissemination	Teaching Effectiveness	Quality of Innovation
Statements of teaching philosophy		x	x			
List of courses taught and developed, representative instructional materials	x	x		x		
Representative student products					x	x
Learning outcomes assessment data					x	x
End-of-course student ratings for the past 2-3 years					x	x
Retrospective senior ratings	x	x			x	x
Alumni ratings	x	x			x	x
Peer ratings	x	x		x	x	x
Self-evaluation			x		x	x
Teaching seminars and conferences attended, books read, journals subscribed to		x	x			
Presentations, invited seminars, and workshops on teaching given		x		x		
Published papers and monographs	x	x		x		x
Published textbooks and courseware	x	x		x		x
Awards and other recognition					x	x
External references					x	x

TEACHING PDE-BASED MODELING TO ChE UNDERGRADUATES

Overcoming Conceptual and Computational Barriers

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Introducing partial differential equations (PDEs) in the undergraduate engineering curriculum can be frustrating for both students and instructors. Many students gain a dislike of differential equations before the core engineering curriculum even begins. As engineering instructors, we then face a number of challenging problems. We must help the students overcome conceptual barriers associated with the math and help them envision the physical phenomena being described. Additionally, we must devise models for which we can obtain solutions in limited timeframes (*i.e.*, class time or homework time). This latter constraint is imposed by computational barriers, which often restrict us to overly simplistic problems that have limited engineering relevance. Although these computational issues have been a stumbling block in the past, modern numerical packages prove to be very accessible, even to the undergraduate student, and have been shown to improve learning in a number of ways.^[e.g.,1]

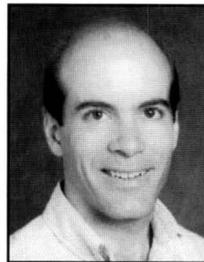
This paper describes an instructional framework that was used for incorporating computational tools into a relatively short section on PDEs during an undergraduate modeling course. The rationale is that by allowing the students to jump headlong into the solution of real engineering problems, the emphasis in the classroom can change. Attention can be diverted away from arduous mathematical details (for the moment) and focused on broader conceptual issues such as the general behavior of classes of equations, or using a model for design considerations. This approach has a number of advantages. The students' concurrent, hands-on solution of problems is a powerful method for illustrating fundamentals (that otherwise seem abstract). More time can be committed to model development and general behavior (which remain with students longer than the details of solution techniques). And, the ability to solve real engineering problems illustrates to the students the true power of mathematical modeling.

A number of computational packages are available and appropriate for undergraduate education. Mathcad, Maple, Mathematica, MATLAB, and Polymath are all common in chemical engineering education.^[1-4] Fluent is especially effective for CFD applications.^[5] We focus on MATLAB in this paper, largely because of its unique PDE Toolbox. At LSU, MATLAB is provided to the students via the department's PC network. (An academic unit can provide MATLAB on a number of PCs without a large investment by purchasing a classroom kit.) Additionally, Mathworks has recently released a student version of MATLAB (which is the professional version plus popular toolkits) that helps students who wish to work at home.

In the remainder of this paper we will discuss the context for this approach and one possible strategy for breaking down conceptual barriers in the classroom. At the end, three example problems will be solved using MATLAB, illustrating the type of modeling exercises that can be assigned to complement conceptual discussions in the classroom.

CONTEXT

The ideas and examples described here were developed as part of a senior-level math-modeling course at LSU, which is described below. When beginning the PDE section of the course, it was helpful to consider the contexts in which our



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students typically are introduced to PDEs. Unfortunately, these encounters are infrequent and generally presented as asides to the main material.

Consider three of the most likely places that ChE undergraduates run into PDEs. First, they may arise at the end of an introductory numerical methods course. But using Chapra and Canale^[6] as a guide, we see that PDEs are relegated to Chapter 29, suggesting that the topic probably receives a quick overview near the end of this type of class. PDEs are usually presented again in the undergraduate fluids course in the form of the Navier-Stokes equations, but the emphasis here is placed on the flow phenomena rather than the mathematics (rightly so), and the solved examples are nearly always one-dimensional problems that reduce to ODEs. Hence, for chemical engineering students, the lasting impression of PDEs usually comes from dealing with the unsteady heat equation. While the equation and its application are fairly easy to grasp, the mathematics are not; the most common introductory solution is for a semi-infinite domain, which calls for abstract boundary conditions, a similarity transform, and an error-function solution. (Surely, the frequent appearance of *erf* on comical student-organization T-shirts should tell us something!)

While experiencing PDEs in a variety of contexts emphasizes their importance, it likewise seems to leave the students somewhat unsettled and without a firm foundation for the subject. These considerations helped formulate an approach that was used when given the luxury of spending three or four weeks on the topic of PDEs with senior-level chemical engineers. At LSU, the class in which this occurs is “Development of Mathematical Models.” It affords a number of unique opportunities for the instructor. Being a math course among other more popular electives, it attracts some of the better undergraduates along with a few Masters students from our graduate program and from industry, and these students have more-or-less completed the ‘principles’ classes. Also, beyond the class’s strong modeling emphasis, the topical coverage is left largely to the instructor’s discretion (see Rice and Do^[7] for a template of the course offered at LSU). Finally, at the point in the semester when PDEs are introduced, the students have themselves derived a number of PDEs governing transport and reaction engineering problems that subsequently were reduced to simpler form. Hence, their foundation for model development is strong, and they can clearly see the need to move beyond algebraic equations and ODEs in order to make full use of their models.

APPROACH

The educational objective is to allow the students to solve complex PDEs of real engineering interest, without sacrificing coverage of fundamental mathematical behavior. To realize this goal, an approach is used whereby classroom coverage includes topics such as the origin of the equations, visualization of the solution space, qualitative behavior, and ties between the physical phenomena and mathematics. These topics are potential conceptual barriers, and overcoming them can make the terminology and the detailed mathematics less intimidating. At the same time, to prevent excessive classroom time being devoted to numerical techniques or specialized software, the students are left mostly on their own to pursue numerical solutions to homework or modeling projects. This approach works well (given good numerical tools) because the solutions that the students have themselves worked out are highly effective illustrations of conceptual topics. In the past, it would have proved less feasible because, until the instructor covered solution techniques, the students lacked the tools to fully explore the mathematical models with which they were working.

The intent is not to de-emphasize the crucial subject of solving PDEs. Rather, these issues are postponed until the foundation is stronger. If implemented properly, this approach shares many positive attributes of ‘just-in-time learning’ employed by Finlayson.^[8] modeling projects evolve so that just as students identify the need for new mathematical tools, the relevant subjects are addressed. The benefit of incorporating software such as MATLAB is that topical coverage in the classroom can remain fundamental without slowing the students’ progress toward quantitative solutions.

The ideas and examples described here were developed as part of a senior-level math-modeling course at LSU, . . . When beginning the PDE section of the course, it was helpful to consider the contexts in which our students typically are introduced to PDEs. Unfortunately, these encounters are infrequent and generally presented as asides to the main material.

CONCEPTUAL BARRIERS

Conceptual barriers are never clear-cut, and they of course depend on background, learning style, and ability. But we will attempt to generalize a set of hurdles that stand between more easily conceptualized physical behavior and the corresponding mathematics. An example is the categorization of PDEs; the mathematical definitions of parabolic versus hyperbolic PDEs probably seem abstract at first, but explaining the analogy to the synonymous heat and wave equations makes this classification more tangible.

This development of strong ties between analogous physical and mathematical behavior provides a basis for breaking down conceptual barriers. Emphasis is placed on the behavior of *general classes* of PDEs, with concrete examples used to illustrate these ties. It is hoped that the foundation and comfort level that can be achieved by this approach offsets the 'risk' of sending the students headlong into numerical solutions (without much knowledge of the associated techniques).

No single list of conceptual barriers is comprehensive. Table 1 shows a list of topics that are addressed sequentially by the author during a three-week section covering PDEs. The first couple of points are general, but the latter part of the list applies to second-order PDEs, for two reasons. First, many second-order equations can be packaged neatly into elliptic, hyperbolic, and parabolic categories, which aids in generalizing behavior. Second, these are the types of equations amenable to solution in MATLAB's PDE Toolbox, which was an essential part of the approach.

The in-class overview of second-order PDEs was taken largely from Crandall,^[9] who does an excellent job of tying qualitative behavior of the equations to quantitative mathematics (numerical and analytic). The approach promotes picturing a PDE as a family of surfaces, the correct surface being pinned down by the appropriate boundary and initial conditions. Crandall explains the difference between equilibrium problems and propagation problems, which ties in nicely to a discussion of the characteristic curves for parabolic and hyperbolic equations.

COMPUTATIONAL BARRIERS

Effective use of a math model requires, of course, a solution. In the past, a significant time investment was required to introduce analytic

solution techniques and the problems were more often than not restricted to one spatial dimension. From a numerical perspective, innovative ideas have been presented for programming solutions to PDEs at an introductory level,^[10,11] but these too are dimensionally restrictive. In contrast, modern numerical software gives the student more flexibility with respect to the type of problems that can be solved and the way in which they can be explored.

Software such as MATLAB's PDE Toolbox allows two-dimensional problems of arbitrary geometry to be set up and solved in a matter of minutes. In MATLAB, the system geometry is entered using a graphical user interface (GUI) that strongly resembles familiar drawing programs. Equations and boundary conditions are chosen from radio-button menus, and clicking with the mouse results in mesh discretization, solution by the finite element method, and a wide range of three-dimensional color graphical output. Numerical output is only slightly harder to manipulate, requiring a review of MATLAB's built-in 'pde-tool' scripts. The PDE toolbox can be used at an introductory level without extensive knowledge of the basic MATLAB software. Hence, the time spent in familiarizing students with the software can be kept relatively small. In 1997, the PDE toolbox was introduced to the students during a single-

TABLE 1
Synopsis of Conceptual Topics Discussed During Classtime
During the PDE Section of a Modeling Course.

<i>Topic used to address conceptual barrier</i>	<i>Synopsis of the classroom discussion</i>
Independent and dependent variables	Use a 'familiar' equation to emphasize independent/dependent and how they define a PDE.
Picturing the solution surface	An ODE describes a family of curves; one or more boundary conditions pin down the curve of interest. Similarly, many PDEs can be pictured as a surface, pinned at the edges.
Second-order PDEs	These are categorized as elliptic, parabolic, or hyperbolic. It helps to understand physical behavior associated with each in the form of Poisson's equation, the heat equation, and the wave equation.
Equilibrium versus propagation	Elliptic equations describe equilibrium or 'jury' problems ^[9] —the boundaries (which are fixed on all sides) wholly dictate the shape of the interior. Propagation problems have an open boundary. The surface evolves with time, pinned on the sides by boundary conditions and at the front by initial conditions.
Characteristic lines	Characteristic lines are sudden changes in the slope of the surface (like creases), brought about by changes in boundary conditions. Parabolic equations have one characteristic line; changes at the boundary are propagated instantly but weakly into the interior. Hyperbolic equations have two characteristic lines. Changes at the boundary are propagated into the interior at full strength but at a finite speed.
Finite difference methods	There are analogous characteristic lines for the finite difference method. These partly dictate step size in propagation problems.
Stability and numerical diffusion	When using numerical solutions, we must be wary of errors inherent to the solution technique. Many of these stability issues relate to the form of the governing equation.

class session held in the department computer lab. In 1999, it was introduced via a step-by-step instruction set handed out to the students, thus requiring no class time.

The use of software should not de-emphasize the importance of teaching analytic and numerical techniques for solving PDEs. Instead it should allow us to embrace the introduction of PDEs at the undergraduate level (if their use enhances the fundamentals being taught) and encourage exploration and critical thinking early on.

Three examples are given below. These were chosen to illustrate a number of points. First, they are indicative of the

types of problems easily solved by MATLAB (most importantly, those with arbitrarily complex boundary geometries). Second, one each of an elliptic, parabolic, and hyperbolic equation are shown. Third, and most important, they typify problems where the student clearly understands the engineering relevance and the manner in which their models can be used in design. This last aspect becomes especially effective when a model can be tied to an experiment, as is shown in Example 1, or, for instance, in reference 12. The MATLAB scripts for these examples can be found on the web at <www.che.lsu.edu/faculty/thompson/education.htm>

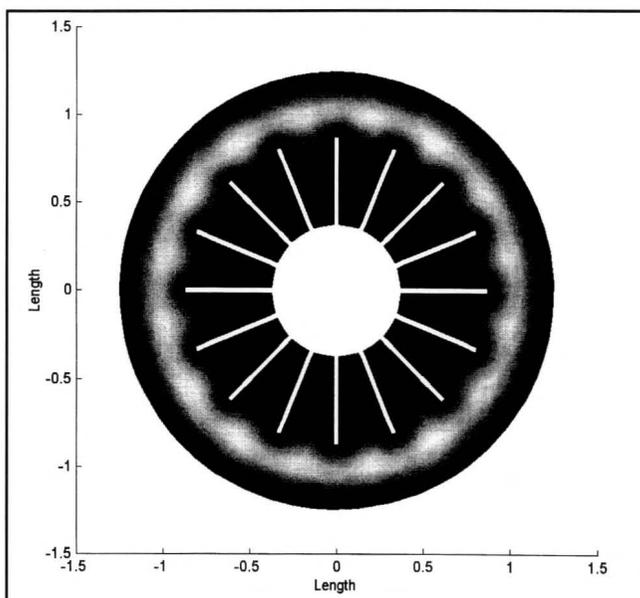


Figure 1. Velocity map in entire heat-exchanger domain taken from undergraduate students' solution.

domain (boundaries along the centerlines of two neighboring fins) or 1/32 of the domain (one boundary along a fin and one along a fluid line of symmetry). We show the former approach below.

For unidirectional flow, the Navier-Stokes equations reduce to^[13]

$$\rho \frac{\partial u}{\partial t} = G(t) + \mu \nabla_2^2 u \quad (1)$$

where u is the velocity in the direction of flow, $G(t)$ is the pressure gradient in this direction, and ∇_2^2 is the Laplacian for the two directions orthogonal to flow. Hence, for a steady flow, G is constant and the equation re-

duces to Poisson's equation

$$\nabla_2^2 u = -G/\mu \quad (2)$$

Zero-velocity boundary conditions are used along all surfaces of the heat exchanger. Depending on how the FEM domain is chosen, lines of symmetry are likely to arise, in which case symmetry boundary conditions ($\mathbf{n} \cdot \nabla u = 0$) are also used. In MATLAB, the elliptic equation is written as

$$-\text{div}[c * \text{grad}(u)] + a * u = f \quad (3)$$

where 'div' and 'grad' are the divergence and gradient operators, respectively. Hence, one would specify $c=1$, $a=0$, and $f=G/\mu$ to perform the calculation. The solution using MATLAB's PDE Toolbox involves four steps:

1. Map the domain using the GUI. (The geometry can be drawn crudely using the mouse, and then refined by double-clicking on the various polygons to type in precise vertex positions.)
2. Select the governing equation and boundary conditions. The GUI contains a radio-button interface that allows the user to specify the type of equations and boundary conditions along with values of parameters.
3. Solve the problem. After step two, the solution consists of clicking two buttons: one to generate and refine the FEM mesh and the second to solve the problem. A wide range of graphical output is available.
4. Quantitative analysis. This last step requires slightly more user experience since the command-line interface must be used. For instance, values of velocity at each node in the mesh are contained in an array that can be exported to the MATLAB workspace. There are a series of 'pde-tool' commands that can then be used to perform interpolation, integration, etc. Integration is used to calculate volumetric flowrate as a function of the pressure gradient that was

Example 1 Steady Laminar Flow in a Finned Heat Exchanger

For parallel laminar flow through a duct, the Navier-Stokes equations reduce to Poisson's equation (a scalar equation since there is only one velocity component). This example is for flow in the annulus of a heat exchanger in LSU's ChE measurements laboratory. This example was of particular interest to students in the math modeling class because many of them had used this apparatus for a pressure-drop-versus-flowrate experiment in which they calculated the friction factor for the annular region. Additionally, the complex geometry in the annulus makes the problem an excellent candidate for solution using MATLAB.

The annular space in the heat exchanger is contained between $r = 1.05$ inches (OD of inner pipe) and $r = 2.469$ (ID of outer pipe). It contains 16 symmetrically placed fins of width 1/32 inch and length 1/2 inch, as shown in Figure 1. Symmetry allows the solution to be performed in either 1/16 of the

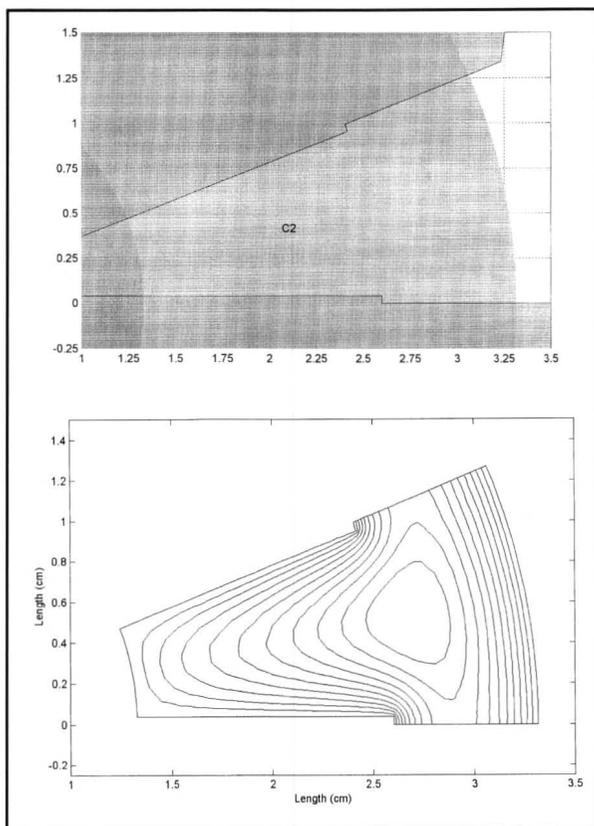


Figure 2. Geometry of 1/16 of flow region in heat exchanger (top); z-direction (perpendicular to page) velocity contours (bottom).

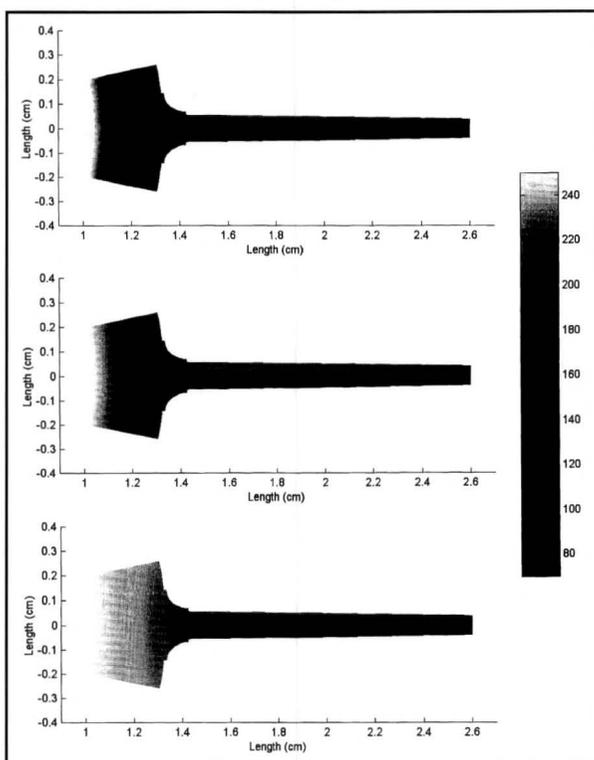


Figure 3. Snapshots of temperature profiles during transient heating ($t=7$ sec, $t=2.4$ min, and $t=12$ min).

imposed during specification of the PDE.

Figure 2 shows how the annulus geometry (1/16 of the entire domain) is defined using various simple geometric shapes and shows contours of the z-direction velocity (*i.e.*, velocity is perpendicular to the page). The contours have not been assigned numerical values in this figure because the velocity depends on one's specific choice of viscosity and pressure gradient. Their shape remains fixed, however.

