

Michael L. Shuler

... of Cornell University



DOW AWARD LECTURE

Membrane Science and Technology
in the 21st Century

(p. 94)

William B. Krantz

Feature Articles ...

- Agitation and Aeration: An Automated Didactic Experiment (p. 100) *Badino, Almeida, Cruz*
Experiments and Other Learning Activities Using Natural Dye Materials (p. 132) *Burrows*
Integrating Biology and ChE at the Lower Levels (p. 108) *Hollar, Farrell, Hecht, Mosto*
Nonideal Reactors in a Junior-Level Course (p. 136) *Lawrence, Beene, Madihally, Lewis*
Random Thoughts: We Hold These Truths To Be Self-Evident (p. 114) *Felder*
Improving Coherence in Technical Writing (p. 116) *Suraishkumar*
Computer Evaluation of Exchange Factors in Thermal Radiation (126) *Henda*
Use of Dynamic Simulation to Converge Complex Process Flowsheets (p. 142) *Luyben*
Using Small Blocks of Time for Active Learning and Critical Thinking (p. 150) *Lombardo*
Teaching Nonideal Reactors with CFD Tools (p. 154) *Madeira, Alves, Rodrigues*
A Simple Open-Ended Vapor Diffusion Experiment (p. 122) *Whitmire, Blaylock*

and ChE at ...

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► EDUCATOR

82 Michael L. Shuler of Cornell University, *Claude Cohen*

► UNIVERSITY

88 Rice University, *Kyriacos Zygourakis*

► DOW AWARD LECTURE

94 Membrane Science and Technology in the 21st Century,
William B. Krantz

► LABORATORY

100 Agitation and Aeration: An Automated Didactic Experiment,
Alberto C. Badino, Jr., Paulo I.F. De Almeida, Antonio J.G. Cruz

132 Experiments and Other Learning Activities Using Natural Dye Materials,
Veronica A. Burrows

► CURRICULUM

108 Integrating Biology and ChE at the Lower Levels,
*Kathryn A. Hollar, Stephanie H. Farrell, Gregory B. Hecht,
 Patricia Mosto*

136 Incorporating Nonideal Reactors in a Junior-Level Course Using
 Computational Fluid Dynamics (CFD),
*Benjamin J. Lawrence, Jason D. Beene, Sundararajan V. Madihally,
 Randy S. Lewis*

► RANDOM THOUGHTS

114 We Hold These Truths To Be Self-Evident, *Richard M. Felder*

► CLASSROOM

116 Improving Coherence in Technical Writing, *G.K. Suraishkumar*

126 Computer Evaluation of Exchange Factors in Thermal Radiation,
Redhouane Henda

142 Use of Dynamic Simulation to Converge Complex Process Flowsheets,
William L. Luyben

150 Using Small Blocks of Time for Active Learning and Critical Thinking,
Stephen J. Lombardo

154 Teaching Nonideal Reactors with CFD Tools,
Luis M. Madeira, Manuel A. Alves, Alírio E. Rodrigues

► CLASS AND HOME PROBLEMS

122 A Simple Open-Ended Vapor Diffusion Experiment,
David Whitmire, Wayne Blaylock

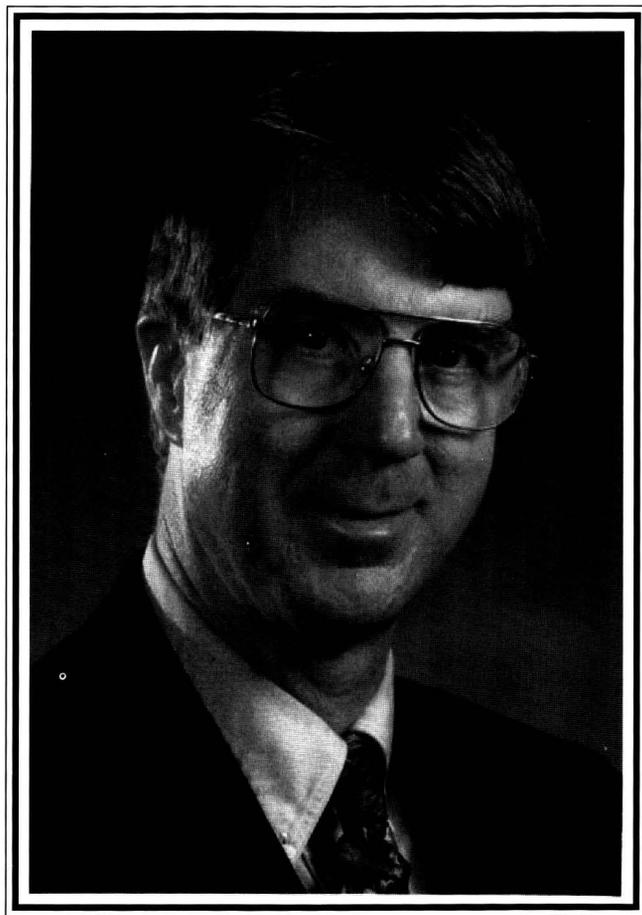
113 Call for Papers

121 Teaching Tips

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Michael L. Shuler

of Cornell University



CLAUDE COHEN

Cornell University • Ithaca, NY 14853

The School of Chemical (now Chemical and Biomolecular) Engineering at Cornell University is proud to have Michael L. Shuler, a true educator and a visionary, among its faculty members. Mike is a great example of what it means to be an educator. He is imaginative, creative, and prolific; most importantly, he is sincerely interested in the advancement of the field. He has a genuine curiosity and enthusiasm in guiding his students to become independent researchers, and he gives them the freedom to explore new research directions.

BACKGROUND AND EDUCATION

Michael L. Shuler grew up in Joliet, Illinois, where as an 8th grader he had already decided to pursue biochemical engineering. All students were required to write a description of the career they wanted to pursue. Mike chose chemical engineering and wrote specifically about building processes to make antibiotics. He felt that making a life-saving drug in large enough quantities to really help people was a noble and ennobling enterprise. It combined his interests in science, society, and service.

Mike's choice of career path was a natural one given his family situation. His father Louis put himself through college (Bradley University) during the depression, majoring in chemistry, and began his worklife at the Army Ammunition Plant in Joliet before joining the Army Air Force in World War II. He spent his Army career as a civilian employee working as an industrial engineer, ultimately coordinating a production schedule of 700 different chemical plants. At the end of the war, Louis married Mary Boylan, who taught English to seventh graders in West Des Moines, Iowa. Not surprisingly, both Mike and his younger brother, Patrick, ended up being chemical engineers. Pat worked for Chevron prior to becoming manager of Oil Field Chemistry and Production Chemicals in the Petroleum Energy and Environmental Center administered by Caltech.

Growing up as a Roman Catholic, Mike's religious beliefs have always been an important part of his life and have greatly influenced his thoughts on service. He always had an interest in teaching, and while at the University of Notre Dame he became committed to the idea of teaching at the university level. Kramer Luks and Nick Sylvester were new, young faculty members there and they both strongly encouraged him to pursue graduate studies at the University of Minnesota.

When Mike graduated from Notre Dame in 1969, the Vietnam War was at its peak; Mike had participated in ROTC both in high school and at Notre Dame and graduated as a second lieutenant in the U.S. Army. He was able to obtain an educational delay to go to graduate school. At that time the only other male U.S. students who would enter graduate

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Mike with Cornell faculty members at the 2002 annual AIChE meeting in Indianapolis, pictured at the NCAA Hall of Champions where Cornell's reception was held. Front row: Fernando Escobedo, Paulette Clancy. Back row: Matt DeLisa, Kelvin Lee, David Putnam, Bill Olbricht, Mike Shuler, Yong Joo, and Abe Stroock.

school had either failed the Army's physical exam, were veterans, or had joined the U.S. National Guard or Reserves and had completed six months of training. While Mike had no interest in the Army as a career, he felt that the experience was useful in developing leadership and teaching skills (the only formal instruction he ever received in pedagogy).

At the University of Minnesota he decided to work with Professors Rutherford "Gus" Aris and Henry Tsuchiya. Gus was a theoretician with exceptional mathematical skills and Henry was a bacteriologist. Mike soon realized that he knew more math than Henry and more biology than Gus, and that part of his role was to help bridge the interdisciplinary divide. This experience prepared Mike well for conducting and leading interdisciplinary research teams as he advanced along his career path. Mike also completed a minor (supporting program of courses) in mathematics, biochemistry, and microbiology and was only one course short of fulfilling the requirements for a Masters of Science in microbiology. A strong, formal background in biology was unusual for a chemical engineering student of that day and time and it provided Mike with an advantage that proved to be important to his early academic success.

When the time came to interview for an academic job, Neal Amundson, head of Minnesota's Chemical Engineering Department, took a great deal of interest in helping Mike (along with Gus and Henry). His perspective and insight were crucial; Amundson thought that chemical engineering at Cornell had great potential and that the faculty there would welcome someone with Mike's talents. The department at Cornell at that time was in transition from a department with a focus on undergraduate education to one that was developing a top-rated research department.

Mike's selection of Cornell was based not only on the advice of the faculty at Minnesota, but also on the supportive environment he found when he visited there. In particular, he found that Bob Finn (a founding father of biochemical engineering) had a well-established laboratory with the entire infrastructure necessary for biochemical engineering. During those days, academic offers did not include start-up packages and none of Mike's three academics offers had included any money for equipment or supplies.

*Mike
is a great
example
of what it
means
to be an
educator.
He is
imaginative,
creative,
and
prolific;
most
importantly,
he is
sincerely
interested
in the
advancement
of the
field.*

Even more important, Bob was by nature a very generous person and was a natural mentor for Mike. When I interviewed at Cornell three years later, I remember visiting with Bob and Mike in Bob's office. Mike remained rather quiet during my visit, and his boyish looks (he is a few years younger than I) led me to the mistaken conclusion that he was one of Bob's students—Julian Smith corrected my erroneous impression later in the day.

When Mike arrived at Cornell, Jim Stevenson and John Anderson were young assistant professors, and their presence and active support helped make Cornell an attractive and stimulating place. Mike was also happy to have the able administrative assistance of Bonnie Sisco right from the beginning.

LEADERSHIP IN BIOCHEMICAL ENGINEERING

Mike has been a leader in biochemical engineering since joining Cornell thirty years ago and he continues in that role today. His work has had an extraordinary influence on academic research, on teaching and curriculum development, and on the industrial development of biotechnology.

Early on, Mike undertook the ambitious and challenging work of building comprehensive mathematical models for the kinetics of metabolic and synthetic pathways in single cells. He and his students integrated a large amount of information from microbiology and cell biology into a theoretical and computational framework to predict cell growth and how the formation of products depends on bioreactor variables. His paper with Mike Domach on single-cell mathematical models for the bacterium, *Escherichia coli*, published in 1984, was recognized as one of the twenty most influential papers published in *Biotechnology and Bioengineering* in the 40th anniversary issue of that journal. Over the years, Mike has been a leader in developing quantitative, numerical models of cellular functions and applying those models to the design and scale-up of biochemical processes. The computer models have been used successfully in identifying conditions that enhance production of desirable compounds while minimizing formation of undesirable byproducts. Gene Network Sciences (Ithaca, NY) uses Cornell's single-cell model as the base for



Research Group – The Shuler research group at a 2003 holiday party in the Shuler home. Each year Karen and Mike host a party for his research group.

bacterial models. The company is developing these models to find and evaluate new antimicrobial drugs.

The area of plant cell culture for the production of bio-chemicals was pioneered in the U. S. by Mike. His group was the first to explicitly demonstrate that the response of cell cultures containing cell aggregates depends on the interplay between mass transfer and chemical reactions in the culture. By combining immobilization, medium optimization,

and *in situ* product extraction, the group was able to obtain significant extracellular production of ajmalicine, a compound previously thought to be constrained to the intracellular compartment. This work opened the door for others to produce a variety of compounds.

The best example of how Mike strives to convert new discoveries into large-scale production of compounds that will benefit people and society is the story of Phyton, Inc., a company founded by two of Mike's former PhD students, Bobby Bringi and Chris Prince. Mike headed an industrial and academic collaboration aimed at understanding the factors that would allow the effective production of the important anti-cancer compound Taxol using plant cell culture techniques. Phyton, Inc., was one of two industrial collaborators. At Phyton, Bobby and Chris applied the principles developed in their theses and described in a joint monograph with Mike, *Plant Cell Tissue Culture in Liquid Systems*,¹¹ to the successful, large-scale commercial production of Taxol from *Taxus sp.* The company has grown in ten years from three to approximately a hundred employees and boasts the world's largest dedicated plant-cell-culture facility with bioreactors of up to 75,000 liters in capacity. Mike's ten-year service on Phyton's Board of Directors has been an important factor in the company's growth. The company has recently been acquired by DFP Pharmaceuticals, Inc.

A major issue in bioprocess engineering has been the production of proteins, particularly therapeutic proteins, using recombinant DNA technology. Mike's group has worked extensively on a variety of host cells to make various proteins: bacterial, yeast, insect, plant, and mammalian. Mike's breadth of experience with this wide-range of host cells is unique. This work not only has increased our fundamental understand-

ing of protein expression, but it has also led to new approaches that enhance productivity and product quality. Working with Al Wood and Bob Granados of Boyce Thompson Institute, Mike developed an insect cell line that is widely used and sold commercially by Invitrogen as the “High Five” cell line. Working with Dave Wilson, Mike demonstrated the possibility of producing large amounts of a desired protein that could unexpectedly be released by the commonly used bacterium, *Escherichia coli*, into the extracellular medium where recovery or purification is relatively inexpensive.

In another area of innovative research, Mike has proposed cell culture analog (or CCA) models that combine detailed cellular/molecular models with traditional physiology-based pharmacokinetic models (PBPK) to guide the construction of a physical analog of the PBPK. The physical analogs can act as human or animal surrogates for estimating the response of an organism to challenges by pharmaceuticals or potentially toxic chemicals. Mike’s group is currently constructing microscale devices with four compartments: “liver-lung-fat-other tissue” and other microscale models of the blood-brain-barrier and of the gastrointestinal tract. The expectation is that these devices will facilitate evaluation of new drugs prior to animal studies and/or human clinical trials. HmREL™, a company cofounded by Greg Baxter (who collaborated with Mike’s group), has licensed patents developed in Mike’s group to commercialize these concepts.

Mike’s research work has been well recognized by numerous awards: the Marvin J. Johnson Award of the Microbial and Biochemical Technology Division of the ACS in 1986; the AIChE Food, Pharmaceutical, & Bioengineering Division Award in 1989; the AIChE Professional Progress Award in 1991; the Amgen Award in Biochemical Engineering in 1997; and the Warren K. Lewis Award in 2003. Besides being elected fellow of the AIChE in 1997, Mike has been honored by election to the National Academy of Engineering in 1989 and to the American Academy of Arts and Sciences in 1996.

Mike has had a lasting educational influence in the field of biochemical engineering. His textbook, *Bioprocess Engineering: Basic Concepts* (with F. Kargi, a former student), has been extremely successful, by any measure, and is now the textbook-of-choice for a course in biochemical or bioprocess engineering. The second edition of the book was published in 2002.^[2] Mike is also very keen on integrating research into undergraduate courses or laboratories^[3,4] and strongly encourages his graduate students to work with undergraduate students on their research.

Mike has been actively involved with the AIChE since his

student days. He was chair of the Food Pharmaceutical and Bioengineering Division in 1994. He has been a member of the publications committee for about 15 years and was founding editor for *Biotechnology Progress*. In addition to serving on numerous AIChE committees and task forces, Mike was a member of the Board of Directors for the last three years (2000-2003). As many readers are aware, the last three years have been a tumultuous period for AIChE, making board membership a very intense experience. The evolution of AIChE in the last three years has been remarkable, and Mike hopes that his work as part of a large team effort will serve the profession well.

Mike is currently serving on a Formation Committee for a new “Society for Biological Engineering” (announced at the November, 2003, AIChE meeting). It is being formed through AIChE but will seek partner organizations. The expectation is that AIChE’s leadership in establishing SBE will result in a clearer understanding of chemical engineering contributions to biotechnology and bioengineering and better link the profession to new opportunities at the interface of biology and engineering.

ROLE IN THE DEPARTMENT AND THE COLLEGE

To be a successful teacher, one should have an excellent command of the subject matter, an ability to inspire students to high achievement, and generosity with one’s time—Mike possesses all these qualities. His success as a teacher has been recognized by several teaching and advising awards at Cornell. He was awarded the prestigious College of Engineering’s Tau Beta Pi Award early in his career, an award given to the best teacher in the college (of 200 faculty members). More recently (1996), he received the Richard F. Tucker award for outstanding teaching from the college, and this past year he received the James M. and Marsha D. McCormick award from the college in recognition of his sustained contributions to freshmen academic advising.

Mike has also been an extraordinarily effective mentor of students at the graduate education level. According to many of his former students (see Table 1), most of whom have gone on to successful careers in academia and in industry, he has always been approachable, kind, and encouraging. Under his guidance, students are given the freedom to take their research in new directions and to act as research mentors to undergraduate students—both of these opportunities have prepared many for academic positions.

Mike served as director of the School of Chemical and Biomolecular Engineering from 1998 to 2002. He demonstrated excellent leadership throughout his tenure, as reflected

His work [in biochemical engineering] has had an extraordinary influence on academic research, on teaching and curriculum development, and on the industrial development of biotechnology.

by curriculum development and resolution of difficult personnel issues during that time. He was successful in encouraging faculty to develop focal areas of research and instruction, and he constantly strived to keep the morale of the faculty, staff, and students high.

Mike was also successful in the hiring, development, and retention of faculty during his tenure as director. He played a valuable role in supporting young faculty (Kelvin Lee and Fernando Escobedo) and in hiring new faculty (Lynden Archer, Yong Joo, David Putnam, Abraham Stroock, and Matthew DeLisa). Besides serving as acting director for one year in 1986 and for one semester in 1993, Mike repeatedly resisted serving as director of the school on a more continuous basis before 1998. Having served as director of the school from 1990 to 1993, I understood his earlier reluctance, but applauded his eventual decision to accept the position when he considered that the time was right to take on the challenge. He subsequently earned the admiration of his colleagues and students for his ability to successfully juggle his large research group, the administration of the department, and his family obligations.

In 1993, the Dean of Engineering asked Mike to head a college-wide committee to develop a plan for intensifying the college's investment in bioengineering. The charge and vision have evolved over the last decade, but Mike has always played a leadership role. He led the development of a new bioengineering curriculum—a long-standing college goal. At the undergraduate level, the new curriculum comprises several series of courses that have been tailored to accommodate students from any engineering major. Students who complete the bioengineering option receive recognition on their transcripts. Early on, Mike recognized the importance of advising, and he developed a system where each student participating in this option is assigned a bioengineering faculty who oversees that part of the student's curriculum. Thus, the students not only receive formal recognition for completing the option but they also obtain sound advice on planning a career in bioengineering. Mike was also instrumental in designing a new Bioengineering Seminar for juniors and seniors that gives students from different engineering disciplines a venue for interaction. The seminar provides students from different engineering disciplines with a venue for interactions and illustrates the inter-

TABLE 1
Mike's PhD Students

David W. Mitchell
Dennis J. Kubek
Fikret Kargi
Michael M. Domach
Om P. Sahai
G. Anders Hallaby
Mohammad Ataai
Sooyoung S. Lee
George Georgiou
Toohyon Cho
Ke Ming Hsieh
Jeffrey Chalmers
Jen Shu
Byung Gee Kim
Lisa A. Laffend
David E. Steinmeyer
Jeffrey Fu
A. Paul Togna
Christopher L. Prince
V. "Bobby" Bringi
Thomas J. Wickham
Peng "Paul" Wu
Olotu W. Ogonah
Lisa M. Sweeney
Naheed "Nina" Mufti
Ronald A. Taticek
Carolyn M. Acheson
Carolyn W-T Lee
Yousuf M. Al-Roumi
Kennie U. Dee
Michael S. Donaldson
Amyl Ghanem
Susan C. Roberts
Ik-Sung Ahn
Patricia Kuo Haller*
Brian A. Wright
Melissa J. Mahoney*
Kathryn Hollar
Mark L. Smith
Aaron Sin
Christoph E. Joosten
Chien-Kuo Wang
Itzcoatl A. Pla
Kwan Viravaidya

**Primary thesis work done in the laboratory of W. Mark Saltzman*

disciplinary nature of the bioengineering field.

The college and university have asked Mike to play important roles in leading university-wide efforts in developing bioengineering and the role of engineering in the university's "New Life Sciences Initiative." Currently Mike is director of the Biomedical Engineering Program (BMEP). The BMEP is responsible for an undergraduate minor in BME available to all engineering students. The BMEP is also the home for an interdisciplinary graduate field in BME. This field draws upon approximately 30 faculty members from 12 different departments including seven faculty from Cornell's Weill Medical College in New York City. Four of the Chemical and Biomolecular Engineering faculty currently belong to the BME field and two new faculty are in the process of election—with six faculty as members, Chemical and Biomolecular Engineering will have the greatest concentration on BME. Such a complicated program is an administrative challenge, but one that is being well met by Mike and his colleagues.

FAMILY AND AVOCATION

While at the University of Minnesota, Mike met Karen Beck, a physical therapy student from Springfield, Minnesota. They married in June of 1972. Mike considers this decision to be the best and most important one he has ever made. During the final year of Mike's PhD thesis, Karen worked at a local hospital, and after defending his PhD thesis in September of 1973, the two of them headed to Aberdeen Proving Grounds in Maryland. There, Mike spent three months in the Army at the Ordinance Officers Basic School (where he graduated at the top of his class).

Mike and Karen then migrated to Ithaca, arriving on January 17, 1974. In those days, wives were not invited to visit during the recruitment process, so Karen had not had the opportunity to see Ithaca before Mike accepted the Cornell offer. They both fell in love with the hills, lakes, woods, and the small city of Ithaca, however. While that area of the country is often considered extremely cold, Karen and Mike had left Minnesota when it was 25 below—so when they arrived in Ithaca and heard a radio announcer say "12 degrees Fahrenheit and bitterly cold," they knew they would be right at home with the weather there.

Mike and Karen have four children (Andy, Kristin, Eric, and Kathy) and one very new grand-

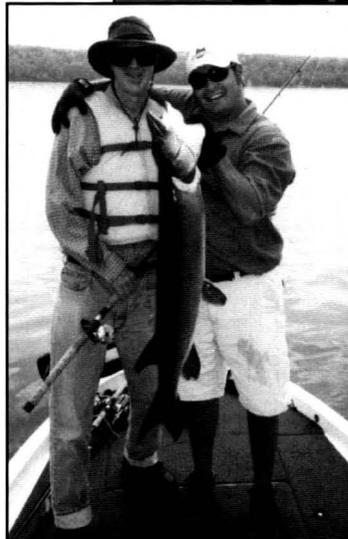


◀ *Mike and Karen relax in front of a quilt made by Karen.*

The Shuler family in Arizona's White Mountains in 2001. Left to right: (first row): Harrey (Andy's wife), Kathy, and Kristin; (second row): Eric, Mike, Louis (Mike's Dad), Andy, and Karen. ▼



Mike (with guide, Mike Williams) and a 45-inch muskie caught on the Kawartha Lakes in Canada. The fish was released. ▼



child (Jeremy). Andy graduated from Cornell in Mechanical and Aerospace Engineering and is currently a PhD student in Aerospace Engineering at the University of Texas, Austin. Andy married a fellow PhD student (Harrey Jeong) from Korea in 2001 and Jeremy was born last December. Having a grandchild is a newfound source of great joy for both Mike and Karen.

Kristin, who has Down syndrome and lives at home with Mike and Karen, works at Cornell in two part-time office jobs. Both Mike and Karen have been active in various community groups supporting developmentally delayed persons.

Eric, who graduated from Cornell with a BA in Religious Studies and History has begun PhD studies in Medieval Studies at the University of Notre Dame. He completed a year of service with Francis Corps between his BS studies and PhD program. Mike is pleased to have one of his children decide to attend his *alma mater*.

The youngest child, Kathy, was adopted from Korea. Kathy arrived in Ithaca when she was only 4 months old. Mike and his family are strongly connected to Korea, both through his family members and through the Korean alumni of the Shuler group. Kathy, a senior in high school, has decided to attend the University of Dayton, where she intends to study psychology with a minor in biology and to focus on animal behavior (especially marine mammals). She is active in dance and the retreat program of the Diocese of Rochester and expects to continue similar activities in college.

Mike's family has always been a source of strength and comfort to him. As is true with any faculty member, his big-

gest challenge has been to balance professional and family activities through the years, and since family and professional obligations are dynamic, the balance has had to be continuously reconfigured.

Mike loves the outdoors in general and fishing in particular. He has successfully passed this interest on to his children. While he enjoys all types of fishing, he particularly likes the challenge of muskie fishing, with fly fishing for trout or smallmouth bass running a close second. Mike got his biggest muskie in Canada last year while fishing with his son Eric and a guide—the fish was just shy of 45 inches.

Mike's advice is that everyone should have a second favorite job as a "fall back" position in case they get discouraged with what they are doing. For Mike, his fantasy job is to be a guide for people who enjoy fishing as a hobby. For now, however, teaching at Cornell is still his "dream" job come true.

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ChE at . . .

Rice University

**KYRIACOS ZYGOURAKIS***Rice University • Houston, TX 77251-1892*

When Rice Institute opened its doors to its first class of students on September 23, 1912, a bachelor's in chemical engineering was among the degrees offered, and in 1916, three chemical engineering graduates (James L. Bramlette, William M. Standish, and Herbert W. Wilber) received their bachelor's diplomas from President Lovett. They were the first in a long line of Rice chemical engineering graduates who went on to have successful professional careers.

The arrival on campus of Arthur J. Hartsook in 1921 marked the true beginning of an independent program in chemical engineering at Rice. Hartsook was educated at MIT and his choice of Rice and Houston was not an accident. At MIT he had gathered information that convinced him that the city and its vicinity would, in time, grow into one of the foremost chemical engineering centers in the country and the world. By the 1940s, Houston had become the petrochemical and energy capital of the world, and Rice graduates began to fill many of the positions created by the growing industrial establishment along the Houston ship channel. For many of these graduates, Houston's ship channel became the launching pad for important leadership positions, first in corporate headquarters in New York or other major U.S. industrial cen-

ters and, subsequently, to key posts all over the world.

The 1950s and 1960s were years of almost exponential growth, and in 1955, the department became a major player in the emerging field of nuclear energy, securing a grant from the Atomic Energy Commission to develop a program in nuclear engineering, supported by a radiation laboratory and a 10-watt operating reactor. Chemical engineering also "annexed" a sanitation laboratory program in civil engineering and began to address the broader problems of environmental pollution.

In the 1960s, the department was ranked among the top seven in the country. Capitalizing on Rice's location, a strong thermodynamics group led by Tom Leland and Riki Kobayashi developed new theories and an extensive database of thermophysical properties for the petrochemical industry. Chemical engineering purchased the first digital computer ever installed at Rice (an LGP-30) and later acquired Rice's first solid-state programmable computer (an IBM 1620) that could be programmed with a (then) new language called FORTRAN.

Perhaps the most significant example of a bold move into new areas, however, was an artificial heart project and estab-

lishment of a Biomedical Engineering Laboratory in the mid '60s. In partnership with Baylor's Department of Surgery, Rice chemical engineers (led by Bill Akers) were instrumental in developing the first left ventricular heart bypass device and carried out a large number of pioneering studies that solidified Rice's national reputation in the field of biomedical engineering. Among their early successes was development of an implantable artificial lens for the eye that restored sight to hundreds of patients. During the late 70s and 80s, however, the Biomedical Engineering lab shifted its research efforts away from medical devices to become one of the strongest centers of applied cellular engineering research.

The 80s and early 90s witnessed continued growth. Many new faculty joined the department to strengthen the areas of thermodynamics (Chapman, Robert), interfacial phenomena and petroleum engineering (Miller, Hirasaki), reaction engineering and applied math (Zygourakis), process control (Badgwell), biochemical engineering (Papoutsakis, San, Shanks) and biomedical engineering (Glacken, Mikos). New laboratories were built in 1982 to house the expanding research programs in bioengineering, catalysis, reaction engineering, and thermodynamics. In 1992, the chemical engineering faculty forming the core of Rice's bioengineering group (Hellums, McIntire, Mikos, San, Shanks, and Zygourakis) moved their offices and laboratories to a new research facility (George R. Brown Hall), especially built to promote interdisciplinary research between biologists and engineers.

Like the chemical engineering profession, the department

reached a major crossroad as it prepared to enter the 21st century. Faculty retirements and the move in 1997 of four faculty members to a new bioengineering department forced the department to redefine its research and educational missions.

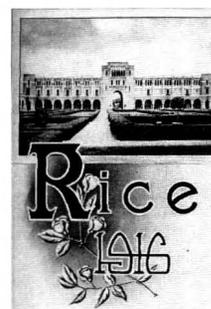
CHARTING NEW DIRECTIONS: FROM MOLECULES TO SYSTEMS

The mission of the department is shaped by the same forces that are redefining the chemical engineering profession. On one hand, revolutionary advances in nanoscale science and molecular biology open exciting new avenues for developing new materials, biological products, and medical therapeutics. At the same time, economic and social forces are driving a transition toward more sustainable and environmentally friendly production methods. Chemical engineers are uniquely qualified to play leading roles in these revolutions. For more than a century, we have been very successful in developing and refining the tools necessary for translating molecular-level discoveries into new and cost-effective products. To meet the challenges of the new century, however, we must integrate molecular biology and nanoscale science into the scientific foundation of our discipline. Such an expanded knowledge base will enable us to engineer new products by scaling up processes from the molecular to the system level.

These challenges and needs form the foundation of the strategic plan formulated in 1998 to guide the future growth of the department. The plan provided a blueprint for research directions, faculty and graduate student recruitment, curriculum development, and facility renovation. At its heart was a dual research and education mission that called for

Capsule History of the Department

- 1912** Rice Institute opens the doors to its first class of students.
- 1916** The first three chemical engineering degrees are awarded.
- 1921** A.J. Hartsook is hired as instructor of industrial chemistry.
- 1927** Hartsook is promoted to Assistant Professor of Chemical Engineering and assumes the leadership of chemical engineering, a post he holds until 1956.
- 1928** Anna Rebecca Lay becomes Rice's first woman graduate in chemical engineering.
- 1938** Chemical engineering ceases to be a part of the department of chemistry and becomes one of the four Rice engineering departments.
- 1941** Rice Chemical Engineering becomes the first chemical engineering department in Texas accredited by ECPD (the precursor of ABET).
- 1941** The first MS degrees in chemical engineering are granted to Sam Bethea (thesis title, "Studies on Decolorizing Clays") and Ervon Eggimann (thesis title, "Performance of an Adiabatic Fractionating Column").
- 1947** The Chemical Engineering Department receives a mandate from Rice President Houston to start a full-scale graduate program.
- 1955** Orrin K. Crosser is awarded the first PhD in chemical engineering (thesis title, "Condensing Heat Transfer Within Horizontal Tubes").
- 1965** The Biomedical Engineering Laboratory is established with the help of a large federal grant. Under the leadership of Bill Akers, this laboratory develops the first successful left ventricular heart bypass in cooperation with the Department of Surgery at Baylor; Bill Akers holds a left ventricular bypass device that was implanted in 10 patients in the late 60s.
- 1967** Fritz Horn and other chemical engineering faculty are instrumental in the formation of the Mathematical Sciences (applied math) department and Horn becomes acting chair of the new department.
- 1968** The Department of Environmental Science & Engineering is created, with chemical engineering faculty at its core.
- 1997** The Department of Bioengineering is created; our chemical engineering faculty transfer their primary appointments to the new department and Larry McIntire becomes its first chair.
- 1998** A strategic plan for chemical engineering is approved by the University and its implementation begins with the help of an Advisory and Development Board.



- ▶ *Conducting world-class research in the areas of advanced materials and complex fluids, biosystems engineering, and energy and environmental systems*
- ▶ *Educating outstanding undergraduate and graduate chemical engineers to rise to leadership roles in academia, industry, law, business, medicine and government*
- ▶ *Promoting interdisciplinary collaborations and forming bridges linking Rice innovations to applications in the chemical, energy, biotechnology and materials industries*

The strategic plan also calls for complementing the department's internal research thrusts with strategic alliances on pollution control with faculty from the Civil and Environmental Engineering Department, and on biomaterials for tissue engineering with faculty from the Bioengineering Department. Because both these departments grew from programs initiated within chemical engineering, our faculty members have many strong connections through research collaborations, joint participation in university-wide research centers and joint faculty appointments. Our new undergraduate curriculum, a very flexible schema that encourages students to build interdisciplinary skills, also calls on these departments as teaching resources, thus solidifying these alliances.

Implementation of the strategic plan began in 1998 with the help of a select Advisory and Development Board whose members include academic, industrial, and professional experts. Over the past five years

- ▶ *Four new faculty members were hired in the areas of materials and biosystems.*
- ▶ *Over 14,000 sq. ft. of laboratory and office space was renovated and now houses state-of-the-art facilities for research on complex fluids, catalysis, and nanomaterials.*
- ▶ *A fundraising campaign for endowed graduate student fellowships has raised more than half a million dollars.*
- ▶ *The undergraduate curriculum was restructured by introducing four focus or specialization areas, by integrating courses or updating their content, and by introducing a biology (or biotechnology) requirement for our BS degree.*

The focus areas in biotechnology, environmental engineering, computational engineering, and materials science are very popular among our undergraduates.

FACULTY RESEARCH

Hiring new faculty has been a top priority and four new colleagues joined our department after 2000 to strengthen the materials and biosystems areas.

Matteo Pasquali joined the department as an assistant professor in January 2000 after receiving his PhD from the University of Minnesota in 1999 and completing his postdoctoral studies at the same University. His research focuses on processing flows of microstructured liquids that are ubiquitous in the chemical, polymer processing, coating, food, and biomedical industries. Current projects include the computational modeling of process flows with mesoscopic rheological properties, the solution of microscopic transport equa-

tions, and the visualization of single DNA molecules in process flows. He recently led a team of researchers who discovered that a sulfuric acid-based superacid makes an excellent medium for dispersing single-walled carbon nanotubes (SWNTs) at concentrations that are useful for industrial processes. This enabled them to process the dispersion into the first continuous fibers of aligned, pristine SWNTs.^[1-3] Fibers like these might be used to make ultralight, and yet ultrastrong, materials with remarkable electronic, thermal, and mechanical properties.