Integration of the velocity profile to determine flowrate gives a fanning friction factor $f=19.5/Re$, whereas students typically obtain values between $f=20/Re$ and $f=25/Re$ in the experiment (using an effective area approach). When quantitative analysis is used, one can introduce the students to issues of numerical accuracy. Grid refinement is trivial in MATLAB, requiring only the click of a button for successive refinements of the FEM mesh. Using various levels of grid refinement in this example (the standard mesh followed by two successive refinements), one obtains the following values for the friction factor: $20.12/Re$, $19.65/Re$, and $19.52/Re$.

Returning to Figure 1, one can see the velocity profile for the entire annular region, where the lighter shading indicates higher velocities. While numerical solution over the entire annular region is less efficient than breaking it along lines of symmetry, the resulting graphic is more appealing than Figure 2. Figure 1 was taken directly from two students' homework;^[14] they were able to work the problem after only a short tour of MATLAB during one of the class periods. (The students used inches rather than cm, causing the discrepancy of scale with Figure 2.)

Example 2 Transient and Steady Heat Transfer in a Finned Heat Exchanger

While the heat exchanger described in Example 1 is not used for heat-transfer experiments at LSU, the concept of heat transfer from a fin is both important and readily amenable to visualization.

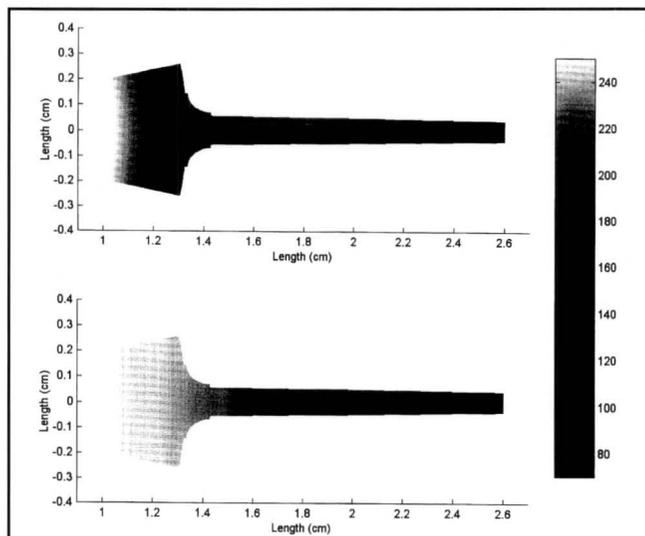


Figure 4. Steady temperature profiles for high (top) and low (bottom) fin-side heat transfer coefficients.

The example shown here can illustrate the unsteady evolution of a temperature profile as well as the steady-state temperature profile for various heat-transfer coefficients. The transient problem underscores the behavior of parabolic PDEs, while the steady problem helps to illustrate engineering fundamentals: the conditions under which fins are useful for increasing heat-transfer efficiency.

Parameters are taken from Example 27-3 in Bennett and Myers,^[15] and the fin dimensions are based roughly on the elliptic example above. The geometry is made somewhat more complex to illustrate the versatility of MATLAB's GUI.

Figure 3 shows the fin at $t=7$ sec, $t=2.4$ min, and $t=12$ min. The shading shows the evolution of the temperature profile in time (an effect that is much more dramatic in color). Figure 4 shows two steady-state profiles, for a high external heat-transfer coefficient [1500 Btu/(hr-ft²-°F)] and a low external heat-transfer coefficient [1 Btu/(hr-ft²-°F)]. The graphics shown here help students conceptualize the conditions under which fins can significantly increase heat transfer.

We make two final points. First, the evolution of the temperature profile (especially in color) is helpful for understanding the behavior of a parabolic PDE: a change in the boundary condition has immediate but weak influence throughout the fin, and the temperature evolution is smooth. Second, one can easily envision numerous exercises that could be performed to illustrate important behavior. For instance, a spatially varying heat-transfer coefficient (discussed in Bennett and Myers) is impossible to impose for even simple analytic solutions, but can easily be incorporated into the MATLAB solution.

Example 3
Wave Propagation in a Heterogeneous Material

Applications of the basic wave equations are less frequent in chemical engineering. While strong convection effects

can produce wave-like behavior, MATLAB (to the author's knowledge) is not equipped to handle convective transport. One can, of course, simulate vibration problems or certain problems involving sound waves. Instead, the example shown here is a highly simplified illustration of seismic exploration. It was chosen because of its intuitive appeal to an engineer of any discipline.

Artificial seismic waves are used in oil exploration or geophysical analysis to map subsurface structure. The wave source may be either on the surface or lowered into a well, and the responses to the wave at various detector locations are interpreted to give the mapping. On a simplistic level, the propagation of pressure waves in the ground is described in the wave equation^[16]

$$\nabla^2 p - \frac{1}{c^2} \frac{\partial^2 p}{\partial t^2} = 0$$

where c is the wave velocity, dependent primarily on the material properties. A time-dependent pressure must be defined at the wave source. Along reflective boundaries of the domain, one specifies $\mathbf{n} \cdot \nabla p = 0$.

Figure 5 shows the geometry used for this simple example. The interesting features are the slope of the lower boundary (which could be interpreted as a geologic bedding plane) and the inclusion of a material heterogeneity at the lower right. These two features make the response more interesting, but preclude solution by analytical means.

To solve the problem, a pressure spike was induced (via a rapidly decaying exponential function) along the top boundary at $t=0$. Figure 6 is a qualitative illustration of the resulting wave's behavior. The lighter shading (which represents the traveling high-pressure front) propagates downward, reflects off of the bottom boundary, and then returns to the surface (where it would be detected). Although length and time scales are not included since the ex-

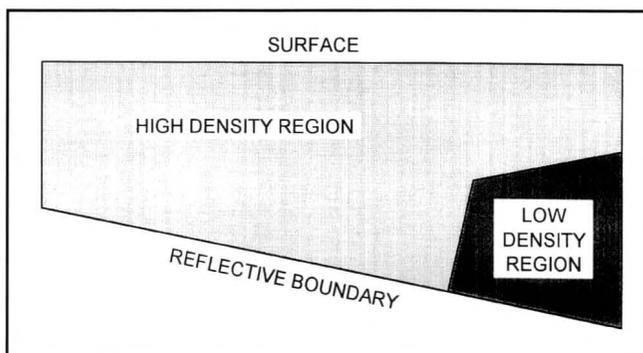


Figure 5. Geometry used for wave propagation example.

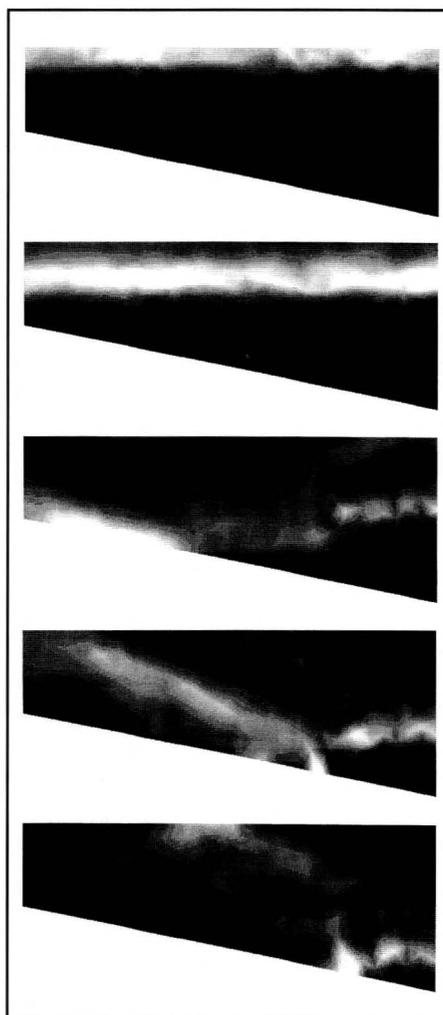


Figure 6. Wave propagation and reflection in a heterogeneous domain. White corresponds to higher-pressure transients.

ample is qualitative, one can see the influence of the lower-density inclusion where the wave gets held up, and one can envision how the surface response allows a map of the subsurface to be generated. From a mathematical viewpoint, this example helps illustrate typical hyperbolic behavior: the response of the interior to a change at the boundary is delayed, but then felt at full strength once the wave reaches a given point. Using this example in the classroom, an otherwise dry discussion of characteristic lines for a hyperbolic equation can become more captivating.

CONCLUSIONS

The use of PDEs in the undergraduate curriculum often has mixed results: Important topics cannot be modeled without PDEs. On the other hand, the simplicity of solution domains for analytic problems often makes for abstract relationships to real engineering problems, and the mathematical details of an analytic solution can distance students from the original objectives.

This paper presents effective uses of modern numerical software for solving real engineering problems at the undergraduate level, which is an increasingly popular approach among chemical engineering educators. The quick learning curve for certain numerical software allows students to begin exploring a model's behavior almost immediately. Classroom time can then be used to break down conceptual barriers associated with PDEs. It is hoped that this approach lays a better foundation and better prepares students for later material on solution techniques, either analytical or numerical.

ACKNOWLEDGEMENTS

The author would like to acknowledge Charles Varnado for providing the numerical code used to generate Figure 1, and to acknowledge the anonymous reviewers for very insightful comments on the original manuscript.

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RANDOM THOUGHTS

Continued from page 145.

The more types of assessment data collected for a specific component (column of the matrix), the more reliable, valid, and fair the evaluation of that component. For explanatory notes and literature citations on the different assessment tools, see Reference 3.

How might the scholarship of teaching be included in tenure and promotion decisions?

Many academic institutions have begun to acknowledge the scholarship of teaching as a valid component of tenure and promotion (T/P) applications. An approach being taken by several of these institutions is to allow faculty members to allocate variable percentages of their total effort to teaching, research, and service, with minimum percentages being specified for each area. If more than a certain percentage is allocated to teaching, educational scholarship must be included in the faculty member's activities and a teaching portfolio containing a subset of the items in Table 1 must be included in the T/P dossier. A review committee assigns separate numerical performance ratings to each of the three areas and weights the ratings by the specified percentages to calculate a composite rating, which provides the basis for the decision on tenure or promotion.

For ratings of the scholarship of teaching to be reliable and valid, the evaluating department should take the following steps:

- *Formulate and announce an assessment and evaluation plan.* Decide which items listed in Table 1 will be collected in the teaching portfolio, taking into account both institutional guidelines and considerations specific to the department. Choose a system to rate each of the items in the portfolio (e.g., rate each item on a scale from 0 to 10), weighting factors for each item, and weighted scores that serve as criteria for ad-

equate and superior scholarship. Describe the rating system to all departmental faculty members who may wish to include educational scholarship in their credentials and display several examples of excellent portfolios as models.

■ *Provide training to portfolio raters.* Give detailed explanations of the evaluation criteria to faculty members who will be serving as raters and provide guided practice on sample portfolios.

■ *Collect at least two independent ratings of each portfolio submitted and have the evaluators reconcile their ratings to arrive at a consensus rating.* Incorporate the consensus rating into the overall tenure/promotion dossier evaluation process.

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EDUCATOR: REKLAITIS

Continued from page 101.

review articles and has received many invitations as an invited lecturer. He supports his research through a number of NSF grants and an industrial/university consortium, CIPAC (Computer Integrated Process Operations Center), at Purdue. He was one of the founders of CIPAC and served as its director until this year when Professor Gavin Sinclair took over. In 1984 he won the Computing in Chemical Engineering Award of the Computing and Systems Technology Division of AIChE. He was again recognized by AIChE for his accomplishments when he was named a fellow in 1994. In that same year he also won the best paper award from *Computers & Chemical Engineering* for the paper by Jayakumar and Reklaitis, "Chemical Plant Layout Via Graph Partitioning: Part 1. Single Level (*Comp. & Chem. En.*, **33**, 441, 1994). 1994 was a very good year for Rex since that year he also won the ASEE Chemical Engineering Division lecture-ship award. His award address on "Computer-Aided Design and Operation of Batch Processes" can be found in *CEE*, **29**, 76, (1995).

Of course, much of the real work of research is done by graduate students. Rex has been advisor or co-advisor for 28 PhD students and 37 MS students. He currently advises or coadvices eight PhD students and one MS student. Seven of his past students are now professors: A. Elkamel (Kuwait University), Carl Knopf (Louisiana State University), I. Karimi (National University of Singapore), B.S. Lee (Pukyong National University), E.S. Lee (Dongguk University, Korea), I.B. Lee (Pohang University, Korea), and G. Yi

(Kyeonghee University, Korea).

Rex has also proved himself to be a good citizen of the chemical engineering community. He has served as secretary, vice-president, and president of CACHE and continues to serve as a trustee of that organization. Equally active in AIChE, particularly in the Computing and Systems Technology (CAST) division (in which he has held all of the offices), he was an elected director of AIChE until December of 1999. He has also been an active member of the Council for Chemical Research and has served on its governing board. He has co-edited several volumes of conference proceedings dealing with process design, simulation, computer graphics, and optimization. He has been Editor-in-Chief of *Computers & Chemical Engineering* since 1994 and was Co-Editor-in-Chief for the eight years before that.

In his research and professional activities, Rex has always been a good team player. He has collaborated with a number of past and current faculty at Purdue on papers, including Paul Andersen, Gary Blau, Frank Doyle, Lowell Koppel, Martin Okos, Joe Pekny, Dan Schneider, Bob Squires, Venkat Venkatasubramanian, and Jack Woods. He has also collaborated on papers and edited proceedings with a number of well-known chemical engineering professors from other schools, including Larry Biegler, Brice Carnahan, James F. Davis, Tom Edgar, Ignacio Grossmann, Dave Himmelblau, Richard Mah, David Rippin, John Seader, Jeff Sirola, Aydin Sunol, and Doug Wilde.

While involved in this work at Purdue, Rex continues to live the good life in West Lafayette, helping raise his two sons and being, in Janine's words, "a wonderful father" who takes the role very seriously—when they were much younger, he would tell the boys wonderful stories of knights and pirates, and take them fishing or sailing, and for family-favorite ski trips in Colorado. George earned his bachelor's degree in history from Purdue, his master's from Wake Forest, and is now working on his PhD in history at Northeastern University in Boston. Victor is a junior in electrical engineering at Stanford University.

Sailing has remained an important part of Rex's life. For sixteen years he participated in the famed Chicago-to-Mackinac race and even won his class a few times in a 34-foot Islander—but most of the time he finished in the middle of the pack. His family, who did not race with him, would watch the boat leave Chicago and then drive to Mackinac Island to watch the boats arrive there. They did, however, enjoy sailing with him in his 19-foot Lightning.

In addition to being close enough to sail on Lake Michigan, the Lafayette area is near enough to visit family in Chicago for the holidays. Rex remains close to his mother and sister and has become close to Janine's large, rowdy extended family.

We are proud to have Rex Reklaitis at Purdue. He is an honest, generous, witty colleague with high standards. Fade out to the tune of *The Wabash Far, Far Away*. □

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.

AN "OPEN-ENDED ESTIMATION" DESIGN PROJECT FOR THERMODYNAMICS STUDENTS

STEPHEN J. LOMBARDO

University of Missouri • Columbia, MO 65211

The project is "open-ended" when the students ask if only one design is right, and an "estimation" will suffice when they cannot find an exact value; the descriptive title for the project intentionally reinforces the expectation of this assignment for the student. The project is a preliminary design to evaluate methods of generating electricity for a resort island. As seen in the accompanying press release (Table 1), written in the form of an advertisement for tourism, a tropical island abundant in leisure activities is described; thinly veiled within the ad are various resources that could be used to produce electrical energy.

This design effort is assigned in a first course in thermodynamics offered by the Department of Chemical Engineering at the University of Missouri at Columbia. All the material typically contained in a "classical thermodynamics" course (first law, second law, and power cycles) is covered in this 15-week semester-long course, and most of the students are first-semester Juniors, having recently completed an introductory chemical engineering course covering material and energy balances. Although the students are still in the beginning stages of their chemical engineering coursework, this project meets the need of providing some early design opportunity in the curriculum. The project also incorporates role playing and decision making, two important elements of active learning^[1] and critical thinking.^[2]

PROJECT ORGANIZATION

The overall objective of this preliminary design is to recommend methods of energy generation that meet the elec-

tricity needs of the island, with some assessment of environmental and safety concerns. The methods proposed by students to date are listed in Table 2.

Organization of the project is shown schematically in Figure 1, and the project deliverables are divided into two parts: A Phase I written report, and a Phase II written report followed by an oral presentation. For the Phase I report, the students, grouped into teams of three or four, propose methods for producing electricity, for which they must provide brief descriptions along with environmental and safety considerations. Each group must also provide block diagrams showing the relationship between the resource and the energy output. The pedagogical role of the block diagram is to force students to contemplate the physical layout of each energy-generation method. For hydroelectric energy, for example, Figure 2 illustrates the relationship between the reservoir, the turbine, and the generator. The groups typically propose one or two methods per team member, and each method requires one to two pages to describe.

Stephen J. Lombardo received his BS degree from Worcester Polytechnic Institute and his PhD from the University of California, Berkeley, both in chemical engineering. He worked for seven years in industry in the areas of ceramic materials and ceramic processing before joining the Department of Chemical Engineering at the University of Missouri-Columbia in 1997.

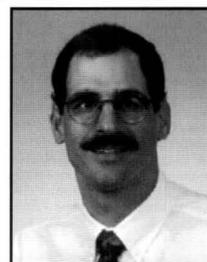


TABLE 1
Press Release for the Open-Ended Estimation Design Project

The island of _____ is a 100-square-mile idyllic spot located _____. Climate, scenery, flora, and fauna all combine to make this a premier vacation spot for families, couples, and those just looking to get away from it all. Abundant recreation activities are available as well as special sightseeing opportunities.

The prime attractions of this island are the miles of scenic beaches with soft, white sand. Breakers pound the shore continuously, making it a year-round haven for surfers. A special locale is the capital port located on the southwest corner of the island. Come spend a languid afternoon visiting this spot and observe the spectacular tidal drop of 40 feet. At low tide, it is a seashell-collector's paradise!

Don't forget the mountains here. Active volcanoes dot the panoramic vistas, and Mount Simone rumbles at least twice a day, spraying a continuous lazy plume of hot gases into the clear blue sky. For the intrepid, guided tours are made to the rim during quieter periods. Come see the most spectacular lava formations on Earth!

Hikers can take trips deep into the heart of the island, where 800-foot waterfalls cascade down into reflecting pools. For those enjoying less strenuous exertions, come spend the afternoon in the hot springs that collect into natural-rock bathing pools. For the conventional individual, we have fresh-water baths; for those looking for something more exotic, we have 2% natural salt baths—guaranteed to improve your skin tone and

leave you feeling healthy. After bathing, come and enjoy a massage at the skilled hands of our staff members. And don't forget, the cleansing effects of a mud bath provide long-lasting therapeutic value to your skin.

Hang gliders will also find plenty of recreational opportunity. The 300-foot lovely cliffs overlooking the ocean afford prime launch locations. The island is renowned for its steady cool breezes that provide year-round hang-gliding opportunities.

And don't worry about bad weather when you come to visit. The sun shines 80% of the time here, with a year-round mean temperature of 85°F and low humidity. Rain, when it occurs, is a late-evening event, so day plans are never ruined.

The island is also abundant with natural resources. Forests of hardwood trees cover over half of the island and contain some of the world's most exotic species of animals and birds. Colorful and extremely rare species of birds can only be found here in the tropical forests.

Spelunkers will also find plenty to do. Mile-long caves provide an opportunity for all levels of cave exploration, from novice to expert. Come down and explore our known caves, or discover new ones of your own! Maybe you will get lucky and find veins of precious metals; large coal deposits have already been discovered.

Don't delay—contact your travel agent now.