Michael Wong joined our faculty as an assistant professor in July 2001 after receiving his PhD from MIT in 2000 and completing a year of post-doctoral studies at UC Santa Barbara. Mike's research program focuses on designing new and improved materials for catalytic and encapsulation applications. His approach is based on the concept that the macroscopic properties of materials can be manipulated and engineered for target applications if their structural features can be controlled at the nanometer scale. Current efforts focus on the development of (a) supported nanoparticle-based metal oxide catalysts for solid acid and oxidation reactions, (b) metal-supported nanoparticles for the breakdown of environmentally-unfriendly organic compounds, (c) "quantum dots" for photocatalysis, and (d) nanoparticle-based hollow microspheres and microshells that can be engineered to encapsulate either enzymes to form micro-bioreactors or drug molecules to form drug delivery devices.

Nikos Mantzaris also joined our department as an assistant professor in July 2001. He received his PhD from the University of Minnesota in 2000 and completed his two-year post-doctoral studies on mathematical biology at the same university. His research lies in the emerging area of biosystems engineering and it aims at understanding, optimizing, and controlling the behavior of biological systems with the use of mathematical modeling and dynamical studies. Specific systems of interest include recombinant *E.coli* cell populations, tumor-induced migration of endothelial angiogenic cells and astrocytic signal transduction systems in the mammalian brain. The fundamental question Nikos is trying to answer for each of these systems is how single-cell events lead to the complex behavior and patterns exhibited by cell populations exhibiting heterogeneous phenotypes. The common thread in these studies is a methodological framework used to accomplish these tasks. This framework includes the development of (a) simplified models that can capture the essential, experimentally observed features of the system under consideration, and (b) sophisticated two- and three-dimensional numerical algorithms that, in combination with the understanding gained from the simplified model results, serve as the basis for studying the asymptotic and transient behavior of the detailed model.

Paul Laibinis joined our department as an associate professor in January 2003. He received his PhD in organic chem-

istry from Harvard University in 1991 and was a member of the MIT faculty from 1993 to 2002. His laboratory employs methods of self-assembly and chemical modification for generating interfaces with enhanced properties. These efforts include generation of molecular and polymeric thin films that are tailored through chemical synthesis to afford specific molecular architectures on surfaces as needed to alter and control surface events. The approach is general and reveals an ability to manipulate macroscopic interfacial events through nanoscopic changes at surfaces. Current research projects include approaches that control the interactions of biological species with surfaces, both to avoid their adsorption and to direct the adsorption of specific agents from solution. Such properties are important in the area of biodiagnostics, where selective recognition of targets in conjunction with the avoidance of nonspecific adsorption events determine the performance of many sensor and microarray technologies.

The research efforts of the new faculty nicely complement the work of the senior faculty in the areas of materials, energy systems and biosystems.

Chapman uses tools such as molecular simulation, computer visualization, statistical mechanics, and NMR to discover how material properties and structure depend on molecular forces. His current research program focuses on polymer solutions and blends, associating fluids, confined fluids, and natural gas hydrates.

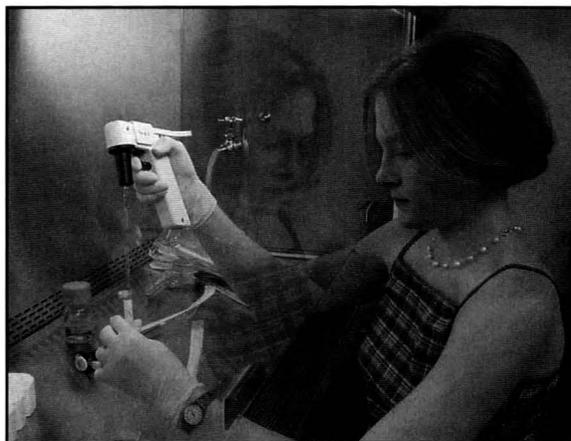
Hirasaki conducts research in fluid transport through porous media ranging from the microscopic scale intermolecular forces governing wettability to the megascopic scale numerical reservoir simulators for field-wide modeling. A recurring theme throughout this research is the dominance of interfaces in the determination of fluid transport processes.

Miller's research focuses on interfacial phenomena, especially those involving surfactants and their applications in detergency, pharmaceutical and food products, petroleum production, ground water cleanup, agricultural chemicals, and personal care products. His current projects include studies on the dissolution rates of surfactants, foam flow in porous media, and transport in emulsions.

Robert conducts theoretical, experimental, and computer simulation studies of the properties of matter. His current efforts focus on magnetic nanoclusters and carbon nanotubes, polymer, colloidal systems, ferroelectrics,

and disordered systems.

Zygorakis studies the mechanisms through which cell migration and proliferation affect the growth of three-dimensional tissues. Experimental data and large-scale simulations are used to analyze the dynamic behavior of large cell populations proliferating on 3-D scaffolds and find how tissue growth rates are modulated by the culture conditions.



Jessica Dunn, an undergraduate, works on her cell migration project.

INTERDISCIPLINARY RESEARCH

Over the past two decades, Rice has established several institutes and centers to promote interdisciplinary research on nanotechnology, biological sciences and engineering, information technology, and environmental engineering. Almost all our faculty members play key roles in these research efforts.

■ **Center for Biological and Environmental Nano-technology (CBEN):** Established in 2001 as one of six Nanoscale Science and Engineering Centers funded

by the National Science Foundation, CBEN is the first to focus on applications of nanotechnology to human health and the environment. The Center's research activities explore the wet/dry interface between nanomaterials and aqueous systems at multiple length scales, including interactions with solvents, biomolecules, cells, whole-organisms, and the environment. Collaborations with industry, entrepreneurs, and the Jones Graduate School of Management are integral to the Center's mission of creating sustainable nanotechnology.

Many chemical engineering faculty members have formed strong collaborations with other CBEN researchers. In collaboration with Richard Smalley and other chemistry researchers, **Pasquali** is studying the rheological properties of suspensions of single walled carbon nanotubes and is working on the production of fibers from concentrated, strong-acid solutions of nanotubes. **Wong** and his collaborators are developing new and improved materials for catalytic and encapsulation applications. Their approach is based upon the concept that the macroscopic properties of materials may be manipulated and engineered for target applications if their structural features can be controlled at the nanometer scale. **Laibinis** is exploring methods of self-assembly and chemical modification for generating interfaces with enhanced properties. Finally, **Mantzaris, Zygorakis, Pasquali, and Wong** are developing transient population balance models and apply them to design reactors and develop optimal control policies for the large-scale production of high-quality

nanoparticles (quantum dots).

■ **Institute of Biosciences and Bioengineering (IBB):** Established in 1986 in recognition of the revolutionary advances in biotechnology and molecular biology, IBB promotes interdisciplinary interactions among scientists, engineers, and clinicians from Rice and neighboring institutions.

Mantzaris and **Zygourakis** are collaborating with faculty from biochemistry and cell biology, bioengineering, and chemistry, to develop a novel framework that combines experimental, theoretical, and computational tools to study heterogeneous cell populations as complex, and highly interconnected systems with interacting components. This system-based approach will change the design principles used to develop effective drugs, tissues with desirable structure, materials with novel properties, and other bio-based, environmentally friendly, and sustainable technologies. **Zygourakis** also collaborates with other IBB members on research focusing on tissue engineering and biomaterials. A Biotechnology Training Grant from NIH and an IGERT grant from NSF provide stipend support for graduate students working in these and related areas.

■ **Shell Center for Sustainability:** Chemical engineering played a key role in the creation of the Shell Center for Sustainability. This Center embraces the central theme of Rice's environmental initiative: that implementation of a strategy for sustainable development requires both new tools and a transformation in our understanding of society's needs.

Administered through Rice's Environmental and Energy Systems Institute, the Center has a three-pronged mission of education, research, and community service to (a) create the knowledge required to remove current technological barriers to sustainability and to enable development of novel "sustainable" processes and products, (b) promote an interdisciplinary approach to sustainability that integrates research, education & public policy, and (c) serve as an independent forum for open discussions on sustainable development issues and policies.

One of the first projects funded by the Center involves research on gas hydrates that offer a vast, untapped energy source and may have played crucial roles in past global warming events. **Chapman** and **Hirasaki** are collaborating with geoscientists to develop mechanistic models describing the accumulation and dissociation of gas hydrates that exist in deep ocean sediments or in Arctic permafrost. Also, **Hirasaki** and **Miller** are working with faculty members from civil/environmental engineering to develop and test new methods for bioremediation of aquifers.

UNDERGRADUATE STUDIES

In today's rapidly changing business climate, industrial sectors from petrochemicals to biotechnology and semiconductor manufacturing offer a multitude of employment op-

portunities for our graduates.

What opens all these career options to our graduates is a broad education that encompasses both fundamentals and applications to give students a sound scientific and technical grounding for further development in a variety of professional environments.

Over the past five years, our department has awarded 146 BS (ABET accredited) and 18 BA degrees, for an average of about 33 graduates per year. After a significant decrease between 2001-03, our enrollments are increasing again and our current sophomore class has about 30 students. The percentage of female students in our classes ranges between 40% and 50%.

Industry employs the majority (about 61%) of our students who graduate with a bachelor's degree. Of the remaining students, about 18% continue their education in graduate schools to prepare for academic careers and industrial research jobs, 12% attend medical or law school, and 9% take government or other jobs.

Courses in mathematics, chemistry, physics, and computational engineering provide a foundation for the chemical engineering core, which introduces students to chemical process fundamentals, fluid mechanics, heat and mass transfer, thermodynamics, kinetics, reactor design, process control, and process design. Chemical engineering curricula place an emphasis on chemistry not found in other engineering disciplines. This background allows chemical engineers to tackle the wide variety of technical problems arising in the chemical, electronic, pharmaceutical, and biotechnology industries.

To complete their technical education, students seeking a BS degree in chemical engineering take course electives in at least two other engineering disciplines to satisfy a "breadth" requirement. Or, they can use their electives to create a focus or specialization area in 1) biotechnology and bioengineering, 2) computational engineering, 3) environmental science and engineering, and 4) materials science and engineering.

Figure 1 shows the components of the chemical engineering BS degree with their credit requirements. A total of 132 credit hours are required for the BS degree. The BA program is more flexible, making it even easier for a student to pursue a double major. Chemical engineering specifies 77 semester hours for the BA degree, including prerequisites and laboratory courses. In addition to these requirements, students must also satisfy the University distribution requirements (24 semester hours) and complete no fewer than 31 semester hours of free electives for a total of at least 132 semester hours.

GRADUATE STUDIES

The department offers programs of graduate study leading to both the Master of Science and Doctor of Philosophy degrees, with the primary emphasis on the latter. A professional master's degree (MChE), involving only course work,

is also offered.

Currently, the department has about fifty graduate students. All are engaged in research activities and receive full financial aid (stipend plus tuition). During the past five years, the department has graduated an average of 7.5 PhDs each year, making it first in per-faculty production of PhD graduates among the eight departments of the Rice School of Engineering. The 1995 National Research Council report ranked our department 16th in the United States in educating chemical engineering PhD students.

Graduate education is aimed at developing each student's ability to conduct independent creative scientific research. To ensure the versatility of our graduates, our curriculum provides a solid background in chemical engineering fundamentals (applied mathematics, thermodynamics, transport phenomena, kinetics, and reaction engineering). It also provides a mastery of engineering tools and ability to set clear goals of professional development so that our graduates become productive and successful in their professional careers.

The graduate program is large enough to offer research topics in several important areas of chemical engineering and related fields, but small enough to retain an atmosphere where students and faculty can have extensive personal contact. In addition, interdisciplinary research projects provide ample opportunities for students to interact with researchers from other disciplines, especially through the interdisciplinary institutes.

THE UNIVERSITY AND ITS CITY

Rice is a leading research university distinguished by a collaborative, interdisciplinary culture and a global perspective. Only a few miles from downtown Houston, it occupies an architecturally distinctive, 300-acre campus shaded by nearly 4,000 trees. State-of-the-art facilities and laboratories, internationally renowned centers and institutes, and one of the country's largest endowments support an ideal learning and living environment. With just 1,600 graduate students and 2,700 undergraduates, it offers an unusual opportunity to form close relationships with its faculty scholars and researchers and the option to tailor graduate programs to specific interests.

Houston is home of the Texas Medical Center, the largest concentration of medical schools, hospitals, and research fa-

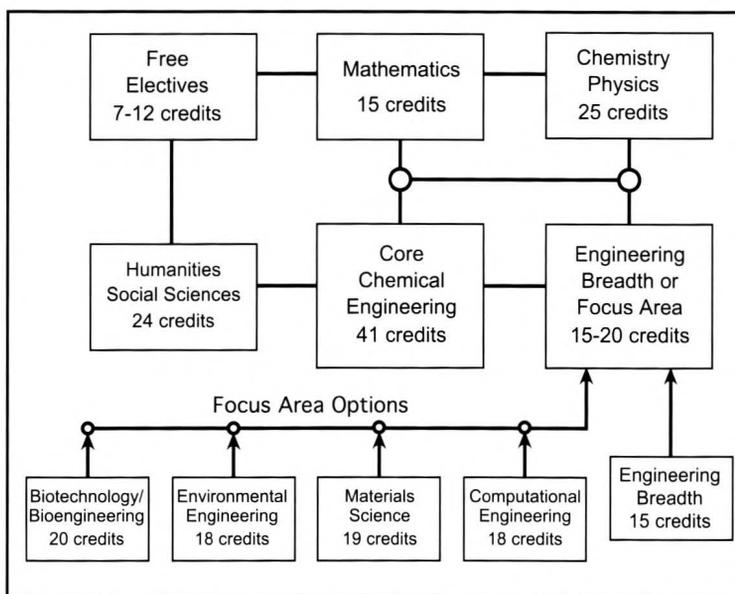


Figure 1. Components of the BS curriculum in ChE.

cilities in the world. Rice has cooperative programs with the University of Houston, Baylor College of Medicine, the University of Texas Health Science Center, and Texas Southern University. Houston is one of the few U.S. cities with resident companies in all four major performing arts (drama, ballet, opera, and symphony). It also boasts a museum district featuring exhibits of national and international prominence. As urban as it is, Houston is also a surprisingly green

city. Houstonians enjoy the outdoors in over 300 municipal parks and 120 open spaces, while the beach at Galveston Island is only a 45-minute drive away.

FORWARD PATH

The Rice chemical engineering department has grown from its embryonic beginnings as an adjunct to the chemistry department to a major research and educational center. To a large extent, this success has been due to the foresight of its faculty and an ability to exploit opportunities in emerging areas.

Past achievements set a precedent for the departmental rejuvenation that is occurring today. Faithful to its tradition, the department is refocusing its research and teaching efforts in areas that address the evolving needs of our society. These efforts are already receiving national recognition.^[1-3] The belief that chemical engineering is an enabling discipline, however, continues to shape our mission. Like our predecessors, we continue to use the same quantitative, systems-based approach in our research, we adapt our curricula to meet the evolving needs of our students, and we apply the same commitment to excellence.

ACKNOWLEDGMENTS

Our special thanks go to Bill Akers, Professor Emeritus, and the staff of the Woodson Research Center, Fondren Library, Rice University.

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Dow Award Lecture

MEMBRANE SCIENCE AND TECHNOLOGY IN THE 21ST CENTURY

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The author's career path in membrane science was anything but direct. Indeed, he embarrassingly admits that he has no formal training in the subject. His interest in membranes began during his tenure as a Director for NSF's (former) Thermodynamics and Mass Transfer Program in 1977-78. This program, which provided the only source of NSF funding for membrane research, had only two grants in the field at the time.

The author's efforts to enhance funding for membrane science ultimately led to establishing NSF's Separations and Purification Processes Program. In the process of doing this, the author also convinced himself that membrane science was a fertile area for challenging research. The actual impetus for initiating a research program in membrane science, however, came from one of his students, who upon completing his MS degree in the author's geophysics research program in 1981, asked if he could pursue a PhD in membrane science. Indeed, we sometimes gain more inspiration from our students than we give to them!

In 1990 the author and Professor Richard D. Noble established the NSF Industry/University Cooperative Research Center (I/U CRC) for Separations Using Thin Films that sub-

sequently became the Center for Membrane Applied Science and Technology (MAST). In 2000 the author accepted the Rieveschl Ohio Eminent Scholar Chair in Membrane Technology at the University of Cincinnati where he established a partner MAST Center site with a particular focus on bio-applications of membrane science.

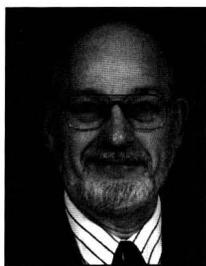
CHRONOLOGY OF MEMBRANE SCIENCE AND TECHNOLOGY

A membrane is a semipermeable medium that permits the passage of some molecules, colloidal aggregates, or particles relative to others. The dawn of membrane science is generally considered to be in the 18th century when Abbe' Nollet used the semipermeable properties of animal bladders to study reverse osmosis. The practical use of semipermeable media dates back many centuries before this, however. For example, the Arawak peoples of the West Indies used microporous stone filters to purify drinking water as early as 1600 BC, and the use of membrane filters for clarifying alcoholic beverages probably predates this by a few thousand more years. An example of one of these primitive stone membrane filters as shown in Figure 1.

It is interesting to note that membrane science developed much faster than membrane technology. For example, dialysis was studied by Graham in 1861 but it was not until 1944 that the first commercial dialyzer was developed by Kolff and Beck—think of how many lives could have been saved if the membrane dialyzer (artificial kidney) had been developed sooner.