The second and main requirement of the Phase I report is including a design equation for each method. The left-hand side of the equation is in terms of energy or power, and the right-hand side is in terms of the fuel or resource and other parameters that will allow for the determination of the amount of energy or power that can be obtained. No calculations are made, however, for the Phase I report, since the resources are not well defined at this point in the project. Rather, the calculations and final recommendation are performed for the Phase II submission.

Separating the development of the design equations in Phase I from the execution of the calculations in Phase II is intentional. Students often find an equation and use it without critical assessment. By delaying the application of the equation from the discovery or derivation, some time will hopefully be spent on critically evaluating the usefulness and correctness of the proposed relationship. The benefit of assessing the design equation becomes apparent to the students when for the Phase II report they have not acquired all the values they need to complete the calculations.

In the case of wind energy, for example, a typical textbook design equation^[3] for the power, P, is

$$P = \eta \rho D^2 v^3 = k D^2 v^3 \quad (1)$$

where v is the wind velocity and D is the blade diameter of the wind turbine. The density of air, ρ , and efficiency, η , are

TABLE 2
Energy Methods Proposed by Students
Hydroelectric
Wind
Geothermal
Hot Lava
Tidal
Ocean Thermal
Fuel Cell
Fossil Fuel
Solar (Photovoltaic)
Hot Springs
Nuclear
Wave
Biomass Conversion
Solar (Thermal)

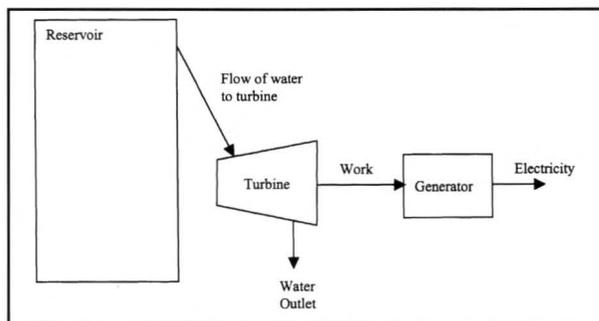


Figure 2. Example of block diagram submitted by a student group for hydroelectric energy.

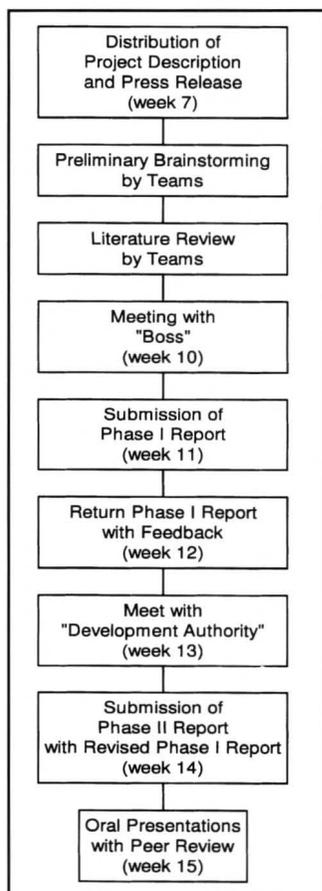


Figure 1. Organization and timeline of the open-ended, estimation design project in thermodynamics.

often lumped into an overall coefficient, k . The correctness of the dependence of the power on the diameter, D^2 , and velocity, v^3 , can quickly be established by observing that the power from wind is related to the rate of kinetic energy change by $\dot{m}\Delta v^2 / 2$ and the mass flow rate, \dot{m} , is equal to $\rho v \pi D^2 / 4$.

The equation for wind energy further illustrates when quantities can be classified as known, easily estimated, or unknown, and thus must be determined by other means. The density of air, for example, can be easily obtained from the ideal gas law, and it is not crucial, for an estimate, if the mean temperature is 65°F or 85°F. The value for the diameter of the windmill, on the other hand, is not necessarily something that can be estimated, but literature sources will typically mention a range of diameters evaluated in actual tests. Finally, it is impossible to estimate the average wind velocity of a location with any certainty; specific values pertain to specific locations.

Wind energy also provides an excellent opportunity to reinforce the usefulness of thermodynamic analysis for calculating energy transformation via the first law. One student, for example, stated that the equation for wind power is not really an outcome of thermodynamic analysis. We then jointly proceeded to evaluate the case of how the kinetic energy change of a gas flowing in a pipe can be related to the shaft work extracted; by extension, wind energy is then linked to the conversion of kinetic energy in the “pipe” swept out by the blades of the wind turbine. Since the wind velocity is also not zero after passing between the blades of the windmill, this point offers partial insight into why the efficiency of wind turbines is low.^[3]

Other methods of generating energy^[3-10] have in their design equations a similarity that is of instructional value for reinforcing the utility of the second law. Burning of fossil fuels, nuclear power, ocean thermal energy, and geothermal energy can all have their design equations represented by the general form

$$P = \eta \dot{m} \Delta H \quad (2)$$

where η is the maximum efficiency, \dot{m} is the mass consumption rate of the fuel, and ΔH is the enthalpy change of the fuel. By casting the design equations in this common format, the maximum efficiency of each method can also be compared on a common basis, namely, the absolute temperature of the hot reservoir, T_h , and cold reservoir, T_c , from the Carnot equation: $\eta = 1 - T_c / T_h$. While some groups choose to use the Carnot efficiency, other teams opt to use an empirical value for η from reference works.

Prior to submission of the Phase I report, the students have an opportunity to schedule a meeting with their “boss,” *i.e.*, the instructor. Since students seem to crave “real world” experience, role playing with their boss provides a good opportunity to get some. Before the meeting, the students are

reminded that their boss does not know the solution to this project. If this were the case, the project would not have been assigned. Furthermore, their boss does not want to solve the problem for them; that is the responsibility of the employee. The boss will, however, guide, encourage, direct, etc.

After submission and acceptance of the Phase I report, the teams “fly” to the island and meet with the director of the local development authority (the instructor), who tries to answer any questions related specifically to the resources of the island. It is at this meeting that location-specific information such as wind velocity, available tidal basin, hydroelectric dam height, and water volumetric flow rate are made available to the students—but only in response to their specific questions. The link between the design equations and known/unknown information then becomes clear. Values for each and every variable in the design equations must be obtained or estimated in order to be able to compute the power. Each group is also given individualized information—no two groups have the same amount of resources or population. In addition, not all of the resources provided are sufficient to meet the energy needs. By tailoring the resources in this manner, groups cannot converge on the same answer and must be comfortable (or uncomfortable) with their own decisions. During the meeting with the local development authority, the values of the resources requested by the students are recorded for later use in grading the reports.

The projects are evaluated for a number of attributes. For the Phase I report, the design equations must be sound and the layouts of the block diagrams logical. Second, the overall organization of the report and writing are assessed. Generally, the Phase I reports have not been graded, but rather feedback for improvement is provided (their boss gives feedback, not grades). The most common shortcoming of the Phase I reports is a poorly formulated design equation. It is either not in terms of a single equation, not in terms of the primary fuel or resource (*e.g.*, for geothermal energy, the power is formulated in terms of the working fluid instead of in terms of the heat available from the hot reservoir), or formulated in a manner for which not all values are easily obtainable.

The format for the Phase II report is a one- or two-page executive summary containing a specific recommendation of how to meet the energy needs of the island. The revised design equations are also presented along with the values used to compute the power. The values of the energy must be roughly correct in light of the fuel or resources specified. Since each group has been given different values for the resources, I calculate the available energy for the methods of each group in a spreadsheet application. In this manner, it is relatively straightforward to determine if each group has correctly calculated the right order of magnitude of energy possible from each proposed method, and it is at this level (namely, the order of magnitude) that the correctness of the calculations is assessed. The revised Phase I report is resub-

mitted as an appendix, and this revision is evaluated for improvements over the original version.

Finally, the soundness of each group's recommendation is strongly weighed. Since at this stage of the design no method of energy generation is strictly right or wrong, as long as sufficient energy to meet the requirements is provided, the recommendation

of each group reflects its evaluation as to what is most acceptable for a resort island and balances what it sees as the competing needs. These are most often a method that is environmentally friendly and aesthetically pleasing. Some groups recommend fossil-fuel power plants as being a tried and true technology, whereas other groups select several methods in combination. The most common recommendation to date has been the use of hydroelectric energy.

The final part of the project is a ten-minute oral presentation by each team for peer review. The three grading criteria are organization of the talk, clarity of presentation, and soundness of the recommendation. The grading process for the oral presentation is conducted in a manner to give students exposure to an assessment practice used in industry. A five-point scale is used, with three as the average, and the students are told that the average of the grades that they award must come close to this average. This is similar to many of the merit raise systems employed in industry where the available "pool" is a fixed percentage of the total salary budget. Use of this method gives the students an opportunity to weigh the consequences of positive and negative assessment and combats any tendency for grade inflation by the teams.

The comments of the students regarding this project were solicited with an anonymous questionnaire, and the results are summarized in Table 3. The most often cited positive aspects of the project were the oral presentations and the open-ended nature of the project. The most negative comments were also related to the oral presentations, two of which can be remedied by better scheduling.

The most frequently cited suggestion by the students pertains to having more specific guidelines for the project. In the experience of the author from seven years in industry, expectations and formats for project presentations and results were limited or non-existent. In general, employees were expected to develop their own presentation formats. The second most frequently cited suggestion pertains to their wish to perform economic estimates. Since this course is offered relatively early in the chemical engineering curriculum, well before their formal design courses with accompanying exposure

TABLE 3
Student Feedback

(Numbers in parentheses indicate the number of times similar types of comments were made in a class of 24 students, 18 of which responded.)

<u>Positive Aspects</u>	<u>Negative Aspects</u>	<u>Suggestions</u>
Oral presentations (7)	Oral presentations on the last day of class (2)	Give more specific guidelines for reports (5)
Open-ended nature (5)	Oral presentations (1)	Require economic estimates (3)
Computationally easy (1)	Problem is too easy (1)	Give more time for project (1)
Opportunity to use people skills (1)		
Role playing (1)		
Research-oriented project (1)		

to engineering economics, this desire to perform economic analyses seems ambitious on their part.

SUMMARY

An open-ended estimation design project has been developed for use in a first thermodynamics course taught early in the chemical engineering curriculum. The project, which contains a number of components

that simulate real-world experience, is designed to emphasize simplification over complexity. A key aspect of the project is decision making; after the values of power for the various methods are calculated, a decision must be made, namely, what ultimately to propose. It is this aspect of the project that is most in line with the expectation of problem solving in industry. The project is also structured to embody many of the elements of critical thinking in that for each team to make a final recommendation, the "students are active, involved, consulting, and arguing with each other..."^[2] Furthermore, several aspects of active learning, such as role playing, writing, and presenting are used to enhance understanding^[1] and retention.^[11] Finally, the project exposes the students to the importance, breadth, and complexity of the numerous issues surrounding the generation of energy.

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LOW-COST MASS TRANSFER EXPERIMENTS

Part 6. Determination of Vapor Diffusion Coefficient

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Molecular diffusion determines the rate of most mass-transfer operations. Determination of the diffusion coefficient of the key component is very important for predicting rates of mass transfer, and many correlations are reported in the literature for binary and multicomponent systems.^[1-4]

This paper describes a simple experimental technique for determining binary diffusion coefficients for vapor (A)-gas (B) systems in which the vapor is generated by the evaporation of a pure volatile liquid and the gas is air. The theory is described in many textbooks on mass transfer and unit operations,^[2-4] and only a brief treatment is given below for immediate reference.

From Fick's first law of diffusion for the case of stagnant B in a binary system, the flux of A at steady state (N_{Az}) is given by^[2]

$$N_{Az} = \frac{D_{AB} p_t}{RTz p_{BM}} (p_{A1} - p_{A2}) \quad (1)$$

where D_{AB} is the diffusion coefficient, R is the ideal gas constant, T is the absolute temperature, z is the length of the diffusion path, p_t is the total pressure, p_{A1} and p_{A2} are the partial pressures of component A at the two extremes of the diffusion path, and p_{BM} is the logarithmic mean of the

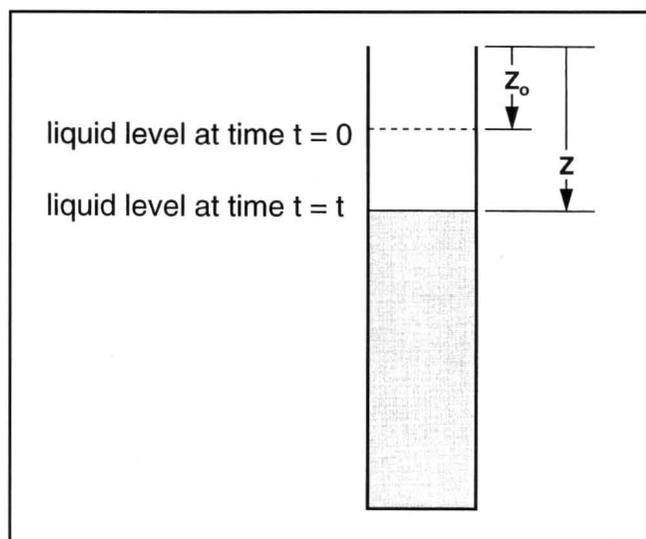
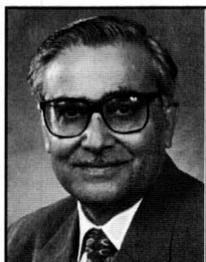


Figure 1. The evaporation tube.

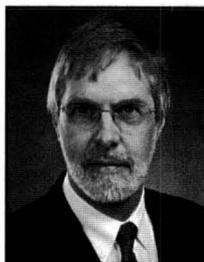
partial pressures of component B at the two ends of the diffusion path.

Let us suppose we have a liquid in a tube (see Figure 1) of cross-section a , and in time, dt , the liquid level in the tube

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This paper describes a simple experimental technique for determining binary diffusion coefficients for vapor (A)-gas (B) systems in which the vapor is generated by the evaporation of a pure volatile liquid and the gas is air.

falls through distance dz . The volume of liquid evaporated will be given by $(a \cdot dz)$. If the density of the liquid is ρ_A and the molecular weight is M_A , the molar evaporation of A will be equal to $\rho_A(a \cdot dz)/M_A$ and the rate of evaporation, $\rho_A a \cdot dz / M_A dt$, can be related to the diffusional flux ($N_{Az} \cdot a$) by the following equation:

$$N_{Az} a = \frac{\rho_A a}{M_A} \frac{dz}{dt} \quad (2)$$

Assuming the liquid level drops very slowly and therefore pseudo-steady-state conditions apply, N_{Az} in Eq. (2) may be substituted for by Eq. (1), giving

$$\frac{\rho_A}{M_A} \frac{dz}{dt} = \frac{D_{AB} p_t}{RT z p_{BM}} (p_{A1} - p_{A2}) \quad (3)$$

which can be rearranged as

$$z \, dz = C \, dt \quad (4)$$

where

$$C = \frac{D_{AB} p_t M_A}{RT p_{BM} \rho_A} (p_{A1} - p_{A2}) \quad (5)$$

Equation (4) can be integrated as

$$\int_{z_0}^z z \, dz = C \int_0^t dt \quad (6)$$

which yields

$$\frac{z^2 - z_0^2}{2} = C t \quad (7)$$

Equation (7) suggests that a plot of $(z^2 - z_0^2)/2$ vs. t will be linear, passing through the origin and having a slope C . The value of D_{AB} can therefore be calculated from the measured slope C by rearranging Eq. (5) as

$$D_{AB} = \frac{CRT p_{BM} \rho_A}{p_t M_A (p_{A1} - p_{A2})} \quad (8)$$

It may be noted that p_{A1} is the vapor pressure of liquid A at T , and p_{A2} may be safely assumed to be zero as fresh air flows over the tube.

EXPERIMENTAL PROCEDURE

The apparatus is quite simple. It consists of a small glass tube of 1- to 2-cm diameter (see Figure 1), a traveling microscope, a source of light to illuminate the liquid meniscus, a thermometer, and a barometer. All these components can be easily found in any chemical engineering laboratory.

The volatile liquids selected should have high vapor pressures to get meaningful results in a reasonable time period—acetone, pentane, and hexane were tested in this study. Tests performed in duplicate indicated that the results were reproducible within the experimental accuracy.

The following procedure is recommended:

1. Fill the tube with the volatile liquid to about 0.5 to 1.0 cm from the top. Care should be taken to pipet the liquid in the tube to avoid wetting the top empty section of the tube with the liquid.
2. Place the tube in a stand and place the stand in an illuminated fume-hood.
3. Note the atmospheric pressure and the temperature in the fume hood.
4. Keep the fume hood fan off and the door fully open (the front glass panel fully raised) to minimize any air turbulence due to suction in the fume hood.
5. Focus the traveling microscope first at the very top of the tube ($z=0$) and then at the liquid meniscus level ($z=z_0$), and immediately start the stopwatch.
6. Record the liquid level (z) in the tube with time to obtain a noticeable drop in the liquid depth. This gives the z -versus- t data.
7. Note the atmospheric pressure and the temperature in the fume hood again.
8. Measure the liquid density at the experimental temperature by weighing a known volume of the liquid.
9. Plot $(z^2 - z_0^2)/2$ versus t and obtain the experimental diffusion coefficient from the slope of the plot as per Eq. (8).
10. Predict the diffusion coefficient from the Hirschfelder-Bird-Spotz correlation^[2] given below and compare with the experimental value obtained in Step 9 above.

$$D_{AB} = \frac{10^{-4} \left(1.084 - 0.249 \sqrt{\frac{1}{M_A} + \frac{1}{M_B}} \right) T^{3/2} \sqrt{\frac{1}{M_A} + \frac{1}{M_B}}}{p_t (r_{AB})^2 f(kt / \epsilon_{AB})} \quad (9)$$

11. Repeat the experiment with a pedestal fan and/or fume hood fan on, and compare the experimental diffusivity values with those with no air circulation in the fume hood.

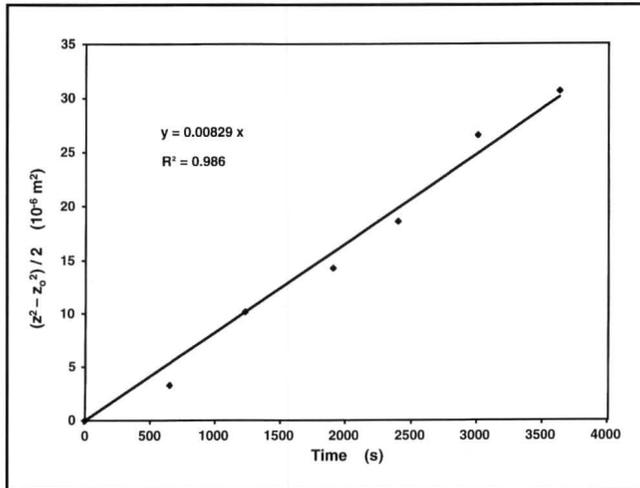


Figure 2. Plot of $(z^2 - z_0^2)/2$ versus time for acetone vapor diffusing through stationary air.

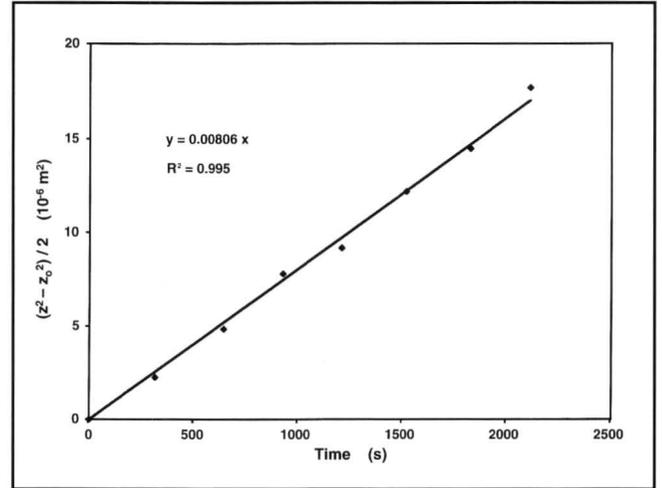


Figure 3. Plot of $(z^2 - z_0^2)/2$ versus time for hexane vapor diffusing through stationary air.

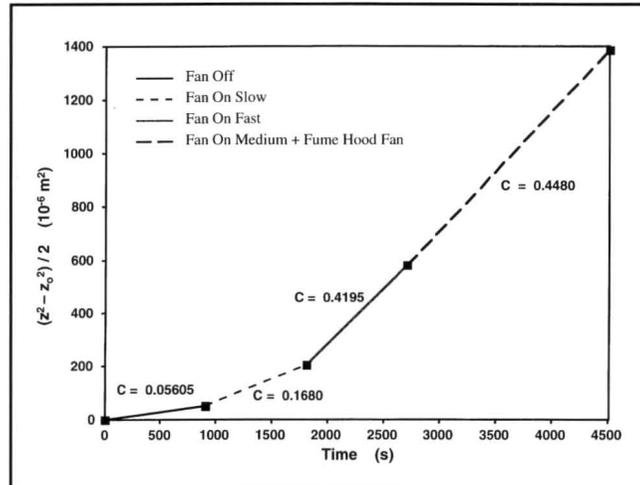


Figure 4. Plot of $(z^2 - z_0^2)/2$ versus time for pentane-air system with varying levels of air circulation

Vapor	p_1 (N/m ²)	p_{A1}^s (N/m ²)	Temp. (°C)	Air Flow		Diffusion Coefficient (10 ⁻⁶ m ² /s)		% Deviation
				Fume Hood Fan	Pedestal Fan	Experimental	Predicted	
Acetone	98960	23905	20	Off	Off	10.1	10.8	-6.5
Hexane	99155	16029	19	Off	Off	8.6	8.1	+6.2
Pentane	100616	76500	27	Off	Off	8.5	9.2	-7.6
Pentane	100616	76500	27	Off	Slow	25.5	-	-
Pentane	100616	76500	27	Off	Fast	63.6	-	-
Pentane	100616	76500	27	On	Medium	67.9	-	-

RESULTS AND DISCUSSION

The results for acetone and hexane at atmospheric pressure, room temperature, and *with no* forced air circulation through the fume hood are plotted in Figures 2 and 3, respectively, and for pentane *without* and *with* forced air flow through the fume hood in Figure 4. As can be noted, the plots of $(z^2 - z_0^2)/2$ versus t for acetone and hexane (see Figures 2 and 3, respectively) yield linear lines passing through the origin with a good fit of data points ($R^2 > 0.986$). The experimental and the predicted values of diffusion coefficients, calculated from the slopes of these plots and the first line on Figure 4 for pentane (with no forced circulation in the fume hood), and from the Hirschfelder-Bird-Spotz correlation^[2] (Eq. 9), respectively, are given in Table 1.

The results suggest that the experimental technique is simple and gives reasonable agreement between experimental and predicted values.

The last three experiments performed with forced air flow in the fume hood (see Table 1 and Figure 4) indicate an increase in the apparent value of D_{AB} , as expected. These results reflect a very important limitation of this procedure, *i.e.*, for ensuring "stagnant B" conditions (to obtain a good agreement between the experimental and the predicted values of D_{AB}) on which the development of Eq. (7) is dependent, undue air turbulence in the fume hood must be absent. Any external turbulence can affect the behavior of the gas mixture in the tube and lead to an increase in the mass-transfer rate.

It may be noted that for this method to work, the density of the vapor (A) should be greater than that of air (B) so that there are no natural convection effects in the tube. This is the case with all common organic liquids.

CONCLUSIONS

1. Rate of fall in liquid level can be used to determine the diffusion coefficient fairly accurately for vapor-gas systems where the vapor is generated by the evaporation of a pure volatile liquid and the gas is stagnant.
2. Experimental diffusion coefficients are within $\pm 10\%$ of the predicted values.
3. Turbulence in the experimental area affects the precision of the results.

GENERAL REMARKS

This laboratory provides students with the opportunity of experiencing how elementary experimental methods can be used to confirm what they read in the classroom. The experiment is extremely simple and can be completed well within the usual three-hour laboratory period. Since linear plots passing through the origin are obtained, only two level readings, about 20 minutes apart, are required for a direct calculation of D_{AB} through Eqs. (7) and (8).

We recommend that the class be divided into groups and that different groups study the effects of 1) nature of component A, *i.e.*, study different volatile liquids; 2) degree of turbulence in the work station (some effort can be made to quantify the results by measuring air velocity in the fume hood with an anemometer); 3) temperature; and 4) natural convection effects in the evaporation tube (this can be studied with any liquid with a molecular weight lower than that for air—water being the safest). The students should also be asked to review the analysis of sources of error in such a procedure provided by various workers.^[6-8]

NOMENCLATURE

a	cross-sectional area of evaporation tube
C	slope of $(z^2 - z_0^2)/2$ vs. t plot
D	diffusion coefficient
f	function
k	Boltzmann's constant
M	molecular weight
N_{Az}	steady-state molar flux of A in the z-direction
p	pressure
R	ideal gas constant
r	molecular separation at collision
T	absolute temperature
t	time
z	vertical distance
ϵ	energy of molecular attraction
ρ	liquid density

Subscripts

A	component A
B	component B
AB	components A and B
BM	log-mean average for component B across the diffusion path
0	initial value
t	total
z	in the z-direction
1	beginning of diffusion path
2	end of diffusion path

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INCORPORATING MOLECULAR MODELING INTO THE CHE CURRICULUM

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Computers have long been used in the teaching of chemical engineering in order to facilitate complex calculations required for the design and analysis of chemical process equipment (plug-flow reactors, multistage distillation columns, etc). The use of computer-based process simulation using commercial software (Aspen Plus, ProVision, Hysim, etc.) is commonplace in most modern chemical engineering curricula. Today, the availability of powerful molecular modeling software is adding an entirely new vehicle for predicting the behavior of systems and processes based on molecular-scale properties. While the principles are not new, only recently has the computational hardware and software become available that can bring these tools (Gaussian, Spartan, Cerius², etc) into the chemical engineering classroom. The capability of combining computation with visualization presents chemical engineering educators with important new opportunities for enhanced teaching and learning.

PARADIGMS IN CHE EDUCATION

Wei^[1] commented on the two paradigms that shaped chemical engineering education during the 20th century. The first of these was based on classification of processes and systems as the familiar unit-operations lexicon; this approach dominated the early stages of chemical engineering teaching. The publication of *Transport Phenomena*^[2] marked the beginning of the second paradigm, that of the fundamental analytical approach based on rigorous mathematical models of physical systems. Recently, a third paradigm for chemical engineering was proposed by Landau,^[3] that of a closer relationship with practice and industry.

It is our opinion, however, that the third paradigm could and should be cast in the context of better integration of the fundamental molecular processes of chemical physics into chemical engineering. Other educators have discussed the importance of the microscopic viewpoint in our teaching and

research^[4,5] but in today's chemical engineering curriculum the basic atomistic concepts learned in organic and physical chemistry are too often left to languish as soon as the specific courses dealing with these subject areas have been completed. This is caused in large part by a lack of continuity between subject matter and by poor integration in terms of teaching of the two disciplines. Important concepts in organic synthesis and molecular structure are rapidly forgotten by third- and fourth-year chemical engineering students, just at the time that these concepts should be applied (for example, in the process design and/or reaction engineering courses).

At the Colorado School of Mines (CSM), we have recently completed a top-to-bottom school-wide redesign of our undergraduate curriculum. As part of this exercise, the undergraduate chemical engineering curriculum was significantly updated and revised. A key philosophical component in this revision process was our desire to incorporate molecular modeling and simulation into the chemistry and chemical engineering course sequence in order to foster a better ap-

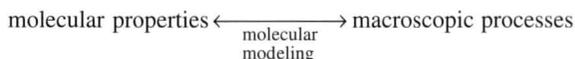
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preciation of the relationship between microscopic and macroscopic phenomena and a better understanding of the importance of chemical physics in determining how molecules interact and react:



As described above, we believe that computer-aided molecular modeling can serve as the catalyst that allows students to make and understand these connections.

MOLECULAR MODELING AND SIMULATION

The two main components of our microscopic approach to understanding macroscopic processes are molecular modeling and molecular simulation. The distinction between these two is somewhat arbitrary, but in our case we define molecular modeling to be the investigation of isolated molecular assemblies (*e.g.*, single molecules, dimers, etc.) and molecular simulation to be the investigation of collections of interacting molecules. The primary tools used to perform molecular modeling are *ab initio* and semi-empirical quantum mechanics and molecular mechanics,^[7] while molecular simulation incorporates the use of molecular dynamics and, for example, Monte Carlo methods.^[8]

The primary use of molecular mechanics is to make empirical estimations of equilibrium molecular geometry (*e.g.*, the most energetically favorable structure) and energy by using parameterized force fields. For homogeneous systems, molecular mechanics describes the total energy of a molecule as the sum of a distortion energy from an “ideal” geometry of connected atoms (E_1)

$$E_1 = \sum_{\text{bonds}} E^{\text{stretching}} + \sum_{\text{bond angles}} E^{\text{bending}} + \sum_{\text{dihedral angles}} E^{\text{torsion}} \quad (1)$$

and the contribution due to non-bonded interactions (E_2) that arise from van der Waals and electrostatic interactions

$$E_2 = \sum_i \sum_j E_{ij}^{\text{VDW}} + \sum_i \sum_j E_{ij}^{\text{electrostatic}} \quad (2)$$

The total energy is just $E_1 + E_2$. Examples of molecular mechanics force fields are SYBYL^[9] and MMFF.^[10] Depending on the nature and applicability of the force field being used to carry out the calculation, this procedure may work well or can give rise to structures, geometries, and hence equilibrium energies that are significantly in error. In so-called computational chemistry programs, force field calculations are often employed to give a refined structure as a starting point for the *ab initio* quantum mechanics calculations.

The second type of computation that is often used for molecular modeling directly involves quantum mechanics, with the general mathematical relationship given by the Schrödinger equation

$$\left(-\frac{\hbar^2}{8\pi^2} \sum_N \frac{1}{m_N} \nabla_N^2 - \frac{\hbar^2}{8\pi^2 m_e} \sum_i \nabla_i^2 - \sum_N \sum_i \frac{Z_N e^2}{r_{iN}} + \sum_N \sum_M \frac{Z_N Z_M e^2}{R_{NM}} + \sum_i \sum_j \frac{e^2}{r_{ij}} \right) \Psi(\{\mathbf{R}\}, \{\mathbf{r}\}) = E \Psi(\{\mathbf{R}\}, \{\mathbf{r}\}) \quad (3)$$

In this equation, ∇ is the momentum operator, m refers to a mass, Z is a charge, e is the unit measure of charge, \mathbf{R} denotes nuclear positions, and \mathbf{r} denotes electronic positions. Ψ is the quantum mechanical wave function for the molecule, and E is the energy of the molecule. According to quantum mechanics, solution for the wave function enables one to calculate the energy and other structural properties of a molecule.

Although this equation may be written down rather simply, it cannot be solved exactly except for the hydrogen atom (one electron, one proton). While exact solution of this equation for polyatomic molecules is still not

Today, the availability of powerful molecular modeling software is adding an entirely new vehicle for predicting the behavior of systems and processes based on molecular-scale properties.

feasible, application of a series of approximations (in particular, the Hartree-Fock approximation) and the advent of powerful desktop computers using high-speed microprocessors has made numerical solutions possible.^[6]

A high degree of computational efficiency can be obtained by using *semi-empirical* quantum mechanical methods that consider only the valence electrons in a molecule and reduce the number of electron-electron interactions by neglecting “overlaps” between atomic orbitals. In addition, these models introduce parameters that have been optimized with experimental data.

In contrast to molecular mechanics and *ab initio* quantum mechanics, molecular simulation techniques examine the behavior of systems composed of a small collection (typically 100 to 10,000) of interacting molecules. The methods used include molecular dynamics (in which the time evolution of the molecular system is simulated and monitored) and Monte Carlo simulation (in which statistical methods are used to sample states of the system according to some pre-defined probability distribution).

The basic method used in molecular dynamics is to solve numerically the classical equations of motion of the molecules (structured mass points) and calculate time averages of quantities such as the configurational energy, pressure, self-diffusion coefficients, local structure, etc. Typically, the molecular system is simulated for picosecond time intervals, which may involve solving the coupled differential equations of motion for several hundred thousand time-steps.

The accuracy of these simulations is governed by the numerical techniques used and the accuracy of the interaction potential(s) that govern the motion and time evolution of the molecules in the system. For structured (polyatomic) molecules, these potentials might include intra-molecular vibration, rotation, and non-bonded interaction potentials as well as non-bonded intermolecular potentials. The non-bonded potentials are typically parameterized intermolecular potential functions such as the Lennard-Jones or Exponential-6 models. An advantage of molecular dynamics is that non-equilibrium properties may be calculated with relative ease.

In Monte Carlo simulations, the energy of the molecular system is minimized by randomly moving molecules according to some desired probability distribution. Again, the user must specify the potential functions, and equilibrium properties can be calculated by statistical (rather than time) averages. A great advantage of this method is the relative ease with which it can be used to calculate phase equilibria.^[11]

Molecular modeling and simulation is finding widespread applicability and increased acceptance in chemical engineering practice. Estimation of thermophysical properties has become routine.^[12]

Simulation of rheological properties of complex fluids has been demonstrated by Cummings and co-workers^[13,14] and

molecular simulation of water has been shown to give structural information that is more reliable than even the most precise measurements can yield.^[15]

In addition, use of molecular mechanics and quantum chemistry calculations to determine orbital occupancy has been shown to be important in understanding and design of new materials such as catalysts,^[16] sorbents,^[17] and reactive polymer membranes.^[18]

MOLECULAR SIMULATION IN THE UNDERGRADUATE CHEMISTRY CURRICULUM

At CSM, students first encounter applications of molecular modeling in their sophomore-level organic chemistry course sequence. Calculations are facilitated using Spartan, which is a user-friendly computational quantum chemistry software package.

Computational quantum chemistry problems are assigned essentially as self-paced “discovery” exercises in Organic I and II. Students first use Spartan to carry out quantum calculations in order to investigate structure/stability relationships for typical hydrocarbons, functional groups, and reactive intermediates (radicals, carbocations, carbenes, etc.). Most calculations are carried out using geometry optimization at the semi-empirical AM1* level: some calculations require *ab initio* methods with higher levels of theory (3-21G)**. In either case, the computations can be rapidly completed using either Spartan’s PC-based software or the Unix workstation version; a total of approximately sixty licensed copies of Spartan are available to chemical engineering students in open computer labs on both platforms.

Spartan’s ability to calculate and display electron density and molecular orbital surfaces is exploited in the organic course sequence where the focus is on understanding the mechanisms of chemical reactions.

The relationships between electronic structure, molecular orbital density, and chemical reactivity are also developed using the visualization capabilities of the software. For example, when studying nucleophilic substitution reactions, the students use Spartan to compute HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) surfaces for the reactants, and then relate the electron transfer taking place in the frontier orbitals to the observed regiochemistry and selectivity of the reaction.

For both the organic and physical chemistry sequences, Spartan’s capabilities of calculating and graphically rendering electron density molecular orbital surfaces greatly facilitates the student’s understanding of the relationship between molecular properties and such important concepts

* Austin Method 1: a semi-empirical molecular orbital method.

** A basis set in which each inner-shell atomic orbital is written in terms of three Gaussian functions and each valence-shell atomic orbital is split into two parts, written in terms of two and one Gaussians, respectively.

as stability and reactivity.

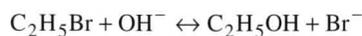
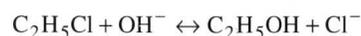
These concepts are further elaborated during the third-year physical chemistry sequence. Here, the students are exposed in class to the theory and some of the mathematical details associated with setting up and arriving at approximate solutions to the Schrödinger equation. As an example, the Morse potential energy diagram for a diatomic molecule is first calculated using measured spectroscopic (IR) data from the lab, and then simulated using Spartan.

MOLECULAR MODELING IN THE CHE CURRICULUM AT CSM

Incorporation of molecular modeling in the chemical engineering curriculum was first accomplished two years ago in our senior-level reaction engineering course. As an example of the approach being used, an outline for one of the computational chemistry homework problems assigned in this class is shown in Table 1.

The problem deals with synthesis of chemical-grade ethanol via a S_N2 nucleophilic substitution reaction in aqueous solution. The objective of the problem is to illustrate use of quantum mechanics and computational chemistry in order to generate the thermochemical information required to carry out an analysis of a simple industrial reaction. Two possible

reactions are proposed, differing only in choice of substrate:



As a first step, students are asked to investigate the thermodynamics of the reactions. For this part of the problem, heats of formation of all products and reactants (including solvation energy effects) are estimated by semi-empirical quantum chemistry methods, and the heat of reaction computed in the normal fashion:

$$\Delta H_R = \sum_j^{\text{products}} \nu_j \Delta H_{F,j} - \sum_i^{\text{reactants}} \nu_i \Delta H_{F,i} \quad (4)$$

Calculation of the equilibrium constant requires the free energy change for the reaction

$$K = \exp(-\Delta G_R^0 / RT) \quad (5)$$

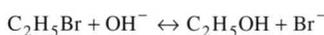
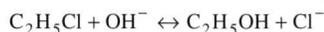
but if entropic effects are not important (a reasonable assumption in this case)

$$\begin{aligned} \Delta G_R^0 &= \Delta H_R^0 - T\Delta S^0 \\ \Delta G_R^0 &\approx \Delta H_R^0 \end{aligned} \quad (6)$$

and the standard free energy change and hence the equilibrium constant for each reaction can be readily estimated

TABLE 1
Example Problem in Reaction Kinetics

Synthesis of chemical-grade ethanol can be achieved by a nucleophilic substitution reaction using hydroxide ion as the nucleophile and a haloethane as the substrate. For this problem, we will investigate the rates of two synthesis reactions, differing only in the nature of the halogen atom (bromine vs. chlorine):



The reaction takes place under aqueous conditions. Both reactions can be assumed to follow a S_N2 (substitution/nucleophilic/bimolecular) mechanism. Hence the geometry and configuration of the transition state can be assumed to be the same for both reactions. We wish to estimate the ratio of the rates of these two reactions.

1. Estimate the activation energies for both the forward and reverse reactions using Spartan. This will require several assumptions regarding the exact geometry of the transition state, namely
 - Assume that the nucleophile (the attacking group) and leaving group are both attached to the same carbon atom and are in axial positions (e.g., 180° apart)
 - For S_N2 reactions, trigonal bi-pyramidal geometry at the carbon atom where the nucleophile is attacking gives a reasonable approximation to the transition state.

To obtain the energy of the transition state, have Spartan carry out a Semi-Empirical Transition Structure calculation using AM1 as the model and water (Water C-T) as the solvent. Remember to set up the correct charge and multiplicity for your assumed transition state. Obtain heats of formation from Spartan for the ionic species (Semi-Empirical, Single Point Energy,

AM1, Water C-T). Obtain heats of formation for the other reactants and products using Semi-Empirical Geometry Optimization as the task, AM1 as the model, and Water C-T as the solvent.

2. Using data on heats of formation of the reactants and the products from Spartan, calculate the heat of reaction for both nucleophilic substitution reactions. Which reaction is favored if the reactions are under thermodynamic control? Calculate the ratio of the equilibrium constants for these two reactions at 25°C.
3. Calculate the ratio of the rate of the substitution reaction for bromoethane as the substrate to the substitution reaction when chloroethane is the substrate in the temperature range from 25°C to 100°C. What assumptions are necessary to carry out this calculation? Are these assumptions reasonable? Does the ratio change with temperature? Why?
4. a) If you were going to engineer a reactor for manufacture of chemical-grade ethanol using one of these two reactions, which haloethane would you recommend be used and why? Are there any important factors that you are not considering in your choice for a substrate?
b) Would you suggest the process be carried out at low temperature or high temperature, and why?