Electrodialysis was reported by Pauli in 1924 but did not become practical until the 1950s. Ultrafiltration was studied in the early part of the 20th century but was not commercialized until the 1960s. Gas separations were studied by Graham in 1864 but the development of the membrane lung oxygenator by Kolff and Balzer did not occur until the 1950s; again consider the impact of this delay on the loss of life. Although the pH meter was developed by Cremer in 1906,

William B. Krantz received a BA in chemistry (1961) from Saint Joseph's College (Indiana) and his BS (1962) and PhD (1968) degrees in chemical engineering from the University of Illinois-Urbana and the University of California-Berkeley, respectively. From 1968-1999 he was Professor of Chemical Engineering and President's Teaching Scholar at the University of Colorado. In 1999 he accepted the Rieveschl Ohio Eminent Scholar Chair at the University of Cincinnati where he is Director of the NSF / U CRC for Membrane Applied Science and Technology. He is the recipient of a Guggenheim, NSF-NATO and three Fulbright fellowships, Special Achievement and Outstanding Performance Awards from NSF, the Innovation in Coal Conversion Award of the International Coal Conference, the George Westinghouse and Dow Chemical Engineering Division Lectureship Awards of ASEE, and the Malcolm E. Pruitt Award of the CCR. He has been named a Fellow of AAAS and ASEE and a Sigma Xi National Research Lecturer. In addition, he has received 27 awards for teaching excellence and service to student organizations.



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the smart sensor industry did not emerge until the 1960s. Nelson and Rose's pioneering studies of controlled release technology were reported in 1955, but this was not commercialized until the 1980s. This delay between scientific discovery and commercial implementation is in stark contrast to the rapid commercialization that we associate with computer- and information-age technologies. Unfortunately this delay is very much associated with our inability to address challenges that have confronted membrane science.

DISADVANTAGES AND ADVANTAGES OF MEMBRANES

The significant time gap between discovery and commercialization of membrane technology is a result of several perceived disadvantages of membrane technology. Since most membranes are made from solids, the permeation rates will be low unless they can be made very thin. Membrane processes scale linearly; that is, the required membrane area is directly proportional to the feed flow rate. Hence, membrane processes do not have the economies-of-scale that are enjoyed by separations technologies such as distillation, extraction, and crystallization.

The attractiveness of membrane technology is also tied to energy costs since they are very energy efficient relative to separations processes that require a change of phase; fortunately (but unfortunately for membrane technology) we have lived during a time of abundant and relatively inexpensive energy. Concentration polarization and fouling have hindered the application of membranes to many liquid separations applications. Most membrane separations employ polymeric membranes that are subject to compaction under high pressure and swelling in the presence of aggressive organic solvents, both of which compromise performance.

Interestingly, membranes have been successful primarily in niche markets where they do not have any competition; consider for example contact lenses, renal dialyzers, artificial lungs, breathable garments, battery separators, *etc.* Polymeric membranes are subject to UV degradation, hydrolysis, and attack by polar aprotic solvents as well as a relatively low maximum use temperature; hence they have limited applications and relatively short lifetimes. Ceramic membranes are brittle, friable, difficult to package into modules and relatively expensive. Finally, polymeric membrane manufacture requires relatively little material; hence, it does not have much influence on the polymer market and the corresponding development of new polymers.

Membranes also enjoy several advantages that will lead to exciting new applications in the 21st century. They are attractive from a First Law of Thermodynamics perspective since they in general require less energy than competitive separation processes owing to the fact that they do not necessarily require an energy-intensive phase change. They are also attractive from a Second Law of Thermodynamics de-

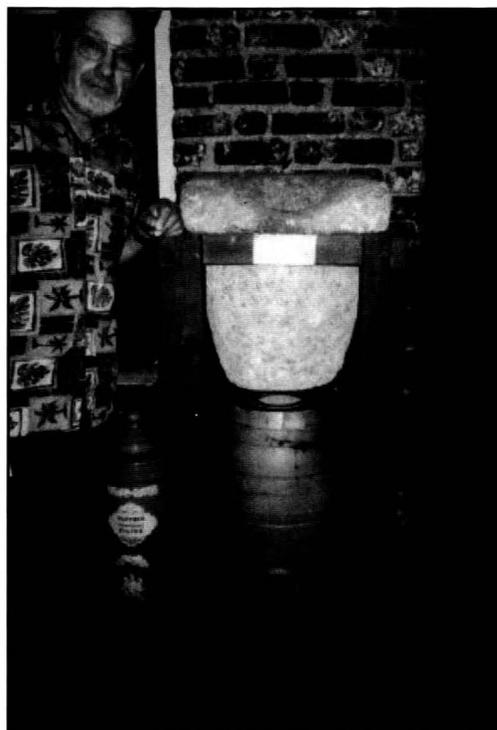


Figure 1. The author and a stone membrane filter of the type used by the Arawak peoples of the West Indies to purify drinking water as early as 1600 BC.

sign perspective since they are not subject to the entropy penalty associated with a phase change. The linear scaling law also has positive implications since it implies that membrane technology is modular and therefore amenable to easy scale-up.

Membrane separations are also easily adapted to both continuous and batch-wise operation. In contrast to many competitive technologies, harsh or extreme operating conditions are not generally required for membrane separations. They can also be used to separate feeds that exhibit an azeotrope that precludes separation via distillation.

Membranes are particularly amenable to hybrid separations in which they are combined with some other technology such as distillation where they can be used to process a slip stream to break an azeotrope. They can also be functionalized to permit highly discriminating separations and can be made from renewable resources such as wood pulp and cotton delinters. Membrane separations are also considered to be environmentally friendly, green technologies. One particular advantage of membranes that has been realized only recently is that they are the only technology that can separate, deliver, or discriminate between solutes on the microchip scale or MEMS (Micro-Electro-Mechanical-Systems) scale.

THE NSF CENTER FOR MEMBRANE APPLIED SCIENCE AND TECHNOLOGY

The challenges and opportunities for membranes led to the establishment of the Center for Membrane Applied Science

and Technology (MAST) (the only NSF block-funded membrane research center in the U.S.) at the University of Colorado in 1990. In 2001 the MAST Center became a Multi-University Industry/University Cooperative Research Center (I/U CRC) by adding a partner site at the University of Cincinnati. This permitted the MAST Center to expand its focus to include biomedical, pharmaceutical and biosensor applications of membranes since the requisite multidisciplinary research was facilitated by having the Colleges of Engineering, Arts and Sciences, Medicine, and Pharmacy on the same campus at Cincinnati.

The objectives of the MAST Center are (1) to conduct basic research and related developmental activities for the use of membrane technology, (2) to provide timely and effective technology transfer between the Center and its sponsors, and (3) to promote education in membrane technology. The MAST site Co-Directors are Professors Richard D. Noble and Alan R. Greenberg at the University of Colorado and Professors Jerry Y.S. Lin and the author at the University of Cincinnati.

The primary source of funding for the MAST Center is its industrial and governmental lab sponsors, each of whom pays an annual fee. Each sponsor designates one representative on the Industrial Advisory Board (IAB) of the Center. Twice each year, the sponsors are invited to submit topics for possible MAST Center research projects. These topics can involve any aspect of membrane science and technology, the undertaking of which would be appropriate to MS or PhD research in any field of pure and applied science. The list of topics along with any supporting information the sponsors choose to provide is sent to faculty spanning a broad spectrum of disciplines at the two MAST sites. Interested faculty then submit pre-proposals that are evaluated by the IAB to determine who will be asked to submit expanded proposals. On the basis of the latter, the IAB selects the proposals that will be funded.

Projects are generally funded for three years at a level adequate to fund one graduate student and to provide a modest budget for supplies, equipment, travel, and some faculty summer support. The return to industry for its investment in the Center is rapid technology transfer, access to University faculty, students, and facilities, a forum to discuss membrane science and technology, and a proven 20:1 leveraging on their annual sponsor fee. The benefit to faculty and students is relevant research, participation of sponsors on the research teams, industry internship opportunities, and access to sponsor facilities. In order to protect the intellectual property interests of the Universities and the sponsors, all MAST Center research is held in confidence until the IAB approves disclosure.

Membrane research at Cincinnati and Colorado impacts not only the graduate programs at each university, but also has had a significant positive impact on undergraduate programs via NSF Research Experiences for Undergraduates (REU) Summer Site Programs that are tied to the MAST Center sites.

Over 175 undergraduates have received financial support and invaluable research experience through the NSF REU programs at the two sites.

Recently the Cincinnati MAST Center site was awarded an NSF Integrative Graduate Research Education and Research Traineeship (IGERT) grant that focuses on bio-applications of membrane science and technology. This program includes a set of prescribed courses in membrane science that provide the impetus for complementary curricular tracks in biomedical, pharmaceutical, and biosensor applications of membranes. Program components include a set of laboratory rotations, training in entrepreneurship, professional ethics, communication skills, industry internships, and the opportunity for an international technical cultural experience. This NSF IGERT program complements the MAST Center in that the membrane research undertaken by the former will be generated by the faculty, whereas that undertaken by the latter is suggested by the MAST sponsors.

Over the past 13 years, the MAST Center has funded 55 research projects that in turn have provided stipend support for 16 MS, 37 PhD, and 6 postdoctoral students. The fact that 77% of the project teams were multi-investigator and 56% were interdisciplinary demonstrates that the MAST Center has successfully promoted the research environment necessary to tackle the difficult challenges facing the advancement of membrane science and technology. This research has led to 90 peer-reviewed and 253 presented papers as well as 10 patents. Most impressive is the fact that MAST Center students have won 27 regional and national awards for their research accomplishments. MAST Center activities have catalyzed more than \$16 million in spin-off funding, primarily as a result of facilitating the formation of faculty research teams.

EXAMPLES OF SUCCESSFUL NSF MAST CENTER RESEARCH

It is interesting to follow the chronology of a successful MAST Center project. In 1993, the U.S. Army Tank and Automotive Research and Development Center (TARDEC) joined the MAST Center. TARDEC's motivation to join the Center was based on problems encountered during the 1991 Desert Storm war in Iraq. Indeed, a major factor that limited our ability to move through the vast desert into Baghdad was the supply of water to the ground forces. TARDEC was responsible for mobile water treatment units, each of which could produce 100,000 gallons per day using reverse osmosis membrane technology.

Approximately one-half of the weight of these units was associated with equipment and chemicals needed to clean the membranes of fouling deposits. Owing to the buildup of fouling deposits on the membranes, the mobile units had to be periodically shut down and de-fouled by circulating chemical cleaning agents through them. Considerable time and cleaning agent materials were wasted owing to the uncer-

tainty in the amount of time required for cleaning the units.

The author participated in a research team that quickly recognized that this problem could be addressed by adapting Ultrasonic Time-Domain Reflectometry (UTDR) to monitor the condition of the membranes. Ultrasound was an established medical technology for imaging centimeter-scale internal organs and fetuses. Adapting it to image micron-scale fouling deposits was a challenging task for our MAST Center research team—one that ultimately led to a U.S. patent.^[1]

TARDEC projects that this UTDR technology will provide a savings of as much as 50% in cleaning time and chemical cleaning agent use. Subsequent publications describe the use of UTDR to monitor membrane fouling,^[2-6] membrane compaction,^[7,8] and membrane formation.^[9] Current research involves the use of UTDR to study membrane swelling, defect detection, and optimal design of membrane modules. This provides an excellent example of how MAST Center projects address both the immediate goals of its sponsors and provide incentives for faculty to pursue new research thrusts that result in scholarly publications and significant external funding.

The MAST Center not only has provided stipend support for many graduate and postdoctoral students, but also has provided financial support and research experience for over 175 undergraduate students. It has been said that if faculty are reasonably confident the objectives of a research project can be achieved, it should be given to a PhD student since they must achieve positive results for their thesis; but if the project is highly speculative, with a low chance of positive results, it is appropriate for an undergraduate researcher! Indeed, undergraduates are delightfully naive; they are not experienced enough to know what is impossible!

One such example is provided by a freshman who came to the author to undertake an independent study research project that involved adapting video-microscopy for imaging the evolution of pore structure during membrane formation via phase inversion. The student happened to be taking physics while he was working on this project and proposed using nonuniform electric fields to eliminate undesirable macrovoid pore defects that compromise the mechanical integrity of polymeric membranes. The author knew that this idea would not work since he had published a paper that explored this same idea,^[10] but he did not want to discourage a young researcher by telling him about the earlier paper. He provided some funds

to allow the young man to explore his 'ill-conceived' idea. What subsequently happened is best described by a beautiful poem of Edgar Guest:

*So he buckled right in
with the trace of a grin
on his face. If he worried, he hid it.
He started to sing
as he tackled the thing
that couldn't be done, and HE DID IT!*

Edgar A. Guest – *It Couldn't Be Done*

Indeed, as it turned out, the student was right and the professor was wrong—wrong in his science, that is, but right in his mentoring of a young researcher! This research led to a U.S. patent^[11] and the 1999 U.S. Collegiate Inventor of the Year award for the young man—and just incidentally, to a new area of research for the professor. Figure 2 shows this young man with a 'hint of a grin' receiving his award!



Figure 2. Andrew Neice, James Hillier (left), and the author (right), at the 1999 Awards Ceremony for the Collegiate Inventors of the Year. Dr. Hillier was honored for his research related to the invention of the electron microscope. Andrew, a freshman at the time, received the Undergraduate Collegiate Inventor of the Year Award for his invention that emanated from NSF MAST Center research focused on macrovoid defect formation in polymeric membranes.

THE FUTURE OF MEMBRANE SCIENCE

Now let us consider the future of membrane science in this 21st century. There are several important considerations regarding membranes that need to be kept in mind when considering where this field of scientific endeavor is going:

- *Membranes are competitive when the desired product is the permeating component.*
- *Membranes thrive in noncompetitive markets.*
- *Membrane processes obey a linear scaling law.*
- *Membranes are the only separations technology that will work on the microscale.*
- *Membranes stand to benefit significantly from the science of biomimetics.*

It might seem surprising that reverse osmosis membrane technology is now used to produce more than 400 million gallons per day of fresh water from seawater; yet, it is not being used to provide fuels-grade ethanol from aqueous biomass solutions. The answer is simple, however—any water that passes through a membrane via reverse osmosis is a useful product. In contrast, to produce a fuels-grade ethanol product from aqueous biomass solutions would require passing nearly all the water through the membrane since the ethanol molecule is larger than water. Indeed, successful membrane technologies usually require that the desired product preferentially permeate.

Any technology would like to be the 'only show on the

road,' but this is especially true for membranes. Consider, for example, life-saving medical technologies such as the membrane lung oxygenator and membrane dialyzer, pharmaceutical devices such as controlled release patches, and consumer products such as contact lenses.

Educators who teach process design are quick to point out the disadvantage of membrane technology in that it obeys a linear scaling law. As stated earlier, it is for this reason that membranes do not have the economies-of-scale that other separations technologies enjoy. It is important to realize, however, that a technology damned for large-scale applications might be blessed for small-scale applications! Indeed, membranes provide the only technology that can separate, deliver, or discriminate between solutes on the micro- or nano-scales.

It is well known that the human body consists primarily of water—the second pervasive component in our bodies is membranes. Indeed, our skin, kidneys, spleen, liver, eye corneas, and every cell in our body involve biological membranes. The science of biomimetics seeks to unravel how living systems accomplish their exceptional performance. We are delighted when we can fabricate a synthetic membrane that will provide a separation factor of 20:1 for some solute. Imagine the impact of being able to make synthetic membranes that can mimic ion channel performance in the bilipid layers of cell walls that can discriminate between sodium and potassium with a separation factor of over one million!

The aforementioned considerations for membrane technology suggest the direction for membrane science applications in this 21st century. For example, changes in federal regulations may soon require that small incorporated municipalities with a population under 10,000 meet the same high water-quality standards that are imposed on larger towns and cities. Membrane technology may provide the economic alternative for these smaller scale applications.

It is well known that the demand for kidney, liver, spleen, and other human organ transplants exceeds the supply of donor organs. There are alternative ways to meet this organ demand that must keep the gods laughing—the animal whose organs are most readily transplanted into humans is the pig! Porcine organ transplants cannot be done directly owing to problems of potential transmission of viruses as well as sensitive religious considerations for some people, but it is possible to encapsulate the porcine organ in the shell of a hollow-fiber membrane module, a device that resembles a tube-and-shell heat exchanger, and to have the blood flow through the fibers. In this way organ functionality is retained by having the solutes permeate through the walls of the hollow fibers without any direct contact between the porcine organ and the blood.

A very desirable alternative to organ transplants is, of course, to cure the disease itself. Tremendous progress is now being made using islet cell transplantation. Islet cells are the 'drill sergeants' of the cell community that can restore healthy organ functionality. Membranes are used both to isolate the

islet cells and to encapsulate them for transplantation via surgical techniques such as laparoscopy.

We have already alluded to controlled release for delivering drugs at the precisely required dosage transdermally. This well-established membrane technology will soon be complemented by smart drug delivery. The latter will involve interfacing devices for sensing the need for treatment and delivering the appropriate drug. Consider, for example, people suffering from heart disease. If they encounter a stressful situation such as a near-accident while driving, they could find themselves in a life-threatening situation if they do not receive one of the drugs that suppresses the adrenaline in their bloodstream. Smart drug delivery might involve a piezoelectric sensor on the chest that would detect an excited heartbeat and send an analog signal to a MEM-MEMS device that would deliver an adrenaline-suppressing drug transdermally into the bloodstream. The latter would close the feedback loop back to the piezoelectric sensor that would gradually reduce the drug delivery as dictated by the heartbeat.

The pharmacy-on-a-chip will use a MEM-MEMS device that incorporates many microscale membranes into a microchip to deliver a solute. The particular advantages of MEM-MEMS technology are miniaturization and analog input/output electrical signals. These devices capitalize on the unique linear scaling characteristic that permits membranes to retain their ability to deliver, separate, or discriminate between solutes even on the micro- and nano-scales. For this reason MEM-MEMS devices will be used in separation devices such as compact portable oxygenators that will greatly improve the quality of life for chronic obstructive pulmonary disease (COPD) patients and in smart sensors for the discriminating detection of solutes such as glucose and insulin levels in the bloodstream of diabetics.