* You may want to consult the Chemical Marketing Reporter (reference room, CSM library) for data that will help answer this question. Up-to-date information on some chemicals can also be found at <www.chemexpo.com> and <www.chemweek.com>.

based on the heat of reaction. Using ratios for the two equilibrium constants in evaluating the thermodynamic feasibility makes this assumption much less restrictive.

This analysis shows that both reactions are favorable thermodynamically, with a preference to chloroethane as the substrate (larger equilibrium constant). The reactions are also shown to be under kinetic control, hence the next step is to see what differences may exist in the activation energies for the two reactions.

This is accomplished by constructing a hypothetical transition state for the nucleophilic substitution reaction for both reactions, and by using Spartan to estimate the energy of these species. This part of the solution process draws heavily on the student's background in organic chemistry theory where substitution reactions are concerned.

Once the transition states for both reactions have been constructed, values for the heats of formation of the reactive intermediates are determined using the Transition Structure Optimization routine (searching for a saddle point on the reaction potential energy surface) in Spartan.

Students can include a calculation of the vibrational spectrum at this point in order to verify that a reasonable approximation for the transition state species has been found by this procedure (at least one imaginary frequency that corresponds to the reaction coordinate of interest). Animation of the largest imaginary frequency in the calculated table of normal mode frequencies provides convincing evidence that the reaction coordinate of interest corresponds well to the transition state structure. Finally, the activation energies for both reactions can be readily estimated from the semi-empirical heats of formation as

$$E_A = \Delta H_{f,TS} - \sum_{\text{reactants}} \Delta H_f \quad (7)$$

Comparison of the relative rates at any temperature, T , then follows directly from

$$\frac{r_{Cl}}{r_{Br}} = \exp\left[\frac{(E_{A,Br} - E_{A,Cl})}{RT}\right] \quad (8)$$

From this process, the students find that the activation

TABLE 2
Course Outline and Instructional Modules
Molecular Perspectives in Chemical Engineering

Learning Objectives

The class introduces students to the use of molecular-scale techniques for the prediction of physical properties, transport properties, and reaction energetics.

Content Summary

This class introduces modern methodologies for the estimation of physical, transport, and reaction properties and parameters needed in the design of chemical processes. In addition, it serves to enhance students' molecular-scale intuition through the use of group contribution methods, molecular simulations, quantum mechanical calculations, and molecular visualization. The class begins with a review of the microscopic world of atoms and molecules; fundamental length, time, and energy scales are discussed. Molecular-scale forces and their representative potentials are presented. Case studies are pursued involving topics such as the estimation of diffusion coefficients,

viscosity, and phase equilibria, as well as transition-state theory for the estimation of rate constants in chemical reactions. Relevant experimental techniques that can serve to verify the molecular-scale calculations are covered. Significant hands-on experience in a computer laboratory and case-study projects is emphasized.

Topics Covered

1. Computers and computer simulation in chemical engineering
2. Properties of fluids and solids; molecular structure prediction methods
3. Computational quantum chemistry, intramolecular properties
4. Intermolecular properties and forces
5. Intermolecular forces and configurational properties
6. Equilibrium molecular dynamics
7. Monte Carlo techniques
8. Nonequilibrium molecular dynamics

<u>Module</u>	<u>Description</u>
Ideal Gas Properties	Simulation and text to illustrate how molecular motions give rise to ideal gas properties.
Vapor-Liquid Equilibria	Simulation to illustrate how inter-molecular interactions affect the dynamics and VLE of mixtures.
Group Contributions	Quantum mechanical calculation of Benson groups.
Diffusion in Polymers	Molecular dynamics simulation and visualization of nitrogen diffusion in polysiloxane.
Thermochemical Properties	Use of computational chemistry to estimate thermochemical properties.
Structure-Property Relationships	Free radical polymerization of vinyl chloride to form PVC.
Activation Energies	Use of quantum mechanics to investigate thermal cracking of ethane.
Intramolecular Quantum Behavior	Quantum mechanics of molecules: potentials, vibrations, IR spectra, and equilibrium geometries.
Intermolecular Forces	Estimation of intermolecular force using quantum chemistry.
Thermodynamics of Rare Gas Mixtures	Application of molecular dynamics simulations to the estimation of mixture properties.

energy for the synthesis using bromoethane as the substrate is significantly lower, thus suggesting that the reaction will be much faster if this compound is used as the reactant. Finally, costs of the two reactants are compared using data from the commodities literature.

The approach to solving this problem relies exclusively on the use of molecular modeling to obtain information that is not readily available from any of the standard data sources—hence the use of quantum chemistry to estimate parameters that are of considerable practical utility for both reactor and process-design purposes is well illustrated.

We have recently added a new senior-level course to our curriculum, “Molecular Perspectives in Chemical Engineering.” This course presents students with a comprehensive overview of the use of molecular modeling and simulation techniques in several different applications, including estimation of thermophysical and reaction rate data, sorption equilibria and diffusion rates, phase equilibrium simulation, and prediction of transport properties.

An outline for this course, including descriptions of the computational exercises that are currently in use, is given in Table 2. Examples of molecular modeling exercises used in the capstone chemical engineering molecular simulation course can also be found by accessing the CSM website at <<http://www.mines.edu/Academic/chemeng>>.

CONCLUSIONS

Molecular-scale modeling has reached a level of sophistication and accuracy that makes it an essential and highly useful tool for chemical engineers, yet the methods, capabilities, and limitations of this tool are not yet well known across the chemical engineering profession. The use of molecular-scale modeling is becoming increasingly important in industry as researchers and product developers look for ways to cut the costs and time associated with development of new products.

At CSM, we have addressed this problem by incorporating atomistic modeling methods throughout our curriculum at the undergraduate level in both the chemistry and chemical engineering course sequences. We believe that this approach represents a new educational paradigm in chemical engineering, and we are committed to integration of these concepts across the curriculum.

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ChE letter to the editor

Dear Sir:

The article by Rugarcia, et al., titled “The Future of Chemical Engineering Education” [*CEE*, **34**, 16, (2000)] is interesting and thought provoking. However, it begins with a caricature of a poor lecture and returns to the theme of the inferiority of the lecture format later in the paper with the assertion that “the superiority of alternative methods. . .has been demonstrated in thousands of empirical research studies.” This view has become widely accepted among the proponents of “new” teaching methods. At the risk of being branded as a Luddite (probably true), I am compelled to offer a modest and purely anecdotal defense of the lecture format.

Looking back on my own experience as an undergraduate, the classes that I most enjoyed were all formal lectures in physics, chemistry, and even geology. These lectures were given to large classes (sometimes several hundred students) and I am sure that the lecturers would have been horrified at the thought of following a course textbook or of presenting worked examples during a lecture. What was presented was an in-depth review stressing the fundamental principles and the logic and coherence of our understanding of the subject. It is perhaps ironic that the notes from several of these courses were later published as successful textbooks! Well-thought-out and well-rehearsed demonstration experiments, performed by a teaching assistant, were sometimes included. Questions, assignments, and practice examples were handled in parallel tutorial sessions, given by either a faculty member or a PhD student, each with no more than

Continued on page 177.

IS MATTER CONVERTED TO ENERGY IN REACTIONS?

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Perhaps the most famous equation of physics is Einstein's mass-energy relation

$$E = mc^2 \quad (1)$$

Although this equation is well known, it is often misunderstood to mean that matter is converted to energy (or vice versa) in reactions; that matter is a form of energy; and that the principle of energy conservation must be modified. Consider, for example, the following excerpt from a general chemistry text:^[1]

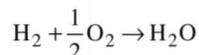
Regardless of the classification used—physical reaction, phase change, ordinary chemical change, chemical change, nuclear reaction—changes in matter involve *the change of matter to energy* if the reaction *evolves energy*, and *the change of energy to matter* if the reaction *absorbs energy*. Energy and matter are thus interchangeable. The scope of the conservation principle is therefore enlarged to include energy as a form of matter or matter as a form of energy. . . . The convertibility of matter and energy is described by the equation $E = mc^2$, predicted by Albert Einstein in 1905. . . .

As we shall see, Eq. (1) does not say that matter and energy are interchangeable, or that matter is a form of energy. Nor does it extend the principle of conservation of energy.

MATTER INTO ENERGY?

One difficulty with the foregoing quote is an ambiguity over the meaning of the word *matter*. There are at least two common ways to measure the quantity of matter in a body: by its mass, or by the numbers of elementary particles it contains. The latter is usually expressed in *moles*.

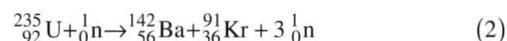
It is easy to show that the constituents of matter are not created or destroyed in ordinary chemical reactions. For example, hydrogen and oxygen react according to the equation



On the left side of the equation we find two moles of hydrogen and one mole of oxygen; the same is true of the

other side. There is no conversion of matter into energy, or vice versa.

What about nuclear reactions? Consider one of the fission reactions that may occur when a neutron is absorbed by uranium-235:

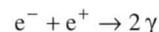


A count of the protons, electrons, and neutrons before and after the reaction shows no change:

Before	After
92 protons	92 protons
92 electrons	92 electrons
144 neutrons	144 neutrons

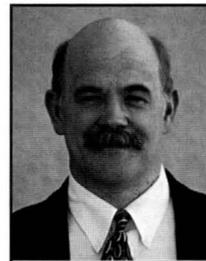
Once again we have an example in which the constituents of matter are conserved in an exothermic reaction. There is no conversion of matter into energy.

To be sure, there are processes in which matter can be created or destroyed. In the reaction between an electron and a positron, for example, both particles are annihilated and two photons are formed:



Nevertheless, we conclude that it is not generally true that matter is converted to energy (or energy into matter) in reactions. If matter is measured by the moles of atoms or nucleons present, the quantity of matter is unchanged in all chemical reactions and in many nuclear reactions.

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Chemical Engineering Education

INERTIAL MASS AND ENERGY

Of course, Einstein's equation refers to mass, not moles. It is worthwhile to consider exactly what is meant by *mass*. In classical mechanics, mass is a measure of two attributes of a material body:

1. The body's resistance to acceleration by external forces ("inertial mass")
2. The force the body experiences in a gravitational field ("gravitational mass")

The title of Einstein's 1905 paper^[2] clearly shows that he was interested in the first concept: "Does the Inertia of a Body Depend on its Energy Content?" (Ist die Trägheit eines Körpers von seinem Energienhalt abhängig?)

The product of inertial mass and velocity is the momentum of a body. Newton's second law of motion can be written as a momentum balance, relating the inertial mass and velocity to the force exerted on the body

$$\mathbf{F} = m \frac{d(\mathbf{mv})}{dt} \quad (3)$$

It has been customary in classical mechanics to regard the mass of a body as a constant, independent of time or velocity (provided the body is not losing or gaining matter). Thus, the mass is usually taken out of the derivation in Eq. (3)

$$\mathbf{F} = m \frac{d\mathbf{v}}{dt} = m\mathbf{a}$$

Einstein challenged the usual assumption that mass is independent of velocity. Using an argument based on the emission of radiant energy (see the Appendix), he derived a relationship between the kinetic energy and the inertial mass. He concluded, "The mass of a body is a measure of its energy content; if the energy changes by L , the mass changes in the same sense by $L/9 \cdot 10^{20}$, if the energy is measured in ergs and the mass in grams." In other words,

$$\Delta E = c^2 \Delta m \quad (4)$$

INTERCONVERSION OF MASS AND ENERGY?

In view of Eq. (4), would it therefore be accurate to say that *mass* and energy are interconvertible in reactions? The answer is still no. If mass and energy were interconvertible, we would expect a negative sign to appear in the equation

$$\Delta E = -c^2 \Delta m \quad (?)$$

But the mass and energy increase or decrease together, so ΔE and Δm must have the same sign.

Consider once again the fission of uranium, as described by Eq. (2). Suppose the reaction is carried out in a closed, adiabatic container, which allows no work or heat exchange with the surroundings. In that case, $\Delta E = 0$, and Eq. (4) yields $\Delta m = 0$. *The reaction occurs without any change in the mass of the system.*

What happens physically is that some of the energy stored in the uranium nucleus is converted to kinetic energy of the

fission products. The temperature of the system rises; but so long as no energy is exchanged with the surroundings, the overall energy of the system does not change. Therefore, according to Eq. (4), the mass does not change.

On the other hand, suppose the thermal energy is withdrawn from the system as it is generated by the fission reaction. According to Eq. (4), this results in a decrease in the mass of the system: $\Delta E < 0$ implies $\Delta m < 0$.

Note that it is the withdrawal of energy from the system that causes the mass to decrease; there is no conversion of mass to energy in the reaction itself. Indeed, if we were to add energy to the system—such as by heating it or accelerating it—the mass would increase again.

FORMS OF ENERGY

Is mass then a form of energy? When speaking of forms of energy, we typically mean kinetic, potential, and internal energy. The total energy of a system may be taken as the sum

$$E = E_K + E_p + U$$

If mass were simply another form of energy, we would have to add another term to the equation

$$E = E_K + E_p + U + mc^2 \quad (?)$$

This is incorrect. According to Einstein, mass is a measure of the energy of the system, not a separate kind of energy. Hence, it would be proper to write

$$m = \frac{E}{c^2} = \frac{1}{c^2} (E_K + E_p + U) \quad (5)$$

Note that the mass varies with kinetic energy and therefore with velocity. We shall return to this point later.

CONSERVATION OF MASS AND ENERGY

An oft-repeated assertion is that Einstein's special theory of relativity modifies the principles of mass and energy conservation. This is only half true. Consider the general balance equation for an extensive quantity in a control volume:

$$(\text{Rate of accumulation}) = (\text{net input rate}) + (\text{net generation rate})$$

For the energy, E , of the system, the balance equation takes the form

$$\frac{dE}{dt} = \sum_i \dot{E}_i + \dot{E}_{\text{gen}}$$

where a dot over a variable indicates a rate, and the summation is taken over the boundaries of the control volume. In thermodynamics, we recognize three ways for energy to cross the boundaries: by heat transfer, by work interactions, and by material flows. Therefore, the energy balance can be written

$$\frac{dE}{dt} = \sum_i (\dot{Q} + \dot{W} + m\dot{E})_i + \dot{E}_{\text{gen}} \quad (6)$$

where

\dot{Q} rate of heat transfer through boundary i

\dot{W} rate of work through boundary i
 \dot{m} rate of material flow through boundary i
 \hat{E} energy per unit mass of material

Einstein assumed that energy is conserved—it is neither created nor destroyed. In other words, the energy generation rate is zero:

$$\dot{E}_{\text{gen}} = 0 \quad (\text{Conservation of Energy})$$

This is the assumption usually made in engineering analysis; therefore, our energy balance need not be modified to account for the effects of relativity.

We do, however, have to modify the usual engineering mass balance:

$$\frac{dm}{dt} = \sum_i \dot{m}_i + \dot{m}_{\text{gen}} \quad (7)$$

We normally assume conservation of mass

$$\dot{m}_{\text{gen}} = 0 \quad (\text{Conservation of Mass})$$

Relativity changes this. Recall that the mass of a system is a measure of its energy content. Dividing the energy balance, Eq. (6), by c^2 and assuming that energy is conserved, we obtain

$$\frac{1}{c^2} \frac{dE}{dt} = \sum_i \left(\frac{\dot{Q}}{c^2} + \frac{\dot{W}}{c^2} + \frac{\dot{m}\hat{E}}{c^2} \right)_i$$

Each term in this equation has dimensions of mass divided by time. Moreover, $\dot{m}\hat{E} / c^2 = \dot{m}\hat{m} = \dot{m}$. Thus

$$\frac{dm}{dt} = \sum_i \left(\frac{\dot{Q}}{c^2} + \frac{\dot{W}}{c^2} + \dot{m} \right)_i$$

This equation can be rearranged to produce

$$\frac{dm}{dt} = \sum_i \dot{m}_i + \sum_i \left(\frac{\dot{Q}}{c^2} + \frac{\dot{W}}{c^2} \right)_i \quad (8)$$

Comparing Eqs. (7) and (8) term by term, we conclude that

$$\dot{m}_{\text{gen}} = \sum_i \left(\frac{\dot{Q}}{c^2} + \frac{\dot{W}}{c^2} \right)_i \quad (\text{Relativity})$$

In other words, mass is “generated” in the system by heat transfer and work. Of course, $1/c^2 = 1 \times 10^{-17} \text{ s}^2 \text{ m}^{-2}$ is so small that the generation rate is usually negligible in practical problems.

RELATIVISTIC AND REST MASS

According to Eq. (5), the mass varies with velocity. To determine the velocity-dependence of mass, consider a closed, adiabatic system initially at rest. Suppose that a force, \mathbf{F} , accelerates the system in such a way as to leave its potential and internal energy unchanged. The energy balance for the system reduces to

$$\frac{dE}{dt} = \dot{W}$$

Substituting $E = mc^2$ and $\dot{W} = \mathbf{F} \cdot \mathbf{v}$ into this equation, we obtain

$$\frac{d}{dt}(mc^2) = \mathbf{F} \cdot \mathbf{v} \quad (9)$$

The mass is related to the force by the momentum balance, Eq. (3),

$$\mathbf{F} = \frac{d(m\mathbf{v})}{dt} \quad (3)$$

Substituting this into Eq. (9), we obtain

$$\frac{d}{dt}(mc^2) = \mathbf{v} \cdot \frac{d(m\mathbf{v})}{dt}$$

Multiplying by $2m$ and rearranging yields

$$c^2 \frac{dm^2}{dt} = \frac{d(mv)^2}{dt}$$

Next we integrate, noting that $\mathbf{v} = 0$ at $t = 0$. The result is

$$c^2(m^2 - m_0^2) = (mv)^2$$

Solving for m , we obtain at last

$$m = \gamma m_0 = \frac{m_0}{\sqrt{1 - v^2/c^2}} \quad (10)$$

In this equation, m is the inertial mass, sometimes called the *relativistic mass*; and m_0 is the *rest mass*, which is the mass of the system at $v=0$.^{*} At velocities much lower than the speed of light, $\gamma \approx 1$ and the relativistic mass coincides with the rest mass. This is usually the case for engineering problems.

CONCLUSION

We have seen that Eq. (1), Einstein’s mass-energy equation, does not predict the interconversion of matter and energy in chemical or nuclear reactions. In fact, the constituents of matter are conserved in chemical reactions and in many nuclear reactions. Nor are *mass* and energy interconvertible. Instead, what Einstein showed was that the mass of a body is a measure of its energy content; consequently, the mass increases when the energy does. Because energy is conserved, there is no need to change our usual energy balance. But in some cases it may be desirable to modify the mass balance to account for the dependence of mass on energy.

We may well ask whether any of this matters, since chemical engineers rarely if ever encounter problems in which relativistic effects are significant. There are at least three reasons why it is important. First, if we are going to mention the theory in our classes or textbooks, we should try to get it right. Second, our students may in the future have to deal with problems in which a sound understanding of $E = mc^2$ is

^{*} In recent years, the preference of many physicists has been to define the rest mass as **the** mass of the system, and to drop the subscript 0. The mass, m , then becomes independent of velocity, which may be considered an advantage; on the other hand, the factor γ must be included explicitly in many equations. For a lively discussion of this issue, see references 4 and 5. This paper has adhered to the more traditional definition, in which the mass, m , is the inertial or relativistic mass.

required. Finally, the Special Theory of Relativity is one of the major scientific discoveries of the 20th century. It could be argued that no scientist, engineer, or mathematician can be truly educated without a proper understanding of this theory.