In the past, profitable applications of membranes such as water desalination have required making membranes via large-scale, continuous-production-line processing. Indeed, heretofore most commercial membranes have been manufactured either via phase-inversion or interfacial polymerization. The application of self-assembly, molecular scaffolding, and other templating techniques for making highly functionalized membranes has been an academic curiosity.

The exciting potential for MEM-MEMS technology, however, has dictated a new paradigm for membrane manufacture in the 21st century—namely making commercial membranes by the millimeter rather than the mile. Consider for example that a single 8.5 x 11-inch sheet could provide 2 million micromembranes having a 200-micron diameter such as might be incorporated into a MEM-MEMS device. A particular advantage of these micromembranes is that the total force on their area for typical operating pressures will be quite small, thereby obviating the need for a thick support layer that reduces the permeation rate.

Making membranes by the millimeter rather than the mile

for MEM-MEMS and other high-tech applications opens the door to an array of techniques for introducing unique structure and functionality. The MAST Center has developed a program that is currently focusing on using Langmuir-Blodgett (L-B) technology to address the MEM-MEMS challenge. The L-B technique involves spreading one or more surface-active components at the water/air interface to form a monomolecular film. This film is subsequently compressed by a moving barrier in the interface. This compression causes ordering of the surface-active molecules and possibly a two-dimensional phase transition. The ordered or phase-separated film can then be collected on a solid support by drawing the latter through the interface. Composite membranes can be fabricated by employing a microporous membrane as the solid support on which the L-B layers are collected. The thickness of these composite membranes can be controlled by adding more L-B films. The functionality of these composite membranes can be engineered by changing the properties of the monomolecular film, either by employing different surface-active molecules or by changing the surface state of the film. Microporous L-B films can be created by first using a monolayer within which a two-dimensional phase separation has occurred and then dissolving the dispersed phase component from the supported L-B film.

It is particularly desirable to make fluorocarbon membranes using this L-B technique. Fluorocarbon membranes are attractive owing to their excellent solvent resistance and approved use in the human body, but many fluorocarbon polymers are not amenable to membrane fabrication via conventional phase-inversion. Blends of surface-active alkyl- and fluoro-trichlorosilanes will phase-separate under interfacial compression to form dispersed two-dimensional microdomains. Moreover, the trichlorosilanes will spontaneously hydrolyze in water and subsequently polymerize under compression to form a robust film that can be collected on a porous support. By appropriately choosing the concentration and chain length of the alkyl- and fluoro-trichlorosilanes, it is possible to make the former the dispersed phase component. The latter then can be easily dissolved from the supported L-B film using common solvents such as benzene.

Challenges in applying the L-B method for fabricating composite membranes relate to achieving the desired functionality, pore size, and mechanical integrity. The NSF MAST Center is exploring the use of chain length, surface compression speed, substrate pH, temperature, and DC electric fields to decrease the dispersed phase domain size in these L-B films. We are optimistic that this research will lead to an enabling technology for manufacturing highly functionalized membranes that will address the demands of 21st century applications!

SUMMARY

Membrane technology has unique advantages that position it to address exciting challenges in the 21st century that relate

to environmental, biomedical, biosensor, and pharmaceutical applications. In particular, it is the only separations technology that retains its functionality at the micro- and nano-scales and thereby has unbounded potential for use in MEM-MEMS and related applications.

ACKNOWLEDGMENTS

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AGITATION AND AERATION

An Automated Didactic Experiment

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Since its foundation, the Federal University of São Carlos' Chemical Engineering Department has traditionally conducted instructional experiments to complement the theoretical knowledge passed on in the classroom. This practice is part of a successful approach to provide students with a good practical background, preparing them to become competent and competitive professionals in the chemical industry. Our undergraduate laboratory follows the principle of designing instructional kits for short experiments to be prepared and conducted by the students themselves.^[1]

Recent advances in equipment design and techniques have facilitated the acquisition of on-line information concerning chemical processes. This reality is undoubtedly becoming part of the daily routine of chemical engineers in research laboratories and industry. Therefore, undergraduate courses should provide opportunities for students to get first-hand practice in the techniques involved in automated chemical processes.

During the establishment of a "Special Training Program" for undergraduate students (called "The Factory of the Future"^[2]), a set of automated experiments was implemented with the financial support of CAPES, a Brazilian education funding agency. One of the kits in this program is an Agitation and Aeration Experiment, which was used in a case study of an important biochemical process, "Aerobic Cultivation of Baker's Yeast." The supervisory system was designed by the authors, and the controllers were programmed by a specialized engineering firm, using commercial software.

Many processes involved in the manufacture of important chemical products, such as the hydrogenation of oils in the production of margarine or the aeration of fermentation broths in antibiotic production, make use of agitation and aeration tanks to promote efficient mass transfer from the gas phase to the liquid phase. Despite its obvious importance, teaching about the operation of agitation and aeration is usually rel-

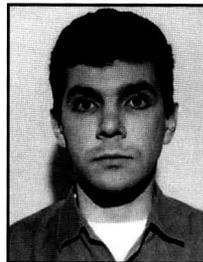
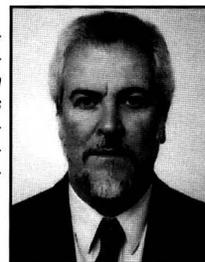
egated to a secondary role in chemical engineering courses.

This paper describes automated equipment developed to run teaching experiments on these unit operations in the laboratory. The purpose of the experiment is to show students a real chemical process. The main adjusted parameters, such as the stirrer speed (N) and gas (air) flow rate (Q), can be monitored. Simultaneously, phenomena involving changes in dissolved oxygen concentration (C) and gassed (P_g) and ungassed (P_0) power consumption can be viewed by the supervisory computer. The continuous acquisition and storage of experimental data allows the volumetric oxygen transfer



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[We have] traditionally conducted instructional experiments to complement the theoretical knowledge passed on in the classroom. . . . Our undergraduate laboratory follows the principle of designing instructional kits for short experiments to be prepared and conducted by the students themselves.

coefficient, ($k_L a$) to be accurately determined, facilitating the students' analyses of the data and writing of reports.

THEORY

Owing to their versatility, conventional agitation and aeration tank fermentors are still the ones most frequently used on bench, pilot, and industrial scale in the fermentation industry.^[3] In fermentation processes involving the cultivation of aerobic and facultative aerobic microorganisms, oxygen is an essential element in the supply of energy for cell metabolism and, hence, a key element in the syntheses of biomass and products.

A convenient way of evaluating oxygen transfer in aerobic cultures is to measure the volumetric oxygen transfer coefficient ($k_L a$). The gassed power consumption per unit volume of broth (P_g/V) and the volumetric oxygen transfer coefficient are still the most widely used criteria in the design and scale up of conventional stirred and aerated tank fermentors.^[4]

Various equations correlating the volumetric oxygen transfer coefficient ($k_L a$) to other quantities have been published.^[5] Cooper, *et al.*,^[6] originally proposed the simplest, correlating $k_L a$ to the gassed power consumption per unit volume of broth (P_g/V), the superficial gas velocity (v_s), and the geometry of the vessel (D_t)

$$k_L a = C_1 (P_g / V)^\alpha (v_s)^\beta \quad (1)$$

where

$$v_s = \frac{4Q}{\pi D_t^2} \quad (2)$$

Although initially developed for fluids different from fermentation broths, the relation given in Eq. (1) has been widely used in fermentation systems.^[5] Values reported in the literature for the constants α and β and the proportionality constant C_1 vary considerably with the geometry of the system, the range of variables covered, and the experimental method used. Therefore, specific correlations for $k_L a$ for use in subsequent monitoring, control, and scale up of aerobic fermentations should be obtained from bench-scale experiments.

Similarly to the volumetric oxygen transfer coefficient ($k_L a$), the gassed power consumption (P_g) can be correlated to the system's geometric parameters (impeller diameter, D_t), to operation variables (impeller speed, N , and gas flow rate, Q), and to the physical properties of the fermentation broth (den-

sity, ρ , and viscosity, μ) that are implicit in the ungassed power consumption (P_0). The power requirements in gassed and ungassed systems can be represented by the traditional equation proposed by Michel and Miller^[7]

$$P_g = C_2 \left(\frac{P_0^2 N D_t^3}{Q^{0.56}} \right)^\theta \quad (3)$$

where the constants C_2 and θ also depend on the system's geometry and on the range of operating variables used.

MATERIALS AND METHODS

Microorganism

Fermentations were conducted using *Saccharomyces cerevisiae* in the form of commercial Baker's yeast (Fleischmann®).

Culture Media

To activate and ferment the inocula, a culture medium containing (in $\text{kg}\cdot\text{m}^{-3}$)

- glucose (15.0)
- KH_2PO_4 (5.0)
- $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ (0.5)
- yeast extract (3.0)
- $(\text{NH}_4)_2\text{SO}_4$ (4.5)
- antifoam ($1.0 \text{ L}\cdot\text{m}^{-3}$)

was used. The initial pH was adjusted to 4.6 with the 4M H_2SO_4 or 3M NH_4OH .

Supervisory and Data Acquisition System

The experiment was monitored and controlled in an automated teaching system, which uses a Programmable Logic Controller (PLC) coupled to a supervisory system that provides the man/machine interface (MMI). The main purpose of this interface is to allow the user to interact with the programmable controller. The system was implemented in a Supervisory Control and Data Acquisition Architecture where the PLC performs control functions while monitored and supervised by a microcomputer.

The computer screen is divided into two windows. The first one shows an animated view of the process with continuous variable updates. The on-line values are displayed in boxes next to the respective variables during the process. The sec-

ond window presents a graphical display of the time course of the process variables. These windows can be seen in Figures 1 and 2.

Experimental Apparatus

The experiment was carried out in an agitated and aerated cylindrical vessel equipped with two six-flat-blade turbines and an air sparger. The stirrer speed (N) was controlled by a frequency inverter (0.5 HP, Siemens, Germany) coupled to the AC 0.4 kW motor. Stirrer speed was measured directly by an optical tachometer (Monarch Instruments, Amherst, NH) on the agitator shaft. The electric signal was used to monitor the stirrer speed.

The air flow rate (Q) through the vessel was monitored by a mass flow meter (0 to 20 SLPM, KURZ Instruments, Inc., Monterey, CA). The temperature was kept at 30°C by circulating water between a thermostatic bath and a water jacket. A polarographic electrode (submersible type, IC Control, Canada) connected to a dissolved oxygen transmitter (model 855, Microprocessor Analyzer, CI Control, Canada) was used to measure the dissolved oxygen concentration (C_E). Figure 3 shows the dimensions of the vessel and Figure 4 illustrates a sketch of the experimental system. All the analog signals between the physical system and the PLCs (GE Fanuc, series 90-30, GE Fanuc Automation North America, Inc.) were provided as current signals (4 to 20 mA).

The power consumption (P) was monitored and controlled through a frequency inverter, which controlled the stirrer speed (N) by modulating the electric power transferred to the AC motor. The volumetric oxygen transfer coefficient ($k_L a$) values obtained at different stirrer speeds (N) and air flow rates (Q) were correlated with the system's operating parameters and physical dimensions. Correlations of this type are useful for the design, control, and scale up of fermentors.

Determination of $k_L a$

The volumetric oxygen transfer coefficient ($k_L a$) was determined using the method proposed by Mignone and Ertola,^[8] based on a step change in stirrer speed during cultivation.

Assuming mixing is complete, the mass balance for dissolved oxygen in the liquid phase during aerobic batch cultivation can be expressed as

$$\frac{dC}{dt} = \underbrace{k_L a(C^* - C)}_{\text{OTR}} - \underbrace{Q_{O_2} C_x}_{\text{OUR}} \quad (4)$$

where OTR is the oxygen transfer rate and OUR is the oxygen uptake rate.

Initially, the culture is maintained under a constant air flow rate (Q) and stirrer speed (N_1). This situation corresponds to the steady state I, in period I shown in Figure 5. During this phase, we have $(k_L a)_1$ and the dissolved oxygen concentration (C_1).

The stirrer speed is changed to N_2 where $N_2 > N_1$. After a short time, a transient state is produced (period II in Figure 5) during which the concentration of oxygen varies until the new steady state II is reached (period III). This new period is characterized by another volumetric oxygen transfer coefficient $(k_L a)_2$ and by another oxygen concentration (C_2).

Each of these periods in Figure 5 can be described by the following equations:

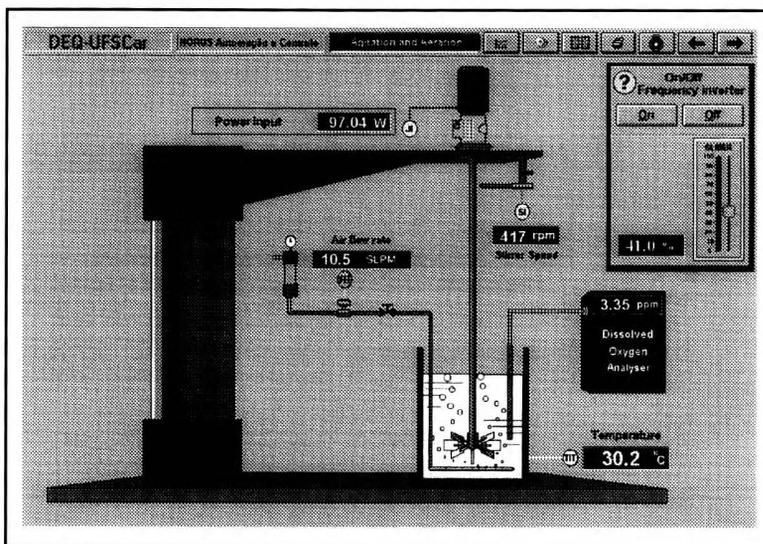


Figure 1. Representative screen of instrumentation created by the supervisory system, showing updated signals (variables) in real time.

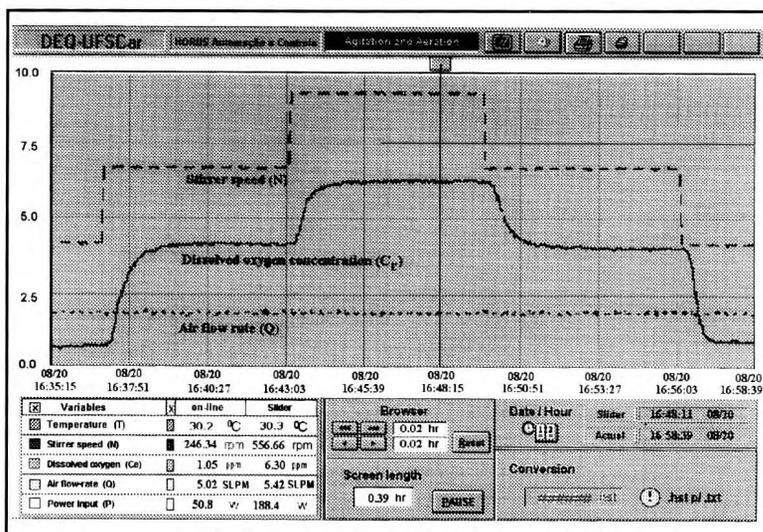


Figure 2. Graphic display showing the time course of process variables.

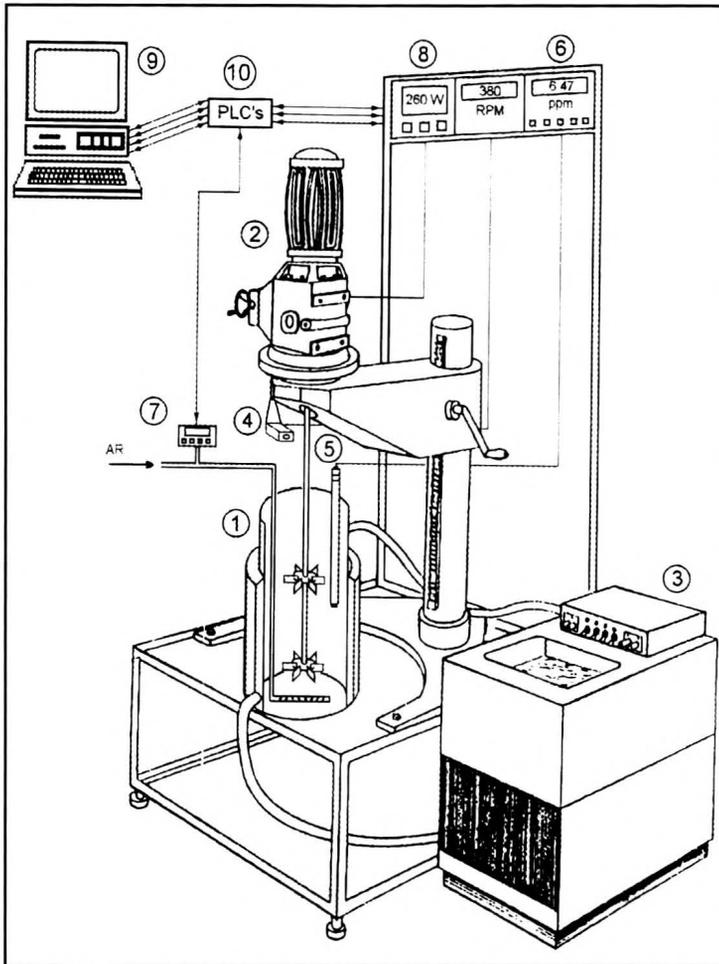


Figure 4. Experimental apparatus: (1) agitation and aeration tank; (2) stirrer motor; (3) thermostatic bath; (4) photo tachometer; (5) dissolved oxygen electrode; (6) dissolved oxygen analyzer; (7) mass flow meter; (8) frequency inverter; (9) supervisory computer (InduSoft Studio 3.0[®] running on Windows 95, Microsoft[®]); (10) Programmable Logical Controllers.

Period I (steady state)

$$\frac{dC}{dt} = (k_L a)_1 (C^* - C_1) - Q_{O_2} C_x = 0 \quad (5)$$

Period II (transient phase)

$$\frac{dC}{dt} = (k_L a)_2 (C^* - C) - Q_{O_2} C_x \quad (6)$$

Period III (new steady state)

$$\frac{dC}{dt} = (k_L a)_2 (C^* - C_2) - Q_{O_2} C_x = 0 \quad (7)$$

In each case, the oxygen concentration was kept above the critical value. For short periods of time, it may be assumed that the oxygen uptake rate ($Q_{O_2} C_x$) remained constant.

From Eq. (7)

$$Q_{O_2} C_x = (k_L a)_2 (C^* - C_2) \quad (8)$$

Substituting Eq. (8) into Eq. (6) gives

$$\frac{dC}{dt} = (k_L a)_2 (C_2 - C) \quad (9)$$

Eq. (9) can be integrated from $t = 0, C = C_1$ to $t = t, C = C_2$, giving

$$C = C_2 - (C_2 - C_1) e^{-(k_L a)_2 t} \quad (10)$$

Defining a dimensionless concentration

$$\bar{C} = \frac{C - C_1}{C_2 - C_1} \quad (11)$$

Eq. (10) can be rewritten in dimensionless form

$$\bar{C} = 1 - e^{-(k_L a)_2 t} \quad (12)$$

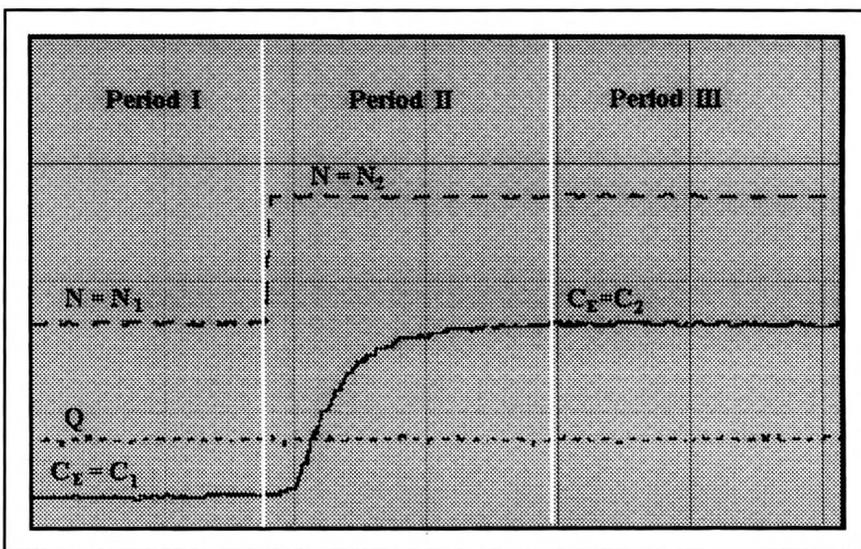


Figure 5. Dissolved oxygen concentration profile (C_p) after steps in stirrer speed (N).

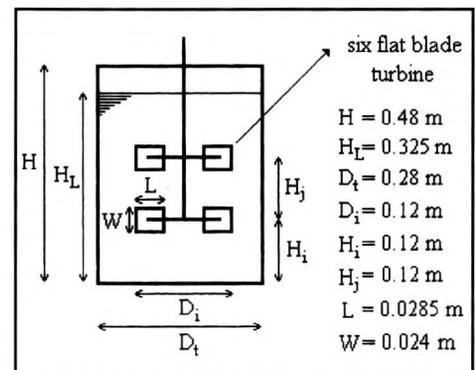


Figure 3. Dimensions of the vessel.

Equation (12) describes the kinetics of the liquid phase. This equation, however, does not take into account the electrode kinetics and the kinetics of the stagnant film that covers the membrane of the electrode. These two phenomena are described by the first-order equations

$$\frac{d\bar{C}_F}{dt} = \frac{\bar{C} - \bar{C}_F}{\tau_F} \quad (13)$$

$$\frac{d\bar{C}_E}{dt} = \frac{\bar{C}_F - \bar{C}_E}{\tau_E} \quad (14)$$

where \bar{C}_F and \bar{C}_E describe, respectively, the dimensionless diffusion film and electrode responses; τ_F and τ_E are the response times for the liquid film and electrode diffusion resistance.

The composition of the gas phase is assumed to remain constant, so it is unnecessary to consider its kinetics.

The value of \bar{C}_E can be derived from Eqs. (12), (13), and (14)

$$1 - \bar{C}_E = \frac{\left(\frac{1}{k_L a}\right)^2}{\left(\frac{1}{k_L a - \tau_F}\right)\left(\frac{1}{k_L a - \tau_E}\right)} e^{(-k_L a t)} + \frac{\tau_F^2}{\left(\tau_F - \frac{1}{k_L a}\right)(\tau_F - \tau_E)} e^{\left(\frac{-t}{\tau_F}\right)} + \frac{\tau_E^2}{\left(\tau_E - \tau_F\right)\left(\tau_E - \frac{1}{k_L a}\right)} e^{\left(\frac{-t}{\tau_E}\right)} \quad (15)$$

The area (α_1) below the electrode response curve, $(1 - \bar{C}_E)$ versus time, is given by

$$\alpha_1 = \int_0^{\infty} (1 - \bar{C}_E) dt = \frac{1}{(k_L a)_2} + \tau_E + \tau_F \quad (16)$$

The response times τ_F and τ_E are determined by a step change in oxygen concentration in the medium, carried out before inoculation (no cells present). The area (α_{IE}) below the response curve versus time is then given by

$$\alpha_{IE} = \int_0^{\infty} (1 - \bar{C}_E) dt = \tau_E + \tau_F \quad (17)$$

The difference between α_1 and α_{IE} then yields

$$\alpha_1 - \alpha_{IE} = \frac{1}{(k_L a)_2} \quad (18)$$

Thus, this method provides a simple procedure to evaluate $(k_L a)_2$ after a step change in the stirrer speed (N).

It is evident that, by returning the stirrer speed to its original value N_1 , the value of $(k_L a)_1$ can be obtained by means of a similar procedure.

Experimental Procedure

The experiment was carried out in the apparatus illustrated in Figure 4, with 20-L (0.020 m³) of culture medium in the tank.

The air flow rate (Q) was initially set to 12.0 SL·min⁻¹ (2.0·10⁴ Sm³·s⁻¹) and stirrer speed (N) to 400 rpm (6.67 s⁻¹), until the dissolved oxygen concentration given by the electrode (C_E) attained the saturation value (equilibrium). The electrode response time (τ_E) was obtained by placing the electrode in the tank after equilibration in an 0.1 M sodium sulfite solution (Na_2SO_3) ($C_E = 0$).

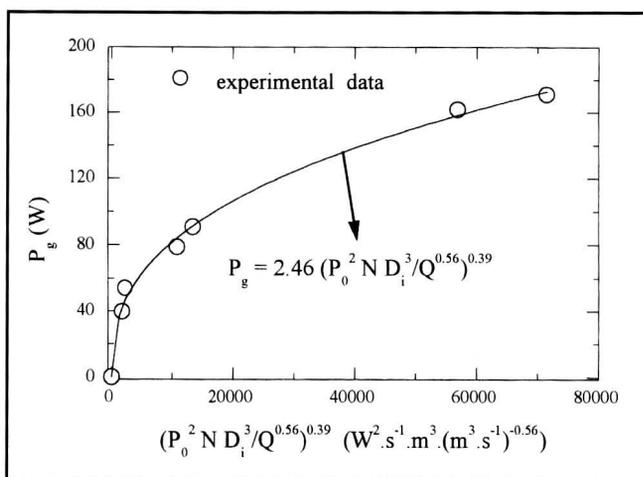


Figure 6. Experimental correlation between gassed (P_g) and ungassed (P_u) power requirements.

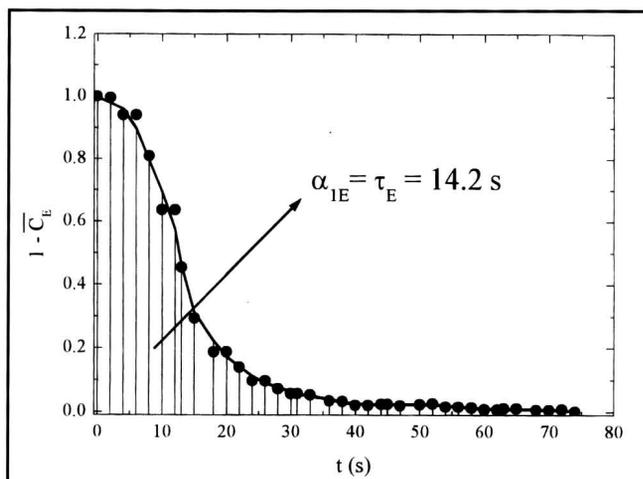


Figure 7. Electrode response in a step assay at 400 rpm (6.67 s⁻¹) in culture medium without cells.

The tank was inoculated by adding 0.40 kg of commercial Baker's yeast (40% on a dry basis), giving an initial cell concentration (C_x) of approximately $8 \text{ kg}\cdot\text{m}^{-3}$.

After inoculation, the air flow rate was kept at $12.0 \text{ SL}\cdot\text{min}^{-1}$, the stirrer speed was altered to approximately 250 rpm (N_1), and the first steady state was produced, with $C_E = C_{E1}$. The stirrer speed was raised to approximately 400 rpm (N_2) and the second steady state was reached, with $C_E = C_{E2}$. The stirrer speed was increased again to approximately 550 rpm (N_3), producing the third steady state, with $C_E = C_{E3}$. After the third steady state was reached, the stirrer speed was returned to approximately 400 rpm (N_2) and 250 rpm (N_1), respectively, as illustrated in Figure 8.

This experimental procedure was repeated at an air flow

rate (Q) of $18.0 \text{ SL}\cdot\text{min}^{-1}$ ($3.0\cdot 10^{-4} \text{ Sm}^3\cdot\text{s}^{-1}$) so that six values of volumetric oxygen transfer coefficient ($k_L a$) could be obtained. After the C_E curves were measured, the air flow rate (Q) was turned off and stirrer speed (N) adjusted to approximately 250, 400, and 500 rpm, respectively. For each agitation and aeration condition, the system recorded the gassed and ungassed power consumption (P_g and P_0).

The total duration of the experiment, which involved three stirrer speeds and two air flow rates, was approximately 2.5 hours.

RESULTS AND DISCUSSION

As described previously, the experiment is totally monitored and controlled through a microcomputer with a software supervisor. The students may alter any given variable and view its effect over time. Experimental data are recorded at 2-second intervals in the form of a binary file that is subsequently transformed into an ASCII file and transferred to a computer worksheet such as Excel®.

Figure 1 illustrates the main screen of the supervisor software and shows the variables, which can be manipulated by using the mouse and keyboard, such as the stirrer speed (N) and the air flow rate (Q). The response variables, which vary according to changes in the manipulated variables, appear in their respective fields, as do the power requirements (P) and the dissolved oxygen concentration given by electrode (electrode signal, C_E).

Power Requirements • Table 1 lists the values of power input in gassed (P_g) and ungassed (P_0) broth, monitored and controlled through a frequency inverter at various stirrer

speeds (N) and air flow rates (Q). As can be seen, the gassed power requirements (P_g) are lower than the ungassed values (P_0) under the same agitation condition (N), which is due to the fact that the introduction of gas into the fluid decreases its apparent density (ρ). It can also be observed that an increase in stirrer speed (N) raises the power requirements (P_0 and P_g), indicating the strong influence of viscous forces in the operation of this important unit.

Gassed power consumption values (P_g) were correlated with the ungassed power consumption (P_0), stirrer speed (N), air flow rate (Q), and the impeller diameter (D_i) through a well-known equation proposed by

TABLE 1
Power Requirements for Various Conditions of Agitation (N) and Aeration (Q)

$N(\text{s}^{-1})$	$Q\cdot 10^4(\text{Sm}^3\cdot\text{s}^{-1})$	$P_0(\text{W})$	$P_g(\text{W})$	$\frac{P_0^2 ND_1^3}{Q^{0.56}} \left[\text{W}^2 \text{s}^{-1} \text{m}^3 (\text{m}^3 \text{s}^{-1})^{-0.56} \right]$
4.15	2.0		53.9	2,228.4
4.18	3.0	51.4	39.7	1,791.5
6.81	2.0		90.8	13,389.7
6.85	3.0	98.3	78.7	10,743.0
9.35	2.0		171.0	71,794.9
9.37	3.0	193.5	161.8	56,850.8

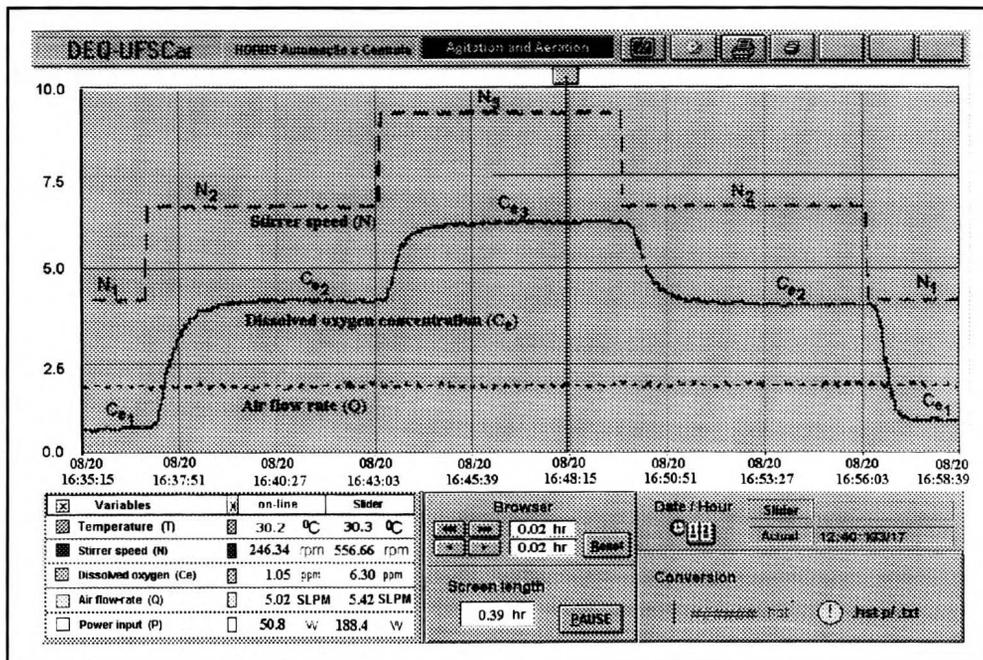


Figure 8. Supervisory screen for viewing the changes occurring during a run.

$$P_g = 2.46 \left(\frac{P_0^2 N D_i^3}{Q^{0.56}} \right)^{0.39} \quad R^2 = 0.995 \quad (19)$$

The experimental data and fitting equation are illustrated in Figure 6. The high correlation coefficient indicates that the equation represents closely the data obtained from the experimental system.

Oxygen Transfer • Similar values of electrode response time (τ_E) were obtained in triplicate assays at a stirrer speed of 400 rpm (6.67 s^{-1}). The resistance of the liquid film covering the membrane of the electrode was considered negligible in the range of stirrer speeds studied. Thus, $\tau_F = 0$, and from Eq. (17), $\alpha_{1E} = \tau_E$. Figure 7 illustrates a typical electrode response curve obtained in the culture medium at 400 rpm (6.67 s^{-1}).

Figure 8 shows the supervisory window where the students can view changes occurring in the dissolved oxygen concentration given by the electrode (C_E) after step changes in the stirrer speed (N), with the air flow rate (Q) maintained constant, as described in the methodology of Mignone and Ertola^[8] for $k_L a$ determination. In the actual window, the variable profiles appear in color, but to facilitate viewing here, the profiles of Q , N , and C_E are illustrated, respectively, with dashed, dotted, and solid lines, and temperature, air flow rate, and power requirement were omitted.

Figure 9 shows typical curves of the electrode response after the stirrer speed is subjected to sudden changes. The symbols (\bullet and \square) represent experimental data acquired and stored by software, which are linked by smooth lines. According to the methodology proposed by Mignone and Ertola,^[8] the area below the response curve obtained by plotting $1 - \bar{C}_E$ vs time corresponds to

$$\alpha_1 = \int_0^{\infty} (1 - \bar{C}_E) dt = \frac{1}{(k_L a)_2} + \tau_E + \tau_F \quad (20)$$

and given $\tau_F = 0$ and $\tau_E = 14.2 \text{ s}$, $k_L a$ values in the second steady state ($(k_L a)_2$) can be determined by Eq. (21)

$$\alpha_1 - \alpha_{1E} = \frac{1}{(k_L a)_2} \quad (21)$$

Table 2 shows the results of $k_L a$ measurements at different values of air flow rate (Q) and stirrer speed (N), as well as the variables of gassed power consumption per unit volume of broth (P_g/V) and superficial gas velocity (v_s) calculated for the experimental conditions used.