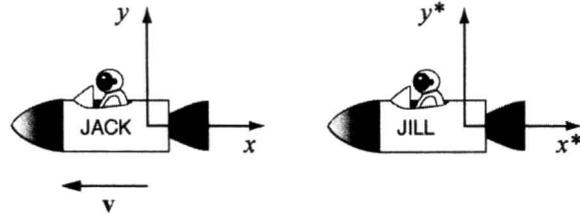
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APPENDIX: Derivation of $\Delta E = c^2\Delta m$

Consider two astronauts, Jack and Jill, riding their space scooters far out in interstellar space. (Space scooters had not been invented when Einstein published his derivation in 1905, but his argument was essentially the same as what follows.) Jack is moving away from Jill at a constant velocity v . For the purposes of our analysis, we define two coordinate systems, as shown in the Figure. The (x,y) -coordinate system is attached to Jack and moves with him; the (x^*,y^*) -coordinate system is attached to Jill. The systems are oriented so that the x -axis and x^* -axis are parallel to the direction of v .



We want to calculate the energy of Jack and his scooter. To do so, we must specify which coordinate system we have in mind. Relative to Jill's (x^*, y^*) system, Jack is moving at speed v , giving him a kinetic energy $\frac{1}{2}mv^2$. Relative to his own (x,y) system, Jack is not moving, so he has no kinetic energy. In either system, Jack and his scooter have the same internal energy. Thus, the difference between Jill's view and Jack's view is

$$E^* - E = \frac{1}{2}mv^2 \quad (A1)$$

Now suppose Jack activates his laser beacon, which fires two pulses of light. One pulse has energy $L/2$ and is emitted at an angle θ relative to the x -axis; the other also has energy $L/2$, but is emitted in the opposite direction.* Jack's velocity does not change, but the internal energy of Jack and his scooter decreases by the sum of the energies of the light pulses

$$E_2 - E_1 = \Delta E = -\left(\frac{L}{2} + \frac{L}{2}\right) = -L \quad (A2)$$

Jill once again sees things differently. As Einstein showed in a previous paper on relativity,^[3] the energies of the light pulses appear from Jill's standpoint to be

$$\frac{L}{2} \left(\frac{1 + v \cos \theta}{\sqrt{1 - (v/c)^2}} \right) \quad \text{and} \quad \frac{L}{2} \left(\frac{1 - v \cos \theta}{\sqrt{1 - (v/c)^2}} \right)$$

Therefore, Jill computes the change in Jack's energy to be

$$E_2^* - E_1^* = -\left[\frac{L}{2} \frac{1 + v \cos \theta}{\sqrt{1 - (v/c)^2}} + \frac{L}{2} \frac{1 - v \cos \theta}{\sqrt{1 - (v/c)^2}} \right] = -L \frac{1}{\sqrt{1 - (v/c)^2}} \quad (A3)$$

Subtracting Eq. (A2) from Eq. (A3), we obtain

$$E_2^* - E_1^* - (E_2 - E_1) = -L \left[\frac{1}{\sqrt{1 - (v/c)^2}} - 1 \right]$$

Regrouping the terms on the left-hand side of the equation yields

$$(E_2^* - E_2) - (E_1^* - E_1) = -L \left[\frac{1}{\sqrt{1 - (v/c)^2}} - 1 \right] \quad (A4)$$

Referring back to Eq. (A1), we see that the left-hand side of the equation equals the change in kinetic energy of Jack and his scooter relative to Jill's (x^*, y^*) system. Moreover, Eq. (A2) shows that $-L = \Delta E$. Thus, we can rewrite Eq. (A4) as

$$\Delta\left(\frac{1}{2}mv^2\right) = \Delta E \left[\frac{1}{\sqrt{1 - (v/c)^2}} - 1 \right] \quad (A5)$$

Einstein made use of the approximation

$$\frac{1}{\sqrt{1 - (v/c)^2}} \approx 1 + \frac{1}{2} \left(\frac{v}{c} \right)^2$$

Substituting this into Eq. (A5), we obtain

$$\Delta\left(\frac{1}{2}mv^2\right) = \Delta E \left[\frac{1}{2} \left(\frac{v}{c} \right)^2 \right] \quad (A6)$$

But if Jack's velocity does not change, $\Delta\left(\frac{1}{2}mv^2\right) = \frac{1}{2}v^2\Delta m$, and Eq. (A6) becomes

$$\Delta m = \Delta E / c^2 \quad (A7)$$

This is the result Einstein obtained in 1905.

* Why two laser pulses? As Einstein noted, light carries momentum. If Jack fired only one pulse, it would tend to accelerate him in the direction opposite the direction of the light. By using two equal but opposite pulses, there would be no acceleration.

A LABORATORY FOR GASEOUS DIFFUSION THROUGH PERMEABLE SOLIDS

The Time Lag

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Mass transfer, one of the core areas of classical chemical engineering curricula, is most often presented to students through laboratory tutorials dedicated to unit operations (*e.g.*, distillation, gas absorption, extraction, etc.). Laboratory tutorials aimed at a more fundamental approach can also be proposed, based for instance on the study of one of the methods leading to diffusion coefficient determination in fluid phases (liquid, gases, etc.)^[1] To our knowledge, however, the study of a strict diffusion process in a less conventional phase, such as a permeable solid (polymer, adsorbent, microporous material), is seldom attempted at an undergraduate level in chemical engineering departments. In this paper, we will describe an experimental setup that enables study of the transitory mass transfer of a permanent gas through a permeable solid; apart from the simplicity and rapidity arguments, this technique, currently referred to as the *time-lag method*, permits us to stress either the mass-transfer or the physical-chemistry aspect in the solution approach proposed to the student.

THEORY

The time-lag permeation technique was originally conceived in 1920 by Daynes in order to study the mass transfer through an elastomeric material.^[2] The method was refined and widely used through the years by authors such as Barrer^[3] and Crank,^[2] and it has been applied successfully to numerous materials—from catalyst particles to metals and polymers—and to different sample geometries. Interest in the time-lag technique has been sustained over the past ten years, as shown by Vieth^[4] in his work on permeation through polymer films.

A time-lag cell consists of an upper and lower chamber separated by an initially gas-free solid sample (see Figure 1). A permanent gas is introduced in the upstream part of the cell at time zero; while maintaining upstream pressure constant, the appearance of permeated gas is continuously monitored in the lower compartment using a pressure transducer. A significant pressure rise only occurs after a period called the *time lag*. This time lag, θ , indicates the onset of a quasi-steady-state diffusion process, which persists until the pressure in the entire cell equilibrates.

Two experimental configurations can be used to perform a time-lag experiment. The first one, called the “Wicke-



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Kallenbach" diffusion cell experiment, consists of two compartments initially containing the same inert gas at the same constant pressure and separated by the solid film to be tested. At time zero, another compound is introduced in the upper chamber and the response to this impulse is monitored in the downstream compartment.

As part of our study, we use another configuration termed the "traditional" time-lag experiment, which differs from the previous one in that a vacuum is initially applied in both compartments. Rutherford has discussed the advantages and drawbacks of each method.^[5]

A theoretical computation of downstream-compartment pressure increase can be obtained starting from Fick's second law applied between the permeable sample boundaries^[2]

$$D \left(\frac{\partial^2 c}{\partial x^2} \right) = \frac{\partial c}{\partial t} \quad (1)$$

It should be stressed that Eq. (1) applies only for a constant diffusion coefficient, which is a special case; the didactic system selected for this study (oxygen/nitrogen/silicone rubber) is in agreement with this assumption. Frisch extensively discussed the more complex general situation of a concentration-dependent diffusion coefficient.^[6] In this case, Eq. (1) has to be rewritten as

$$\frac{\partial}{\partial c} \left[D(c) \frac{\partial c}{\partial t} \right] = \frac{\partial c}{\partial t} \quad (2)$$

For a flat sample, the following boundary conditions can be postulated: a film initially free from gas, the attainment of equilibrium at the inlet gas-polymer interface according to a Henry-type expression, and a near-zero concentration of gas at the downstream face:

$$c(x, 0) = 0 \quad (3a)$$

$$c(0, t) = c_0 = SP_0 \quad (3b)$$

$$c(L, t) = c_L \equiv 0 \quad (3c)$$

where L is the sample thickness, P_0 the upstream pressure, and S (deriving from Henry's law expression) is usually called sorption coefficient. Again, Henry's law validity corresponds to a simple and special case; it is important to note that numerous systems, especially those involving glassy polymers (*e.g.*, polyethyleneterephthalate used in carbonated beverage packaging) show strong deviations from Henry's law. Nevertheless, the assumption of a constant sorption coefficient is correct for the system selected for this study.

Equation (1), subject to the experimental boundary conditions, Eq. (3), can be integrated by Laplace transform^[2]

$$c = c_0 \left(1 - \frac{x}{L} \right) - \frac{2c_0}{\pi} \sum_{n=1}^{\infty} \left[\frac{1}{n} \sin \left(\frac{n\pi x}{L} \right) \exp \left(-\frac{Dn^2 \pi^2 t}{L^2} \right) \right] \quad (4)$$

where n is an integer.

The net gas flowrate can be computed from the concentration profile based on the integration of Fick's first law with respect to time. The resulting downstream pressure increase is

$$P_L = A \frac{RTDP_0}{VL} \left[St - \frac{SL^2}{6D} + \frac{2SL^2}{\pi^2 D} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^2} \exp \left(-\frac{Dn^2 \pi^2 t}{L^2} \right) \right] \quad (5)$$

When a quasi-steady-state prevails, the transient summation terms are negligible and an asymptotic solution is reached

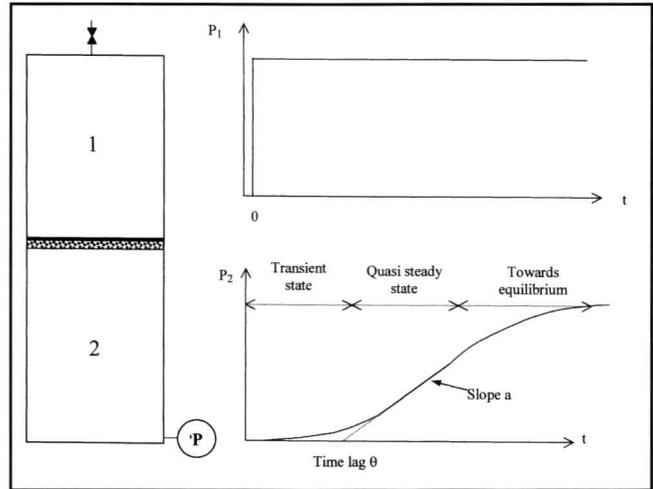


Figure 1. Schematics of a time-lag apparatus and experiment.

for the downstream pressure P_L

$$P_L(t) = A \frac{RTSD P_0}{VL} \left(t - \frac{L^2}{6D} \right) \quad (6)$$

This equation reveals that the pressure-time plot shows a linear rise and allows determination of the following parameters (see Figure 1):

$$\theta = \frac{L^2}{6D} \quad \text{known from the intercept} \quad (7)$$

$$a = A \frac{DRTS P_0}{VL} \quad \text{known from the asymptotic slope} \quad (8)$$

In other words, the above analysis shows that an interpretation of the early events of a time-lag experiment allows simultaneous determination of the three main quantities characterizing mass transfer: the diffusion coefficient (D), the Henry law sorption coefficient of the gas in the solid (S), and the product of both, usually called permeability,

$$\wp = SD \quad (9)$$

The objective of the laboratory tutorial described in this paper is to show and analyze the possibilities and limitations of a time-lag experiment performed according to the preceding data treatment.

MATERIAL AND METHODS

The experimental apparatus we set up consists of a stainless-steel permeation cell (see Figure 2), within which a circular polydimethylsiloxane film purchased from Dow Corning (Silastic™ sheeting, thickness 125 μm, diameter 8 cm, active surface area 30 cm²) is inserted. The film is mechanically supported by a brass or Inox frit (Poral) sufficiently porous to assert that its mass-transfer resistance is far lower than the one of the analyzed material. A Viton™ seal ensures the airtightness of the cell and also reduces the film surface area exposed to the gas.

An overview of the complete laboratory setup designed in our workshop is shown in Figure 3. For the sake of convenience, a simple, low-cost stainless-steel filter holder can be purchased (for instance, Millipore model 4404700) and works equally well in this application. The two compartments of the cell are connected to a vacuum pump (Alcatel Pascal 1015 SD), while the upper one can be fed by a permanent gas (nitrogen or oxygen) from a bottle by opening a needle valve (Nupro ABVT 1). The upstream compartment pressure is controlled by a Bourdon manometer. An active strain gauge (Edwards ASG NW16 2000 mbar) enables downstream compartment pressure to be monitored. The electric signal ranging from 0 to 10 volts is sent to a digital display (Edwards ADD). Afterwards, an analog-to-digital 24-bit converter (Sigma Delta) with an integrated oscillator (Linear Technology LTC2400) is used to allow a computerized acquisition at a maximum frequency of 20 Hz.

A personal computer with the Test Point™ program carries out the analog data processing. It permits screen display of the downstream pressure rise in millibars versus time in seconds and the information backup in a data-extended file. This file is then imported into a spreadsheet program (such as Excel™) to determine the diffusion and sorption coefficient. Figure 4 shows an example of the complete pressure rise for illustrative purposes.

LABORATORY TUTORIAL

After a short review of the principles and the theoretical development underlying the technique (see the section on “Theory”), we ask the students to familiarize themselves with the equipment and then operate

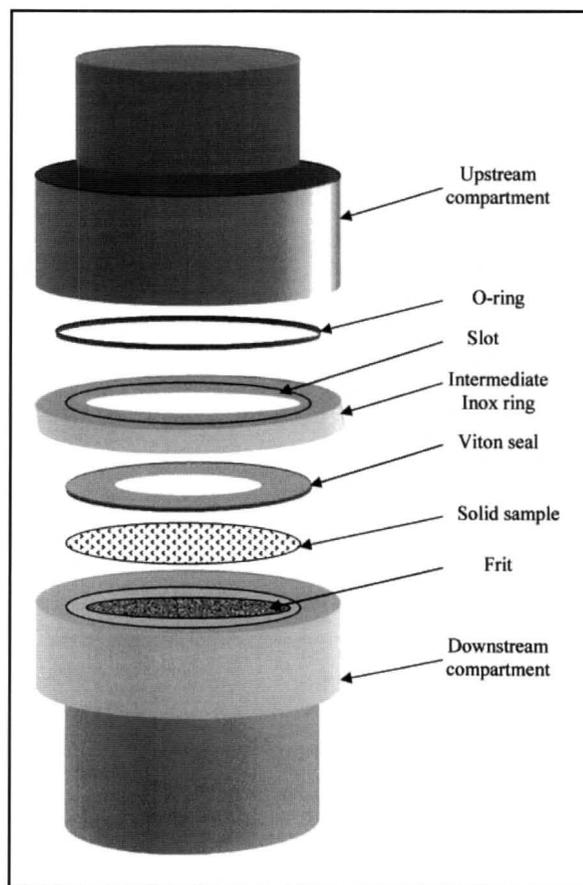


Figure 2. Exploded view of the permeation cell.

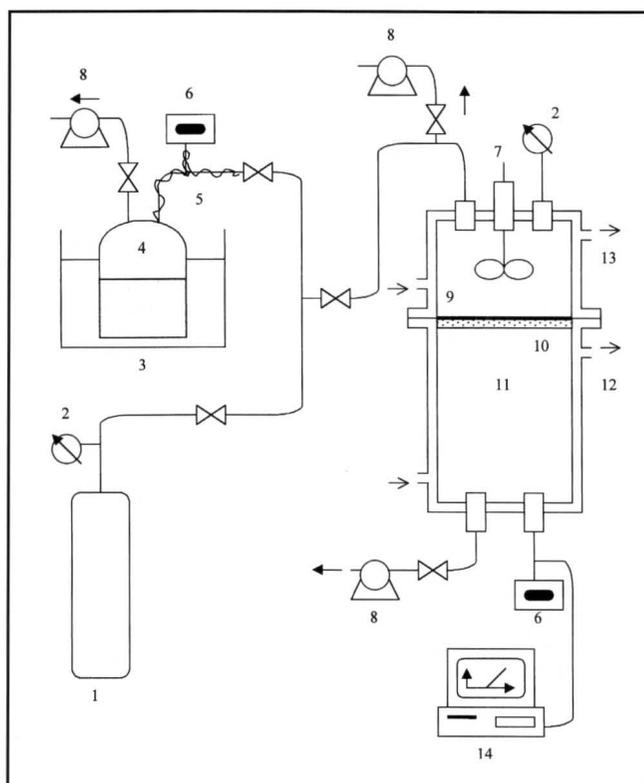


Figure 3.

Overall set up:

1. Gas bottle (pure oxygen or nitrogen)
2. Bourdon manometer
3. Thermoregulated bath
4. Solvent reservoir
5. Heating resistance
6. Pressure gauge and digital display
7. Magnetic stirrer
8. Pump
9. Solid sample
10. Porous support
11. Downstream volume
12. Thermoregulated water flow
13. Thermoregulated water flow
14. Computerized data acquisition.

it according to the following instructions:

① Start thermostated bath and apply a primary vacuum in both compartments. Attention should be paid at this stage to the fact that the downstream side only has to be degassed in a first step, before treating the upstream part. If not, film disruption will occur as soon as a reverse pressure differential takes place (the sample is not supported on the upstream side).

② Evaluate the cell's leakage rate by closing all connections around the module (vacuum pump, gas bottles, etc.). This is of crucial importance since any background in downstream pressure increase will affect data treatment. An average value of about 0.1 millibar per hour should be achievable; if not, cell screws should be tightened, as well as the O-ring and sample positioning checked. The above value should be kept in mind if error calculation on D or S are needed. Nevertheless, it is negligible in regard to PDMS permeability and experiment duration in the present case.

③ A typical time-lag experiment can then be undertaken for a given pressure and temperature. Depending on the duration of the tutorial, 2 to 4 different pressure and/or temperature values (typically ranging between 20 and 80°C and 0.5 to 5 bar) can be explored with pure nitrogen and oxygen. The student is asked to assess D and S values and check the consistency with literature data.^[7-9] The key importance of downstream compartment volume V can be discussed at this stage (see Eq. 8); in our case, direct as well as indirect measurements credit this chamber with a 585 cm³ volume, which fits the needs regarding gauge sensitivity, air losses, and material permeability.

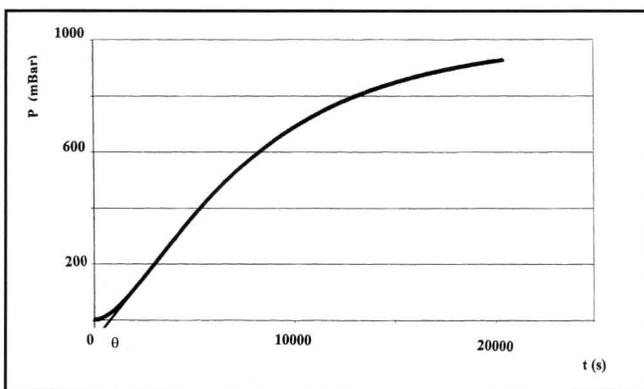


Figure 4. Example of an experimental result obtained by the setup described in this work (downstream pressure vs. time), including the determination of time-lag intercept (θ). Oxygen permeation through a 125- μm thick SilasticTM film; upstream pressure 4 bar, temperature 50°C, acquisition frequency 5 Hz.

④ An error calculation can be optionally performed, based on an analysis already discussed by Paul and DiBenedetto^[10] and later by Siegel and Coughlin,^[11] showing that the technique can lead to small errors in permeability but far greater errors in the diffusion coefficient. For instance, the relative error on θ is about five times larger than that on the slope for data collected at $t \cong 4\theta$:

$$\left| \frac{\Delta\theta}{\theta} \right| \cong 5 \left| \frac{\Delta a}{a} \right| \quad (10)$$

Thus, a 2% error on the slope means a 10% error on the diffusion coefficient—which are commonly assumed values for a single measurement. Therefore, the duration of the time-lag experiment should be carefully considered. While data taken at times greater than 10θ will lead to sizeable errors in diffusivity, the attainment of steady state requires duration times around 4θ .

Nevertheless, the error in steady-state slope can be greatly minimized by simply re-evacuating the downstream chamber with the feed pressure still applied to the top face of the membrane. Reclosing the receiver valve ahead of the vacuum pump (item 8 in Figure 3) allows measuring the steady-state slope without bend-over problems up to a downstream pressure below 1% of the feed pressure. This repeated evacuation and retesting of the slope gives students an easy way to evaluate measurement reproducibility.

⑤ Based on the D and S values, permeability \wp can then be calculated from Eq. (9). The student is asked to express the results in Barrers, the most common permeability unit:

$$\wp (\text{Barrer } 10^{10}) = \frac{273}{T(\text{K})} \frac{V(\text{cm}^3)}{P_0(\text{cmHg})} \frac{L(\text{cm})}{A(\text{cm}^2)} a (\text{cmHg s}^{-1}) \frac{1}{76} \quad (11)$$

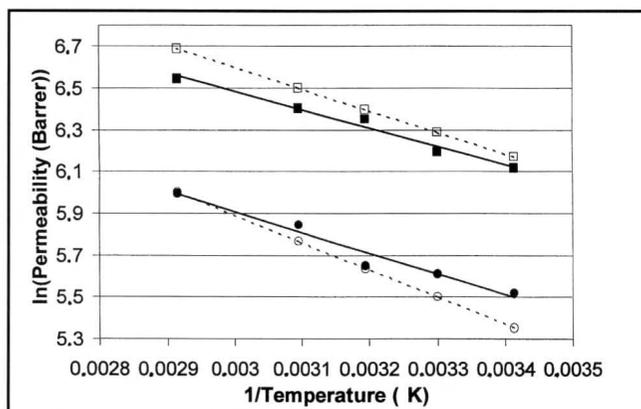


Figure 5. Example of Arrhenius plots for oxygen and nitrogen permeability variation with temperature through SilasticTM film (upstream pressure 2 bar). Comparison between experimental (solid line) and literature (dashed line) values.

Typical oxygen permeability values in PDMS obtained by the setup can be seen in Figure 5 where the good reproducibility of measurement is illustrated.

⑥ For a more physicochemical insight, undertaking the study of the influence of temperature on sorption, diffusion, and permeability can be worth the time. A simple expression is often shown to describe correctly the results for all three parameters:

$$X = X^0 \exp\left(-\frac{E_X}{RT}\right) \quad X = D, S, \text{ or } \wp \quad (12)$$

While the analogy to Arrhenius expression is correct for rate parameters (leading to the often-used vocable activation energy of diffusion and activation energy of permeability), it should be explained to students that the same is incorrect for sorption, which is not an activated process (E_S corresponds to the heat of sorption ΔH_S , as classically obtained by a van't Hoff plot). The following relationship, linking the two activation energies E_P and E_D with ΔH_S can be derived by using Eqs. (9) and (12)

$$E_P = \Delta H_S + E_D \quad (13)$$

Figure 5 illustrates the good accordance between the experimental and the literature values for oxygen and nitrogen permeabilities^[7,12,13]

$$\begin{aligned} E_P^{O_2} &= 7.4 \text{ kJ / mol} & E_P^{N_2} &= 8.2 \text{ kJ / mol} \\ \wp_{O_2}^0 &= 9180 \text{ Barrer} & \wp_{N_2}^0 &= 7150 \text{ Barrer} \end{aligned}$$

These results are satisfactory in that the oxygen permeability is greater than the one of nitrogen and conversely for the energies of activation. At this stage, students can be asked to explore potential separation applications based on this peculiarity, such as gas-separation membrane processes.

Typical experimental results are summarized in Table 1. The already-discussed inaccuracies on the intercept lead to significant errors on D values; however, $D_{O_2}^0$ remains always greater than $D_{N_2}^0$, which agrees with the theory because nitrogen's kinetic diameter is larger than oxygen's.

⑦ The influence of upstream pressure can also be optionally investigated, similar to the work already addressed by Koros and Jordan with a silicone-nitrogen system.^[14]

CONCLUSION

The objective of this work was to point out an easy-to-carry-out experiment of didactical importance for the understanding of gas mass transfer in different solid media. The time-lag permeation method is a flexible and powerful technique that can give both equilibrium (sorption coefficient S) and transport properties (diffusivity D and permeability \wp)

TABLE 1
Experimental (exp) and Literature Values ([7])
for Oxygen Sorption, Diffusion, and Permeability
through PDMS for 1 Bar Upstream Pressure

T(°C)	\wp exp (Barrer)	\wp literature (Barrer)	D exp (m ² s ⁻¹)	D literature (m ² s ⁻¹)	S exp (Pa ⁻¹)	S literature (Pa ⁻¹)
20	454	479	1.0E-09	1.6E-09	0.34	0.31
30	492	539	7.1E-10	1.8E-09	0.53	0.31
40	574	601	1.1E-09	2.0E-09	0.41	0.30
50	605	667	1.6E-09	2.2E-09	0.29	0.30
70	696	806	2.1E-09	2.7E-09	0.25	0.30

in a single experiment; based on the setup described in this work, we have shown that reliable and accurate data with regard to the permeabilities of permanent gases can be obtained, while estimation of D and S is achievable. We focused first on simplicity, especially regarding the data-treatment aspects. We want to stress, however, that more sophisticated approaches (such as those proposed in advanced mass-transfer topics) can be equally well-proposed based on the same setup. A few examples, listed below, show how to open various didactical extensions.

- ▶ A first possibility consists in replacing the silicone rubber membrane with a glassy polymer. For instance, polyethyleneterephthalate (PET), which is readily available since most overhead transparency materials used in projectors are composed of PET; a more permeable Lexan™ film, produced by General Electric, can also be used. If carbon dioxide is used in place of oxygen or nitrogen, experiment duration would remain compatible with a laboratory tutorial providing that a thin enough film (25 μm or less) is available. Investigating the more-complex case of gas permeation through glassy polymers is of value for the students in order to point out polymer barrier properties.
- ▶ In place of permanent gases, organic-vapors transport could be equally well investigated, based on the vapor generator system connected to the module (see Figure 3); in that case, complications arising from the non-constancy of the diffusion coefficient with concentration can lead to complex, but interesting, transport behavior (and thus, data treatment). The incidence of a variable D on the experimental time lag has been explored by Frisch.^[6] Attention should be paid, however, to explosion hazards or O-ring damage when manipulating organic vapors.

- In this work, the solid sample is considered as the single mass-transfer resistance; nevertheless, boundary-layer resistance can arise, particularly when binary mixtures are transported through a very permeable media; in that event, the influence of hydrodynamic conditions on overall transfer (concentration polarization phenomenon) is a good indication that can be best achieved by a magnetic Rushton turbine already existing on the setup.
- The independent temperature jackets for the two compartments also offer an opportunity to experiment with the incidence of non-isothermal conditions, already shown to strongly affect the observed transfer rate of a pure organic vapor.^[13]

ACKNOWLEDGMENTS

The authors gratefully acknowledge the numerous valuable comments of the manuscript's reviewers.

NOMENCLATURE

- A sample surface area
- a asymptote slope
- c concentration
- c_0 upstream concentration
- c_L downstream concentration
- D diffusion coefficient
- $E_{D,P}$ energy of activation for diffusion (D) and permeability (P)
- L sample thickness
- P pressure
- ρ permeability
- R perfect gas constant
- S sorption coefficient
- t time
- T temperature
- V downstream volume

Greek Symbols

- θ time lag
- ΔH_s heat of sorption

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Letter to the Editor

Continued from page 167.

three undergraduates.

Used in this way, a lecture course provides a highly effective way not only for the dissemination of information but also for capturing the interest of students. The formal lectures does *not* provide a good format for developing problem-solving skills, for dealing with engineering design, or even for presenting and discussing solutions to pre-assigned problems.

Unfortunately, in many (if not most) universities the lecture format has been widely misused since it has become the universal workhorse. This may be a more serious issue in engineering education where "design" and "problem solving" constitute a major portion of the curriculum. Nevertheless, within the chemical engineering curriculum, there are many subject areas that are well-suited to the lecture approach and, in the hands of a skilled practitioner and especially if supported by appropriate tutorial sessions, this approach can be very effective. Essentially this same point is made by Wankat and Oreovicz in *Teaching Engineering*. This is one of the references cited in the present article as showing the superiority of alternative approaches! Such a conclusion is hardly surprising since, in any attempt at a quantitative assessment, it would be very difficult, if not impossible, to establish whether the apparent disadvantages of a lecture course are really intrinsic to the format or stem from an inappropriate application of this format. There seems to be a clear danger that, in the current enthusiasm for "new" instructional methods, the very real advantages (and equally real limitations) of the lecture format will be overlooked.

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USE OF AN EMISSION ANALYZER TO DEMONSTRATE BASIC PRINCIPLES

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In choosing and developing experiments for undergraduate laboratories, instructors often try to avoid those experiments that require lengthy or sophisticated chemical analysis, such as experiments related to environmental engineering. But the development of electrochemical and infrared sensors has made gas analysis much easier to accomplish.

This paper describes experiments based on the use of a portable stack gas analyzer, or emission analyzer. In a sense, the analyzer is modern technology's replacement for the classical Orsat analysis of flue gases,^[1] but the analyzer does not measure carbon dioxide levels directly, calculating them instead from the knowledge of fuel type using basic stoichiometry. The modern analyzer provides a relatively quick and painless way of doing chemical analysis for a gaseous system.

The analyzer used here costs \$6,350 and was purchased under an NSF-ILI grant.^[2] With the additional purchase of other more modest components for about \$250, simple combustion experiments with a laboratory burner and a make-shift flue were run. The results were used to demonstrate: 1) the principles of a rotameter, 2) material balances based on the measured molar flow of the fuel gas and the measured volume fraction of oxygen in the exiting flue gases, 3) energy balances based on the temperature of the exiting flue gases, and 4) how the kinetics of nitric oxide formation can be used to estimate temperatures in the hottest part of the flame.

The chemical engineering program at the University of Minnesota, Duluth, is relatively small, with five full-time faculty, three temporary instructors, and a graduating class in the range of 20-30 students. Without the amenities of larger departments (*e.g.*, shop facilities), it is difficult to develop experiments requiring considerable construction of apparatus or faculty time. The experiment described here is relatively straightforward to do—the analyzer does the hard work. It is intended as an undergraduate experiment, how-

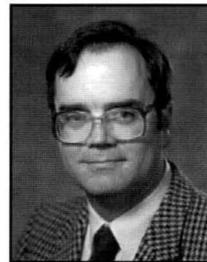
ever, and should not be construed as a research-level experiment or an experiment with which to do thorough studies of combustion.

The analyzer is self-contained in a carrying case the size of a large brief case, so storage of the experiment's components is not a problem. The department also offers a minor in environmental engineering, and the intention is to use this analyzer in a new environmental-engineering laboratory course; other experiments for this course have been described elsewhere.^[3] A group of our students used the analyzer as part of their project in our capstone design course and the project was successfully entered in a national competition.^[4]

EXPERIMENTAL

The apparatus comprises a section of double-walled galvanized flue pipe (18 in long and 3 in wide) mounted vertically with a flue cap positioned on top; these items were purchased from a hardware store. A Veriflow burner, fitted with an N-2 nozzle (Fisher Scientific) was positioned at the center of the bottom opening of the flue; it was connected via a rotameter (Cole Parmer E-32461-58), calibrated in liters of air per minute (L air/min), to the laboratory supply of natural gas. To obtain temperatures in the exiting flue gas that vary with the flow of natural gas, controlled by the rotameter, it was essential to restrict the flow of air into the bottom of the flue. A can of suitable dimensions was cut in

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half, and a 1-in square hole was punched in the bottom of one half. This half was fitted into the bottom of the flue and the burner was positioned at the center of the hole. The rotameter was calibrated with a household gas meter (Equipmeter S-275). For the experiments described here, air was not premixed with natural gas before entering the burner, so the combustion was controlled by diffusion of air.^{15]}

The emission analyzer is a COSA 6000 portable stack gas analyzer. This measures the volume fractions of O₂, CO, NO_x, and SO_x using electrochemical cells. (The lifetime of the O₂ cell is the most limited, being in the range of 1-2 years; the other cells will last between 2 and 3 years.) The analyzer pumps the gas to be sampled through the end of a hollow metal probe (12 in long) at the tip of which is a thermocouple (type K) for measuring the gas temperature. The gas passes from the metal probe via flexible tubing (10 ft long) to a condensate trap clamped to the outside of the main case containing the analytical components of the analyzer. This passage of the gas to the analyzer results in the gas entering the train of electrochemical cells at essentially ambient temperature.

From the measurements of gas levels and temperature, the instrument's firmware calculates various quantities. The volume fraction of CO₂ and the excess air are of most concern here. This requires the user to select the fuel type; the selection includes natural gas, propane, butane, coal, oils light no. 2 and no. 6, as well as a programmable option. Other calculated quantities include efficiency and effectiveness; these are not considered here.

For the experiments described here, the tip of the probe was positioned just below the center of the flue cap. Two to four sets of data for each of six different flows of natural gas were collected. It was important to let the rotameter setting stabilize after changing it. The data presented here were comfortably obtained within 3 to 4 hours; the treatment of the data may take most students a lot longer!

RESULTS AND INTERPRETATION

Calibration of the Rotameter • Volumetric flows were measured under ambient conditions (25°C and 1 atm) throughout. The volumetric flow rate of natural gas, V_{ng}, read directly from the household gas meter in units of ft³/min, regressed against the reading of the rotameter, V_{air}, in units of L/min leads to

$$V_{ng}(\text{ft}^3/\text{min}) = (0.0504 \pm 0.0005)V_{air}(\text{L}/\text{min}) \quad r^2 = 0.987 \quad (1)$$

This is transformed to

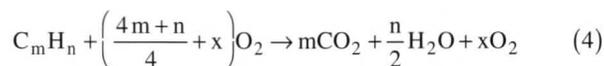
$$V_{ng}(\text{L}/\text{min}) = (1.43 \pm 0.01)V_{air}(\text{L}/\text{min}) \quad (2)$$

What useful information can we obtain from the value of the slope? The theory of the rotameter^[6,7] applied to gases leads to

$$V_{ng}/V_{air} = \sqrt{\rho_{air}/\rho_{ng}} \quad (3)$$

Using the density of air at 25°C and 1 atm, the density of our natural gas is 0.579 g/L under the same conditions. Methane is usually the major component of natural gas, and its density^[8] under the same conditions is 0.657 g/L. Such discrepancies can cause concern, but it should be realized that the composition of natural gas is dependent on its source and upon the life of the well from which it is extracted. For example, the analysis of natural gas from 18 locations^[9] in the U.S. yields the following ranges and median values for the following components: CH₄, 98-24%, 85%; C₂H₆, 70-0%, 8%; N₂, 8-0%, 1%; and CO₂, 25-0%, 1%.

Stoichiometry and Material Balances • The emission analyzer provides a measure of the oxygen in the gas sample as a volume fraction; with the ideal-gas assumption, here and throughout, this corresponds to a mole fraction, Y_{O₂}. From this measurement, the instrument calculates the volume fraction of carbon dioxide and the fraction of excess air. For the complete combustion of a general hydrocarbon, C_mH_n, in excess air, represented by the stoichiometric coefficient x, the reaction is



The stoichiometry is summarized in Table 1 for various bases, and in Table 2 the corresponding molar flows and mole fractions in the exiting flue gas are listed.

In understanding the operation of the gas analyzer, it is recognized that various quantities are calculated from the measured mole fraction of oxygen; these are the mole fraction of carbon dioxide and the excess air. The basic procedure is to get an expression for the stoichiometric coefficient of excess air, x, in terms of the mole fraction of oxygen (see Table 2, Eqs. T1 and T4). Then the mole fraction of carbon dioxide is calculated (see Table 2, Eq. T3). The fraction of excess air is usually defined^[10] by

$$E_{air} = \frac{\left(\frac{\text{moles of air fed}}{\text{moles of air required for complete combustion}}\right) - \left(\frac{\text{moles of air required for complete combustion}}{\text{moles of air required for complete combustion}}\right)}{\left(\frac{\text{moles of air required for complete combustion}}{\text{moles of air required for complete combustion}}\right)} = \frac{4x}{4m+n} \quad (5)$$

To apply the appropriate stoichiometry, two cases under which the analyzer operates are identified. For Case 1, it is recognized that the sample stream passes through a condensate trap at room temperature. When the quantity excess air varies from zero to a value $x = x_{crit}$, the water produced will condense to form liquid; this is treated as vapor and liquid in equilibrium. Then, quantities applicable to the wet-product stoichiometry from Tables 1 and 2 are used. Upon increasing the excess air above x_{crit} , there is no longer sufficient water vapor in the product stream to maintain liquid and vapor in equilibrium; this is Case 2, in which all the products are gaseous, and the gaseous-product stoichiometry is applied.

The value of x_{crit} is calculated by setting the vapor-phase mole fraction of water, on the gaseous-product basis, to its saturation value of

$$y_{\text{H}_2\text{O}} = (n/2) \left(F_0 / F_T^{\text{gas}} \right) = y_{\text{H}_2\text{O}}^{\text{sat}} \quad (6)$$

The solution is

$$x = x_{\text{crit}} = \left(\frac{1}{1 + r_{\text{N/O}}} \right) \left[\frac{n}{2 y_{\text{H}_2\text{O}}^{\text{sat}}} - m - \frac{n}{2} - \frac{(4m+n)}{4} r_{\text{N/O}} \right] \quad (7)$$

If the products from the combustion of methane are passed through the condensate trap at 25°C, the value of x_{crit} is 11.2 mol (corresponding to about 560% excess air). This value is exceeded in the experiments described here.

The dry-product stoichiometry is important for understanding the relationships between quantities measured by the gas analyzer and those measured by the traditional Orsat analysis; the mole fractions of gases in the Orsat analysis are on a dry basis.^[1,10] When $x < x_{\text{crit}}$, then

$$y_{\text{O}_2} (\text{gas analyzer}) = (1 - y_{\text{H}_2\text{O}}^{\text{sat}}) y_{\text{O}_2} (\text{Orsat}) \quad (8)$$

At 25°C, $1 - y_{\text{H}_2\text{O}}^{\text{sat}} \cong 0.97$, so the difference in the mole fractions between the two methods is not great. For the other case, when $x > x_{\text{crit}}$

$$y_{\text{O}_2} (\text{gas analyzer}) = y_{\text{O}_2} (\text{Orsat}) \left/ \left[1 + \frac{n/2}{q + x(1 + r_{\text{N/O}})} \right] \right. \quad (9)$$

The quantity q is defined in Table 2. If methane is burned in 600% excess air (just above the critical value), then

$y_{\text{O}_2} (\text{gas analyzer}) \cong 0.97 y_{\text{O}_2} (\text{Orsat})$. As the excess air increases further, the two measures of the mole fraction get closer together.

In principle, the calibration of the rotameter can be used to calculate the molar flow of fuel to the burner if the composition of the natural gas is known. To keep things simple, the natural gas is treated as pure methane, following the usual practice.^[10] In this case, the molar flow of methane into the burner at 25°C, as a function of the rotameter setting, is

$$F_0 (\text{mol CH}_4 / \text{min}) = \frac{\sqrt{\rho_{\text{air}} \rho_{\text{CH}_4}}}{16.043} V_{\text{air}} = 5.50 \times 10^{-2} V_{\text{air}} (\text{L} / \text{min}) \quad (10)$$

This is used in calculations that follow.