Experimental data for $k_L a$, determined by the proposed method, ranged from 0.0187 to 0.0469 s^{-1} ($67.3 - 168.8 \text{ h}^{-1}$), in complete agreement with the various agitation and aeration conditions tested. Therefore, the results confirm the method's reliability and consistency.

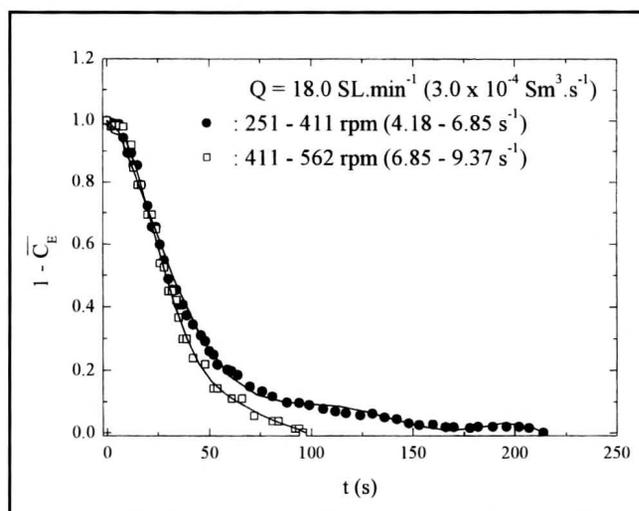


Figure 9. Electrode response at a constant air flow rate ($Q = 3.0 \times 10^{-4} \text{ Sm}^3 \text{ s}^{-1}$), after the following step changes in stirrer speed:

- (\bullet) 251-411 rpm (4.18 - 6.85 s^{-1}); $k_L a = 0.0346 \text{ s}^{-1}$;
- (\square) 411-562 rpm (6.85 - 9.37 s^{-1}), $k_L a = 0.0469 \text{ s}^{-1}$;
- (—) continuous lines.

TABLE 2
Results of $k_L a$ Measurements at Various Air Flow Rates (Q) and Stirrer Speeds (N)

$N(\text{s}^{-1})$	$Q \cdot 10^4 (\text{Sm}^3 \text{ s}^{-1})$	$P_g/V (\text{Wm}^{-3})$	$v_s \cdot 10^3 (\text{ms}^{-1})$	$k_L a (\text{s}^{-1})$
4.15	2.0	2,695	3.25	0.0187
4.18	3.0	1,985	4.87	0.0201
6.81	2.0	4,540	3.25	0.0253
6.85	3.0	3,935	4.87	0.0346
9.35	2.0	8,550	3.25	0.0331
9.37	3.0	8,090	4.87	0.0469

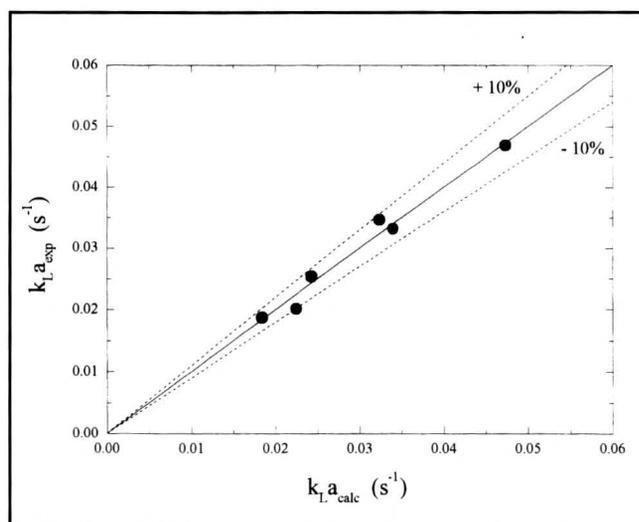


Figure 10. Comparison of the experimental values of $k_L a$ compared with the values of $k_L a$ calculated by the equation (Eq. 1) proposed by Cooper, et al.^[6]

As mentioned earlier, the most classical relation for the volumetric oxygen transfer coefficient ($k_L a$) in agitated and aerated tanks, proposed by Cooper, *et al.*,^[6] is given by Eq. (1). This equation was fitted to the experimental values and the parameters were estimated through nonlinear regression.^[9] The criterion for the best fit and parameter optimization was the sum of squares of residuals (SSR). The fitted correlation is

$$k_L a = 0.046(P_g / V)^{0.53} (v_s)^{0.89} \quad R^2 = 0.98 \quad (22)$$

The parameters estimated by the nonlinear regression are unequivocally within the range of values mentioned in the literature.^[10]

Figure 10 illustrates the congruence between the experimental $k_L a$ values and the data calculated by Eq. (22). The correlation coefficient (R^2), as well as Figure 10, demonstrate that a good fit was obtained, indicating that Cooper's correlation (Eq. 1) can be used to estimate, with good precision, the volumetric oxygen transfer coefficient ($k_L a$) in these systems.

CONCLUSIONS

- The experiment can be completed rapidly, *i.e.*, in about 2 1/2 hours, which is appropriate for an undergraduate experimental class.
- All the transient phenomena can be monitored and controlled on-line by the students, and the data can be stored for subsequent manipulation and calculation. This procedure, which is typical of an industrial supervision process, puts students in direct contact with a reality they will face in their careers as process engineers.
- The easy handling of data facilitates data processing in optimization programs for the industrial operation processes the students are learning to deal with.
- Student training in automated laboratory facilities that simulate industrial processes offers opportunities for acquiring and enhancing their professional skills in today's competitive industrial environment.

NOMENCLATURE

C_1	constant of Eq. (1)
C_2	constant of Eq. (3)
C	dissolved oxygen concentration in the broth in steady state ($\text{kgO}_2\text{m}^{-3}$)
C^*	dissolved oxygen saturation concentration in the broth ($\text{kgO}_2\text{m}^{-3}$)
C_E	dissolved oxygen concentration given by the electrode or electrode signal ($\text{kgO}_2\text{m}^{-3}$)
C_F	dissolved oxygen concentration on stagnant film ($\text{kgO}_2\text{m}^{-3}$)
\bar{C}_E	dimensionless electrode signal (-)

\bar{C}_F	dimensionless oxygen concentration on diffusion film (-)
C_X	cell concentration ($\text{kg}\cdot\text{m}^{-3}$)
D_i	impeller diameter (m)
D_t	tank diameter (m)
$k_L a$	volumetric oxygen transfer coefficient (s^{-1})
N	stirrer speed (s^{-1} or rpm)
OTR	oxygen transfer rate ($\text{kgO}_2\text{m}^{-3}\text{s}^{-1}$)
OUR	oxygen uptake rate ($\text{kgO}_2\text{m}^{-3}\text{s}^{-1}$)
P	power consumption (W)
P_0	ungassed power consumption (W)
P_g	gassed power consumption (W)
Q	air flow rate (Sm^3s^{-1} or $\text{SL}\cdot\text{min}^{-1}$, where S indicates standard condition: 0°C and 1 atm)
Q_{O_2}	specific oxygen uptake rate ($\text{kgO}_2\text{kg}^{-1}\text{s}^{-1}$)
$Q_{O_2} C_X$	global oxygen uptake rate ($\text{kgO}_2\text{m}^{-3}\text{s}^{-2}$)
R^2	correlation coefficient (-)
t	time (s)
v_s	superficial air velocity (ms^{-1})
V	broth volume (m^3)

Greek Letters

α	constant of Eq. (1)
β	constant of Eq. (1)
α_1	area below the response curve obtained by plotting $1 - \bar{C}_E$ vs time during cell growth (s)
α_{1E}	area below the response curve obtained by plotting $1 - \bar{C}_E$ vs time after step assay (s)
θ	constant of Eq. (3)
τ_E	electrode response time (s)
τ_F	film response time (s)

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INTEGRATING BIOLOGY AND ChE AT THE LOWER LEVELS

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Instilling a working knowledge of biological principles in students and developing their ability to apply engineering principles to biological systems (and vice versa) is recognized nationwide as a goal for chemical engineering programs.^[1-5] Many schools offer specialized bio-focused curricula or courses at the senior or graduate level,^[6-8] and there is a significant movement to change chemical engineering department names to reflect faculty expertise in bio-focused engineering. Integration of biology and chemical engineering at the lower levels, however, is difficult in an already overloaded curriculum.

We have developed an integrated, collaborative approach between engineering and biology faculty to introduce chemical engineering students to the application of engineering principles in biological systems at the lower levels. Through specially designed courses and active learning modules that can be easily adapted to any course, students are exposed to this newest pillar of the chemical engineering curriculum.

The systematic implementation of this philosophy exposes students to key areas of collaboration between biologists and chemical engineers in the early stages in their undergraduate education. This strategy also enables faculty to build increasing detail and technical content into problems and projects that address the interface between biology and engineering as students progress through the curriculum because students develop a cumulative knowledge of biological principles.

Revisions to the chemical engineering curriculum include a "Biological Systems & Applications" (BS&A) course designed to introduce students to a variety of biological principles that are directly relevant to chemical engineering. Additionally, several laboratory modules and projects that can be easily incorporated at the freshman and sophomore levels have been developed. These modules include reverse engineering of the human body, reverse engineering of the beer-

making process, and design of a microbial fuel cell.

These modules in the freshman year expose students to chemical engineering principles as they apply to living systems. The BS&A course, specifically designed for sophomore chemical engineering students and taught by faculty in biology, introduces students to a wide variety of topics, from prokaryotic and eukaryotic regulatory systems to food microbiology. A sophomore-level engineering project on microbial fuel-cell design reinforces concepts in microbial growth and nutrition that are covered in the BS&A course.

This collaborative approach to integrating biology and chemical engineering helps prepare students for industrially sponsored projects at the junior and senior level, and for careers in the food, biotechnology, and pharmaceutical industries. The projects, courses, and activities that we describe in this paper address key areas in which chemical engineering

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Gregory B. Hecht has extensive research experience in prokaryotic genetics and molecular biology. With Dr. Mosto, he has developed a new course for chemical engineering students, "Biological Systems & Applications." He is the creator and coordinator of the Rowan University Student Research Symposium, an annual forum at which Rowan students from all of the STEM disciplines present the results of their independent research.

Patricia Mosto has extensive environmental science experience. She has been actively involved with field and laboratory projects related to water quality and water pollution issues for the last thirty years. She worked with the Department of Water and Power and the Department of Sanitation in Los Angeles for ten years. During her ten years at Rowan, she has supervised 41 independent undergraduate projects, taking many students to national and international conferences.

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and biology have a strong connection, such as bioprocess engineering (biochemical reaction engineering for production of commodities and waste treatment), bioseparations, biocatalysis, and metabolic engineering. We will discuss the implementation and impact of these modifications in the engineering curriculum.

EXPERIMENTS AT THE FRESHMAN LEVEL

A two-semester freshman clinic sequence introduces all freshman engineering students to engineering at Rowan University. In the clinic we immediately establish a hands-on, active learning environment for the reason explained by scientist and statesman Benjamin Franklin: "Tell me and I forget. Show me and I may remember. Involve me and I understand." Multidisciplinary engineering experiments using engineering measurements are the common theme of the first semester of the clinic, while in the second semester, students reverse engineer a product or process. In the following paragraphs, we describe two experiments that have been incorporated in the first and second semesters of this unique course sequence. The experiments, of varying lengths (from one three-hour lab to a semester project), illustrate various methods for integrating biological concepts at the lower levels.

Biomedical Experiment • The human body is an exquisite combination of interacting systems that can be analyzed through the application of chemical engineering principles. Familiar examples include fluid flow of blood through arteries and veins, mass transfer in the lungs, pumping of the heart, and chemical reactions in cells. Biomedical topics in chemical engineering are explored in many curricula through advanced-level elective courses, and they are sometimes worked into homework problems in core courses. Freshman and sophomore chemical engineering students are rarely exposed

to real biomedical applications of their discipline, however, and are unaware of the analogies between physiologic systems and chemical engineering operations.

We developed a freshman-level experiment that is used to introduce students to a wide range of chemical engineering principles through their application to physiological processes. The details of the experimental procedure and analysis are provided elsewhere.^[9] Students take measurements of physiologic variables both at rest and during exercise, and then perform engineering calculations that involve basic principles of mass and energy balances, fluid flow, chemical reactions, energy expenditure, mechanical work, and efficiency.

During the three-hour experiment, students measure volumetric breathing rate and heart rate both at rest and during exercise on a bicycle ergometer. They also measure blood pressure at different elevations in the body using a blood pressure cuff (sphygmomanometer). Students use their physiologic data for breathing rate and heart rate to estimate their rate of oxygen consumption, blood flow rate, and rate of energy expenditure. The blood pressure measurements are used to calculate hydrostatic pressure differences to compare with expected values. This experiment provides an initial exposure to a variety of principles from engineering, physiology, and cellular metabolism, and provides motivation and framework for future courses on related topics.

Reverse Engineering of Beer Production • The theme of the second semester is the reverse engineering of a commercial product or process. Previous reverse engineering projects have involved products such as automatic coffee makers,^[10-12] hair dryers, and electric toothbrushes.^[13] One of these semester-long modules, an investigation of the beer production process, incorporates the biology and reverse engineering of a *biochemical process* into our freshman clinic. A detailed structure of the course has been previously described.^[14-15] In this paper we describe the integration of principles from biology and engineering into this introductory, multidisciplinary engineering course. The principles are summarized in Table 1.

Near the beginning of the laboratory-intensive part of the project, a biology professor gives a guest lecture to provide an overview of the biological processes involved in the production of beer. The addition of this guest lecture emphasizes not only the interdisciplinary aspects of biochemical processes, but also illustrates the collaboration between engineering and biology faculty and the importance of multidisciplinary teamwork. Once this foundation is laid, students work in teams to investigate and reverse engineer the major steps of beer production.

TABLE 1
Biological Principles and Topics
Related to Beer Production

<i>Principles/Topic</i>	<i>Where Applicable</i>
Germination and enzyme production	Malting
Enzymatic reactions	Starch hydrolysis to sugars during mashing; protein breakdown to amino acids during mashing
Yeast growth curve	Fermentation process
Fermentation	Fermentation
Fermentation monitoring	Fermentation
Disinfection and contamination	Fermentation and sampling

The students' investigation focuses on three of the major steps of the brewing process: mashing, boiling, and fermentation. The brewing process is shown in Figure 1. Mashing is the first major step in the brewing process. Using the raw materials of malted barley and water, this process produces a nutritionally complete wort for fermentation. Students mash both malted and unmalted barley and then compare the worts obtained from each type. Analyses of the total extract and concentrations of fermentable sugars using an enzyme test kit reveal that only the malted barley produces a wort containing fermentable sugars, as shown in Figure 2.

After mashing, the wort is boiled for stabilization and chilled rapidly to avoid contamination. Yeast is added and the fermentation process takes place over the next 8 to 14 days, with most vigorous fermentation occurring within the first three days. Students may also perform experiments to determine yeast viability and activity.

The fermentation process provides an impressive visual show of biological systems in action. As the fermentation proceeds, students can observe changes in color and turbidity, the formation of bubbles, and eventually the settling of yeast. The fermentation pathway and yeast growth curves are followed analytically as sugars are consumed to produce more yeast, alcohol, and carbon dioxide; analytical measurements include yeast, sugar, alcohol concentrations, and pH. Students also learn about disinfection techniques and contamination issues as they clean and sterilize the glassware and other supplies used for fermentation and subsequent sampling. At the end of the experiment, engineering problems such as disposal of wastewater, organic wastes, and biochemical oxygen demand may be addressed.

EXPERIENCES AT THE SOPHOMORE LEVEL

The two freshman-level modules discussed above introduce the interplay between biology and engineering using familiar systems. These modules also expose students to two different areas in which engineering principles can be applied to biological systems: 1) using engineering principles for analysis in biomedical applications (reverse engineering of human body) and 2) using engineering principles for manipulation of microbial cultures to generate products for human use (beer-making process). The experiments illustrate basic principles and excite students about careers for which a chemical engineering degree can prepare them.

Before tackling in-depth analysis and manipulation of biological systems using engineering principles, however, students must have a firm grounding in biological principles that only a course can provide. A chemical

engineer who is well-versed in biological, biochemical, and microbiological applications is an attractive candidate for employment in the pharmaceutical, biotechnology, and food manufacturing industries. To meet the anticipated growing demand for biology-literate engineers in these industries, biological sciences and chemical engineering faculty worked closely together to develop a course that prepares chemical engineering students for these careers. The 4-credit, lab-intensive course is open only to fall-semester sophomore chemical engineering majors who have completed Advanced Chemistry I. Concurrently with this specially designed biology course, students also are enrolled in a multidisciplinary engineering course that has a biological component.

Biological Systems and Applications Course • The BS&A course was designed to meet the following four objectives:

1. To provide engineering students with a basic understanding of fundamental biological principles and a working vocabulary that would enable them to expand their knowledge base during their academic and professional careers.
2. To convey to the students an appreciation of the wide variety of engineering applications that are related to the fields of biochemistry, cell biology, genetics, general microbiology, and environmental microbiology.
3. To provide laboratory experiences that teach "hands-on" mechanical skills such as micropipetting and culturing techniques.
4. To provide additional laboratory experiences that collectively instill in the students a general "biology common sense" that can be applied to work in any microbiology laboratory or project.