The mole fractions of oxygen and carbon dioxide and the excess air are plotted against the volumetric flow rate of natural gas in Figure 1. As the flow of natural gas to the burner increases, the excess air and the fraction of oxygen decrease while the fraction of carbon dioxide increases with the increasing flow. The largest fraction of carbon dioxide (7%) observed here corresponds to the smallest fraction of excess air (60%). The maximum fraction of carbon dioxide possible is 11.7% and occurs under stoichiometric conditions (no excess air); the student can deduce this from Eq. (T3) in Table 2. The student can calculate the maximum fractions of carbon dioxide possible for other hydrocarbons in a similar way; a standard reference contains the values.^[8]

Energy Balance • The first law of thermodynamics for steady-flow systems is applicable. There is no shaft work

TABLE 1
Stoichiometry for the Complete Combustion of a Hydrocarbon

Species	Molar flow into the burner and the flue	Molar flow out of the flue		
		gaseous-product basis	dry-product basis	with liquid water as product, wet basis
C_mH_n	F_0	0	0	0
O_2	$\left(\frac{4m+n}{4} + x \right) F_0$	$x F_0$	$x F_0$	$x F_0$
N_2	$\left(\frac{4m+n}{4} + x \right) r_{\text{N/O}} F_0$			
CO_2	0	$m F_0$	$m F_0$	$m F_0$
H_2O	0	$\frac{n}{2} F_0$	0	$y_{\text{H}_2\text{O}}^{\text{sat}} F_T^{\text{wet}}$

- F_0 is the molar flow of hydrocarbon into the burner.
- $r_{\text{N/O}}$ is the molar ratio of nitrogen to oxygen in air, $r_{\text{N/O}} = 79.01/20.99$
- F_T^{wet} is the total molar flow out of the flue.
- $y_{\text{H}_2\text{O}}^{\text{sat}}$ is the mole fraction of water in the vapor phase when liquid and vapor are in equilibrium.

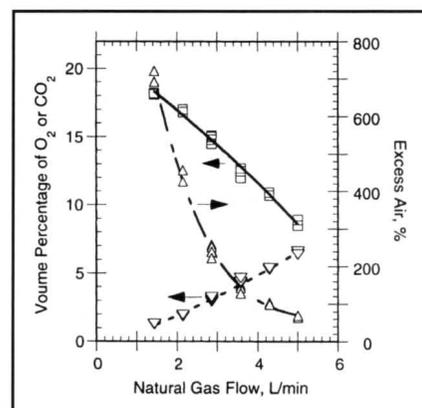


Figure 1. The measured mole fraction of oxygen (\square) in the exiting flue gas as a function of the volumetric flow rate of natural gas to the burner measured under ambient conditions (25°C, 1 atm). The quantities calculated from measured mole fraction of oxygen are the mole fraction of carbon dioxide (∇) and the percentage of excess air (\triangle).

and it is assumed that kinetic energy and potential energy effects are negligible.

$$\Delta H = Q \quad (11)$$

The flue pipe is regarded as an open system; ΔH is the enthalpy change from inlet to outlet, and Q is the heat transferred between the system and the surroundings. Because calculation of the adiabatic flame temperature, $Q=0$, is standard for this system, only the bare details are given here. Many authors^[10-14] present methods for calculation of the adiabatic flame temperatures. In calculating them here, the molar heat capacity functions of Smith and coauthors^[14] were used, and Visual Basic functions for them within an Excel spreadsheet were written. "Goal Seek" was used to solve for the flame temperatures. The resulting adiabatic flame temperatures and the measured flue gas temperatures are plotted against the volumetric flow rate of natural gas in Figure 2.

The measured flue gas temperatures are used to calculate Q directly; this, the net heat transferred, turns out to be negative as heat is lost from the system, the flame and the flue, to the surroundings. The absolute values of Q as a function of the difference between the temperatures of exiting flue gases and inlet gas temperature (considered to be the same as the surroundings, taken to be 25°C) are plotted in

TABLE 2
Molar Flows and Mole Fractions
in the Gas Stream Leaving the Flue

Molar Flows

Gaseous-product basis $F_T^{\text{gas}} = F_0 [q + x(1 + r_{N/O}) + n/2]$
 Dry-product basis $F_T^{\text{dry}} = F_0 [q + x(1 + r_{N/O})]$
 Wet-product basis $F_T^{\text{wet}} = F_0 [q + x(1 + r_{N/O})] / (1 - y_{H_2O}^{\text{sat}})$

General Expressions for Mole Fractions

$$y_{O_2} = xF_0 / F_T \quad [T1]$$

$$y_{N_2} = \left(\frac{4m + n}{4} + x \right) \frac{F_0}{F_T} r_{N/O} \quad [T2]$$

$$y_{CO_2} = mF_0 / F_T = (m/x)y_{O_2} \quad [T3]$$

Mole Fractions of Water Vapor

Gaseous-product basis $y_{H_2O} = (n/2)F_0 / F_T^{\text{gas}}$
 Dry-product basis $y_{H_2O} = 0$
 Wet-product basis $y_{H_2O} = y_{H_2O}^{\text{sat}}$

Expressions for x , the stoichiometric coefficient of excess air, in terms of y_{O_2}

Gaseous-product basis $x = (q + n/2)y_{O_2} / [1 - (1 + r_{N/O})y_{O_2}]$

Dry-product basis $x = (q \times y_{O_2}) / [1 - (1 + r_{N/O})y_{O_2}] \quad [T4]$

Wet-product basis $x = (q \times y_{O_2}) / [(1 - y_{H_2O}^{\text{sat}}) - (1 + r_{N/O})y_{O_2}]$

In the Equations Above $q = m + 0.25(4m + n)r_{N/O}$ and $r_{N/O} = 79.01/20.99$

Figure 3. This shows that the rate at which heat is lost from the system increases with this temperature difference in a nonlinear way; this provides an example of the temperature difference as the "driving force" for heat transfer.

Kinetics of NO Formation • Using other electrochemical cells, the analyzer measures volume fractions of nitric oxide, carbon monoxide, and sulfur dioxide. In Figure 4, the levels of nitric oxide and carbon monoxide are shown as a function of the volumetric flow of natural gas; no sulfur dioxide was detected (detection limit ≤ 1 ppm). The level of nitric oxide increases steadily from 6 to 65 ppm with the flow of natural gas; in contrast the level of carbon monoxide starts off at about 17 ppm, decreases to zero and then increases again at the highest flow rate. It is interesting that nitric oxide is

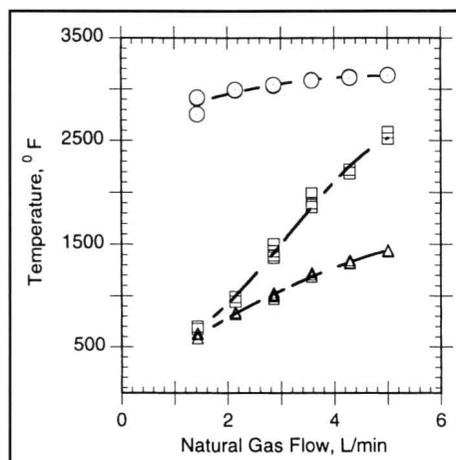


Figure 2. The measured temperature of the exiting flue gas (Δ) as a function of the volumetric flow of natural gas to the burner, measured under ambient conditions (25°C, 1 atm). The calculated adiabatic flame temperature (\square) and the estimated temperature under which nitric oxide is formed (\circ) are shown.

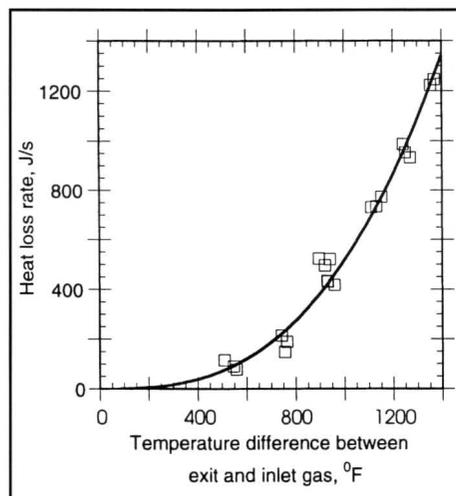


Figure 3. The heat loss rate from the flue as a function of the difference between the temperatures of the exiting and incoming gases.

produced in this experiment; this is a major concern in many industrial processes^[5,15] because of its potential for release into the atmosphere and its subsequent contribution to the formation of acid rain.

In contrast to the combustion of a hydrocarbon, the formation of nitric oxide from oxygen and nitrogen is endothermic.



Because of this, the formation of nitric oxide is only significant at elevated temperatures. It is instructive to use the known equilibrium and kinetic properties of the reaction to estimate the temperatures that must exist inside the flue. First, the rate of generation of NO within the flue is estimated; then a simplification of the known kinetics is used to estimate the reaction temperature.

The mole fractions of the reactants are about 10,000 times larger than the mole fraction of the product; that is, very little of the reactants is converted to product. So the flame within the flue may be treated as a differential reactor^[12,16] running at steady state as far as the formation of nitric oxide is concerned. Under these assumptions, the mole balance leads to

$$F_{\text{NO}} - F_{\text{NO},0} - r_{\text{ave}} V = 0 \quad (13)$$

where F_{NO} and $F_{\text{NO},0}$ are the molar flows of nitric oxide out and into the flue, respectively, and r_{ave} is the average rate of generation of nitric oxide within the reactor volume, V . It is reasonable to take $F_{\text{NO},0} = 0$, and so

$$r_{\text{ave}} = F_{\text{NO}} / V \quad (14)$$

The molar flow of nitric oxide out of the reactor is calculated from

$$F_{\text{NO}} = y_{\text{NO}} F_T^{\text{gas}} \quad (15)$$

where y_{NO} is the mole fraction of nitric oxide, the measurement provided by the analyzer, and F_T^{gas} is the total molar flow of gas out of the flue, given in Table 2. Strictly, the molar flow of nitric oxide should be included, but this flow is negligible in comparison to the combined flow of the other species. The effective volume of the reactor is unknown, but the internal volume of the flue available to the flame is about 1 L, and this is used as an approximation for V in the absence of any other information. The estimated rates of generation of nitric oxide are in the range of $0.6\text{--}3.0 \times 10^{-6} \text{ mol L}^{-1}\text{s}^{-1}$.

Now an expression for the rate of generation of nitric oxide in terms of the concentrations of the chemical species involved is required. Because of its importance in combustion, the mechanism has received much attention; it is widely believed that the reaction follows the Zeldovich mechanism.^[5,17] When this mechanism (under fuel-lean conditions) is applied to our data, it turns out that the forward reaction is

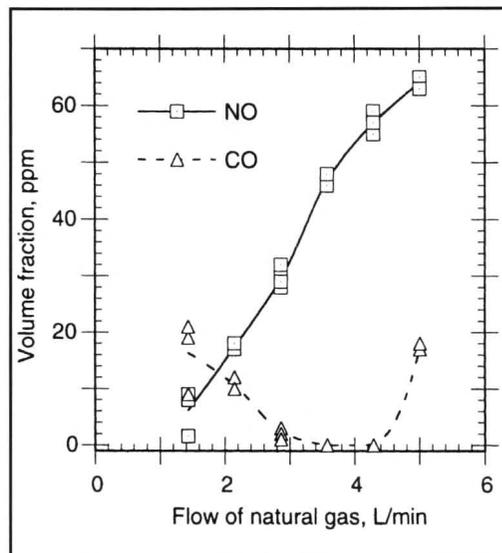


Figure 4. Mole fractions of nitric oxide and carbon monoxide measured in the exiting flue gas as a function of the volumetric flow of natural gas to the burner, measured under ambient conditions (25°C, 1 atm).

dominant; the low levels of nitric oxide seen here are far from equilibrium values, being approximately an order of magnitude smaller than equilibrium values. An abbreviated form of the mechanism that is sufficient to account for the data observed is described; it is also simpler for students, who are encountering mechanisms for the first time, to understand. This abbreviated mechanism is shown in Table 3.

From the slow steps, the rate of generation of nitric oxide in terms of the concentration of oxygen atoms and concentration of molecular nitrogen is obtained.

$$r = 2k_1[\text{O}][\text{N}_2] \quad (16)$$

This expression is obtained from the Zeldovich mechanism in the limit of small concentrations of nitric oxide. To evaluate this, the concentration of oxygen atoms in terms of measured quantities is needed. This is a useful exercise in thermodynamics.

$$[\text{O}] = [\text{O}_2]^{1/2} \left(\frac{P_0}{RT} \right)^{1/2} K_{\text{eq}}(T) \quad (17)$$

where P_0 is the standard pressure of 1 bar. Taking the enthalpy for the dissociation of molecular oxygen to be independent of temperature, the van't Hoff equation gives

$$K_{\text{eq}}(T) = K_{\text{eq}}(T_0) \exp \left[\frac{\Delta H^0}{R} \left(\frac{1}{T_0} - \frac{1}{T} \right) \right] \quad (18)$$

where $K_{\text{eq}}(T_0) = \exp[-\Delta G^0/RT_0]$ and $T_0 = 298 \text{ K}$. Finally, the gas concentrations in terms of the quantities measured by the analyzer are required.

$$[\text{O}_2] = \frac{y_{\text{O}_2} P}{RT} \quad [\text{N}_2] = \frac{y_{\text{N}_2} P}{RT} \quad (19)$$

Here, P is the pressure of the reaction, taken to be 1 atm. Table 2, Eq. T2, contains the expression for the mole fraction of nitrogen, y_{N_2} .

The mole fractions in Eq. (19) should strictly be those calculated on the basis of the gaseous-product stoichiometry, as these are the conditions under which the reaction occurs. Most data were obtained under conditions of excess air for which $x < x_{\text{crit}}$. So, in principle, the measured mole fractions should be corrected to give the corresponding values on the gaseous-product basis.

$$y_i = y_i(\text{measured for } x < x_{\text{crit}}) \left(\frac{F_T^{\text{wet}}}{F_T^{\text{gas}}} \right) \quad i = \text{NO, O}_2, \text{ or N}_2 \quad (20)$$

The smallest value of the correction factor is about 0.9; in view of the severe assumption adopted here regarding the reaction volume, the correction is hardly justified.

The reaction temperature is obtained by solving

$$r = r_{\text{ave}} \quad \text{or} \quad r / r_{\text{ave}} = 1 \quad (21)$$

where r and r_{ave} are defined in Eqs. (16) and (14), respectively. This equation was solved using "Goal Seek" within an Excel Spreadsheet. If values of the kinetic parameters typically found in the combustion literature^[15,17-19] are used, then the abbreviated mechanism leads to the same results as the full Zeldovich mechanism. But the enthalpy and Gibbs Free energy data were taken from a source to which the student is more likely to have ready access,^[20] the temperatures are about 100°F higher with these data, and these

higher temperatures are those shown in Figure 2.

DISCUSSION

The calibration of the rotameter for the flow of natural gas is useful because it leads the student to an understanding of its principle of operation. The same result can be obtained by asking the student to transform the rotameter's scale from L air/min to L methane/min. The household gas meter used for calibration is a quantity meter; it measures the net volume of gas that passes through it using a displacement method,^[6] so its calibration does not depend on the type of gas. To show this, the gas meter was calibrated using the laboratory supply of compressed air, giving

$$V_{\text{air}}(\text{gas meter, ft}^3 / \text{min}) = (28.3 \pm 0.6) V_{\text{air}}(\text{rotameter, L / min})$$

$$r^2 = 0.91 \quad (22)$$

The somewhat low value of the correlation coefficient is attributed to a dirty air supply and the age of the gas meter! But the calibration compares favorably with the conversion, 1 ft³ \equiv 28.32 L. In contrast, the calibration of the rotameter depends on the density of the gas. By direct calibration of our rotameter, the density of our natural gas was obtained. If the composition of natural gas is known (*e.g.*, by gas chromatography), then the student could be asked to reconcile measured density with the measured composition.

The complete combustion of a hydrocarbon leads to three different ways of expressing the stoichiometry; this may seem strange to the student. This feature arises because of the ways by which the combustion products are analyzed. The traditional Orsat method, providing volume fractions on a dry basis, is specific for O₂, CO₂, and other gases (*e.g.*, CO and H₂). In contrast, our gas analyzer, providing volume fractions on a wet or gaseous-product basis depending on the amount of excess air, is specific for O₂, NO, and SO₂; for the levels of CO₂, the analyzer requires knowledge of the fuel's chemical composition. In environmental applications, it is important to be aware of this feature when attempting to measure levels of CO₂ in situations where the fuel may be inhomogeneous, as in a waste incinerator.

The three bases upon which the stoichiometry is described do not lead to mole fractions that differ by very much in the application considered here. To the practicing engineer, the attention to detail may seem unduly fussy, but it is desirable to train students to formulate a sound theoretical framework from which they can make good practical assumptions and judgments. This is an example of such a process. For whichever basis is appropriate, the mass balance is closed for the primary combustion reaction, assuming it goes to completion. An additional exercise for the student is the explanation of how the molar flow of air

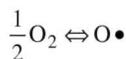
TABLE 3

Mechanism for the Formation of NO from O₂ and N₂ in the Initial Stages Under Fuel-Lean Conditions

Step 1	$\text{O}_2 \leftrightarrow \text{O} \bullet + \bullet \text{O}$	Rapid equilibrium with equilibrium constant K_{eq}
Step 2a	$\text{O} \bullet + \text{N}_2 \xrightarrow{k_1} \text{N} \bullet + \text{NO}$	Slow step
Step 2b	$\text{O} \bullet + \text{N}_2 \xrightarrow{k_1} \text{N} \bullet + \text{NO}$	Slow step repeated to preserve stoichiometry
Step 3	$\text{N} \bullet + \bullet \text{N} \rightarrow \text{N}_2$	Fast step

Net reaction $\text{O}_2 + \text{N}_2 \rightarrow 2 \text{NO}$

Data (from ref. 17) for



$\Delta H^0 = +249.17 \text{ kJ / mol}$ Enthalpy of formation at 298K

$\Delta G^0 = +231.73 \text{ kJ / mol}$ Gibbs free energy of formation at 298K

Step 2 $k_1 = A \exp(-E_a / RT)$ $A = 1 \times 10^{11} \text{ L mol}^{-1} \text{ s}^{-1}$
 $E_a = 315 \text{ kJ/mol}$

into flue varies with the flow of natural gas.

The various temperature data presented here will help the student form a simple picture of a flame, a complicated reacting system.^[5] The first observation is that the model to explain the formation of NO leads to temperatures larger than the adiabatic flame temperature, the maximum possible flame temperature, and the measured exit gas temperature. A flame is far from being a homogeneous reaction mixture, either in its temperature distribution or species distribution. The primary reaction, the combustion of a hydrocarbon here, occurs in a zone defined by mixing the fuel and air and their subsequent reaction; this is the so-called combustion zone. Because the combustion is highly exothermic, the heat generated raises the temperature of unreacted gases, such as excess O₂ and N₂, to such a level that they start to react in a zone, the post-combustion zone that is spatially distinct from the combustion zone. Also, it is interesting to note that the NO-formation and adiabatic-flame temperatures appear to converge upon extrapolation to higher natural gas-flow rates where the fuel-air mixture becomes stoichiometric. This suggests that NO is formed in zones within which the local fuel-air mixtures are stoichiometric. So, qualitatively, the first observation can be explained on the basis of reaction zones with non-uniform temperatures and composition.

A second observation supports the idea of non-uniform temperature distribution. After running the experiment at the highest exit temperature (about 1450°F), it was noticed that the burner's nozzle had become partially coated with zinc. This means that the inside wall of the flue must have reached a temperature of 787°F, the melting point of zinc. This is much lower than the NO reaction temperature. The use of a stainless steel flue, or even better a quartz tube, so the structure of the flame can be observed, would be a worthwhile improvement. It would also be safer.

The discrepancy between the adiabatic flame temperature and the exiting gas temperature may seem large. The flue cap used is designed to allow for air infiltration through perforations fabricated in its walls just as the gas leaves the main part of the flue. The astute student will notice this and realize that it will lead to errors in the gas compositions and temperatures; they will be lower than they should be. The cap is designed to ensure a temperature reduction in the gas just before it enters the surroundings. No attempt was made to modify this, or rather to change the position of the probe, because the maximum operating temperature of the probe is 1550°F for continuous service and 2200°F for short-term use. Such imperfections in laboratory experiments, in our opinion, are not a bad thing; they often help students exercise their critical faculties.

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