Beyond the basics of cell and membrane biology, highlights in the lecture portion of the course include units about prokaryotic and eukaryotic regulatory systems, biotechnology, genomics, microbial growth and nutrition, the physiological diversity of microbes, environmental microbiology, industrial microbiology applications and concerns, and food mi-

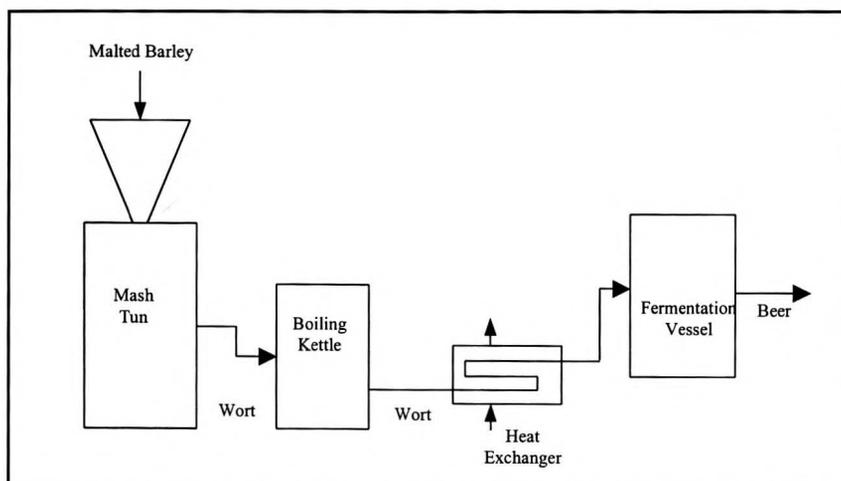


Figure 1. Schematic representation of the brewing process showing major process steps.

crobiology. The laboratory exercises in the course are all devoted to skill development and/or directly connected to lecture topics.^[16] The BS&A course has benefited from using the “project-based” learning approach^[17] and from strong interactivity between chemical engineering and biological sciences faculties. Extensive assessment data demonstrating the effectiveness of the course have been presented elsewhere.^[16]

Microbial Fuel Cell Semester Project • Chemical engineering students who are taking the BS&A course also take Sophomore Clinic I, a multidisciplinary engineering design-and-practice course that is integrated with technical communications. It combines a 1-credit multidisciplinary engineering laboratory with the 3-credit college composition and rhetoric requirement and is co-taught by engineering faculty and composition/rhetoric faculty.^[18] The 1-credit lab for the course includes a semester-long project in which student teams design and create a microbial fuel cell(MFC) that powers a

Lego® Mindstorms robot. The project combines mechanical, chemical, civil/environmental, and electrical/computer engineering skills. Students determine how changing certain fuel cell parameters and conditions affect voltage and current, then construct a Lego Mindstorms robot that derives its energy from a MFC stack. The project reinforces concepts from earlier courses such as chemistry, biology, and physics.

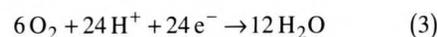
Fuel cell technology and alternative energy sources such as biofuels and photovoltaics are developing technologies that are exciting to students. MFCs operate on the same principles as the more widely used (and more powerful) hydrogen fuel cells. Rather than a nonrenewable source such as natural gas, however, MFCs use biomass as the substrate and microorganisms as the catalyst. While MFCs in which various types of substrates and waste products are converted to energy by a range of microorganisms, this project focused on yeast as the catalyst and glucose as the primary substrate.

The project was inspired by the University of South Florida’s research on the “Gastrobot,” (a self-sustaining, semi-autonomous robot^[19,20]) and educational materials available from the National Centre for Biotechnology Education at the University of Reading.^[21-24] This combination of readily available educational kits and supplies (see <<http://www.ncbe.reading.ac.uk>> for supplies) and accessible literature (see <<http://www.eng.usf.edu/~wilkinso/gastrobotics/>>) that describes cutting-edge research makes the project feasible yet stimulating for the students.

A microbial fuel cell takes advantage of the metabolic reactions of microbes to generate electricity. Organisms carry out the following respiration reaction:



to draw energy from food or carbohydrates.^[21] The above reaction can be broken down as shown in Eqs. (2) and (3)



which follows the activity of electrons.

A redox mediator (methylene blue) can traverse the cell membrane and scavenge electrons from intermediates in which the electrons are stored. The mediator can then present these electrons to an electrode, and if an electron sink is provided (potassium ferricyanide), the circuit is completed. This process is shown in Figure 3. Voltage and current can be monitored using a multimeter. A single microbial fuel cell is capable of producing approximately 0.5 V.

The microbial fuel cell project introduces and reinforces several key concepts (summarized in Table 2): stoichiometry, cells as biocatalysts, cell

TABLE 2
Biological Principles and Topics
Related to Microbial Fuel-Cell Design

<i>Principle/Topic</i>	<i>Where Applicable</i>
Reaction stoichiometry/yield	Calculating theoretical yield of electrons based on initial glucose concentrations
Metabolic pathways	Investigating pathways for metabolism of glucose
Yeast growth curve, doubling time, fermentation	Determining “feeding time” for cell to continuously produce current
Fermentation monitoring	Current and glucose monitoring

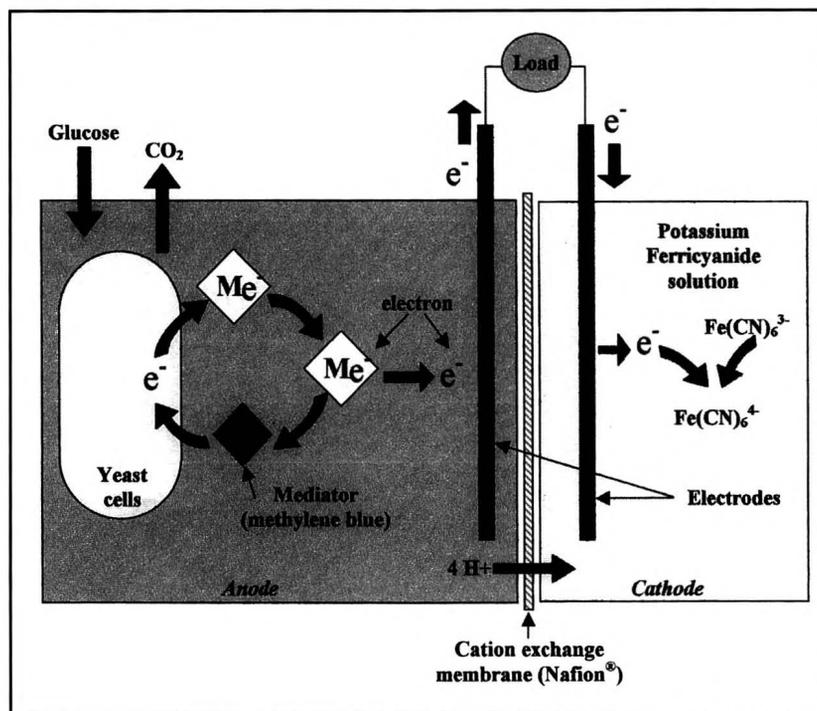


Figure 3. Microbial fuel cell schematic, adapted from Ref. 20.

metabolism, and modeling of the system to enhance design and performance. Student teams are asked to design a microbial fuel cell based on optimization experiments performed with a prototype. They investigate the effect of glucose and yeast concentration on voltage and current produced by the cell. As the yeast consumes the glucose, the current produced drops until no glucose remains and the cell is unable to produce current. By varying the initial amount of glucose and yeast and plotting the concentrations of these two variables, students are introduced to the kinetics of batch fermentation.

IMPACT ON THE CURRICULUM

The combination of experiments and modules at the freshman and sophomore level and a Biological Systems & Applications course specifically designed for chemical engineers helps prepare students for research and industrial projects at the junior and senior levels. As part of the clinic sequence at Rowan, students participate in sponsored research projects during their junior and senior years. Each semester, students work in multidisciplinary teams as part of a 2-credit course. Project funding is provided through government or industrial grants or sponsorships. Located in southern New Jersey, Rowan interacts with many companies in the pharmaceutical and food industries through its junior/senior clinic sequence. Accordingly, the chemical engineering faculty's expertise reflects this bio-intensive regional interest; over half of our faculty have training in biomedical, bioprocess, and biotechnology fields. This research interest is reflected in the types of projects offered in the junior/senior clinic, from experiment development in drug delivery to the effect of packaging conditions on product spoilage.

Students often cite a potential career in biochemical engineering as the motivator for pursuing a chemical engineering degree. This interest in the interplay between biology and engineering is apparent in the student demand for bio-oriented research projects at the junior and senior levels. One measure of student interest in bio-related projects is their participation in the University's Science, Technology, Engineering, and Math (STEM) Symposium. As shown in Figure 4, the percentage of bio-related engineering projects presented at the symposium has increased from 10% in 1998 to almost 50% in 2002.

In some cases, such as the Food Microbiology laboratory exercise, the lab component of the BS&A course has directly benefited students working on research projects. In an industrially sponsored clinic project in which the effect of packaging on food spoilage was studied, a (junior) student who had taken the BS&A course became the leader of the group and taught the other members (two seniors) the techniques necessary for determining bacterial counts. This student's experience in the course helped the group hit the ground running. As the beginning cadre of students who have been exposed to these innovations in the curriculum progress, we expect to

see similar results in future junior/senior clinic projects, as well as in engineering courses that have a biotechnology or bioengineering component.

Like many chemical engineering schools, Rowan offers several bio-related technical electives at the senior and graduate-student level on a rotating basis. Students may enroll in courses on drug delivery, biomedical engineering, or biochemical engineering. Other courses at this level, such as food engineering, polymer engineering, and membrane process technology, have increasing applications in the biotechnology and pharmaceutical industries. Preparing students with a course in biological systems and bio-related modules during their freshman and sophomore years aids in developing material for these courses that explore the link between biology and chemical engineering at a much deeper level. Additionally, we anticipate being able to cover more material and applications in the time that is traditionally spent in an introduction to biological principles.

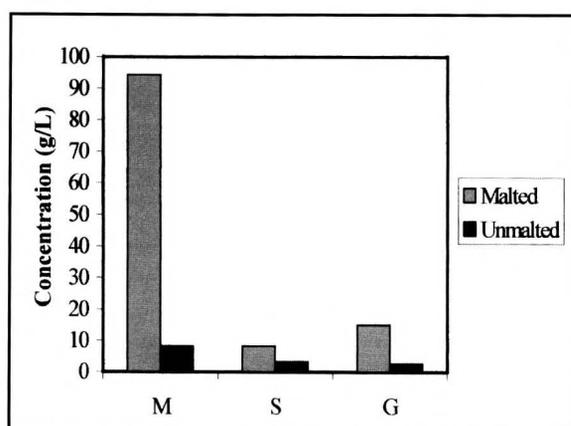


Figure 2. Fermentable sugars in the wort from malted and unmalted barley: M=Maltose; S=Sucrose; G=Glucose

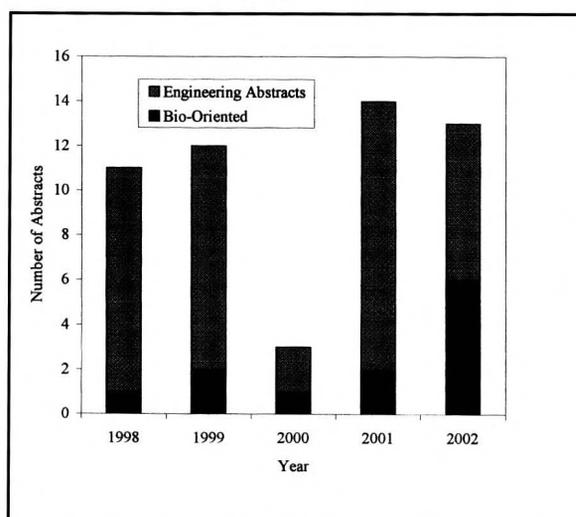


Figure 4. Number of bio-oriented abstracts and total abstracts submitted by engineering students at Rowan's STEM Symposium.

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Random Thoughts . . .

WE HOLD THESE TRUTHS TO BE SELF-EVIDENT

In 1991 I wrote a column listing several widely accepted academic myths for which I've never seen a shred of evidence. I glanced over it today to see if anything has changed in the intervening 13 years. It hasn't. So, I'll re-run it. Tune in again in 13 years.

Rich

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Being engineering professors, we all know about the need to make assumptions... and we also know that if the assumptions are invalid, the results can be worthless. We learn early in our careers to check our results (*Does the model fit the data? Does the algorithm converge? Does the product meet quality specifications?*) and if they are not satisfactory, to question our assumptions (*Is the solution ideal? Is the reactor isothermal? Is flow laminar?*), and we try to develop the same critical, questioning mentality in our students.

When it comes to education, however, our mentality changes. We generally do whatever it is we do without much critical evaluation of how well or how poorly it is working, and we accept without question what Armando Rugarcia^[1] calls *academic myths* - assumptions that have never been shown to have any basis in reality and often defy common sense. Here are some of them.

MYTHS ABOUT . . . FACULTY RECRUITMENT

- People who (1) don't have Ph.D.s , or (2) have spent their careers in industry and have no research publications, are not qualified to be engineering professors.
- When filling faculty vacancies, an engineering department benefits most by selecting the candidates in the hottest and years is more important than whether they know enough engineering to teach the core courses and to change research areas if their present one goes out of fashion.
- The best way to handle required courses that no one wants to teach, such as the unit operations laboratory or the

capstone design course, is to rotate the faculty so that no one gets stuck with them too often. An inferior solution is to fill a vacant faculty position with someone who has the desire to teach these courses and the expertise to teach them well.

- When selecting a department head, the faculty benefits most by choosing the candidate with the strongest research record, regardless of administrative experience or ability. How he or she runs the department in the next five to ten years is less important than what he or she does in research after that.

MYTHS ABOUT . . . RESEARCH AND TEACHING

- Excellence in research and excellence in teaching are highly correlated.
- Requiring EVERY faculty member to build up a strong research program as a condition for promotion and tenure is in the students' (professors', department's) best interests.
- Excusing new professors from teaching responsibilities



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so they can write proposals is a good thing to do. Excusing them from research responsibilities so they can develop a couple of good courses makes no sense.

- Professors who are excellent at research and mediocre-to-adequate at teaching deserve tenure. Professors who are excellent at teaching and mediocre-to-adequate at research don't.

MYTHS ABOUT . . . CURRICULUM DESIGN AND PEDAGOGY

- Our graduates routinely say they never use 90% of what we taught them. Since we're engineering professors, 90% of what they're doing must not be engineering.
- It makes sense educationally to teach students a generalized theory (e.g., transport theory) before teaching them anything about the specific phenomena and devices that the theory was invented to describe (e.g., unit operations).
- Tensor calculus, quantum chemistry, and statistical mechanics should be taught to every chemical engineering undergraduate; statistical process control, project management, and technical writing they can pick up on their own—there's no room for those subjects in our crowded curriculum.
- The best thing to do with ethics, safety, environmental science, and all those other important things ABET says we have to teach, is stick them all in the capstone design course.
- I accomplish something useful when I spend fifty minutes in class writing detailed derivations on the chalkboard for the students to copy.
- We can't teach students to think critically or creatively—they can either do it or they can't.
- Students who complain that our lectures have nothing to do with the real world don't know anything about the real world—and we do.
- If I have covered the syllabus, I have done my job successfully.

MYTHS ABOUT . . . EVALUATION OF STUDENTS (GRADING)

- How well our students will do as engineers correlates highly with (a) their undergraduate GPA; (b) their ability to solve problems with unfamiliar twists on 50-minute

exams; (c) anything else that we typically use to evaluate them.

- An average score of 40 on my final exam proves (a) I set high standards; (b) they didn't understand the material. There is no possibility that it proves (c) the test was lousy.
- An average score of 85 on your final exam proves (a) it was a trivial test; (b) you're a soft grader; (c) there was widespread cheating. There is no possibility that the result proves (d) they learned the material.

MYTHS ABOUT . . . EVALUATION OF TEACHING

- All methods of evaluating teaching are unreliable, and student evaluations are the most unreliable of all.
- If you get consistently outstanding student evaluations, it must be because you are (a) an easy grader; (b) an "entertainer." It is certainly not because you are (c) an outstanding teacher.
- If I get rotten student evaluations it is because (a) the students are ignorant and lazy; (b) I don't water down the material for them; (c) they don't understand what I am doing for them now but in later years they'll come back and thank me. It is **definitely** not because (d) I am doing a rotten teaching job.

I could go on, but you get the idea.

When I classify these points as myths I am not saying there's nothing to them; it's just that as far as I know they've never been scientifically or even empirically validated. (Mentioning someone who is great at both teaching and research, for instance, doesn't quite do it.) If you can justify one or another of these assumptions, let me know and I'll set the record straight.* If, on the other hand, you conclude that the assumptions might be faulty, then how about considering whether some alternative assumptions might lead to better ways of doing things? Couldn't hurt.

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* Before you attempt it, though, you might want to check out the literature: McKeachie^[2] provides invaluable summaries of the research on most of the topics in question, and Rugarcia^[1] makes some interesting points specifically on the research/teaching dichotomy. □

All of the *Random Thoughts* columns are now available on the World Wide Web at
http://www.ncsu.edu/effective_teaching and at <http://che.ufl.edu/~cee/>

IMPROVING COHERENCE IN TECHNICAL WRITING

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It is a well-recognized fact that effective technical communication is a skill that graduate/undergraduate students in engineering disciplines need to develop, and many good suggestions have been made^[1-6] to improve it. Although good communication involves good skills in writing, speaking, reading, and listening (<www.writing-reading.com> accessed on 3 Feb 2003), we usually concentrate on developing only the speaking (presentation) and writing skills in students. Between the two, it is usually more difficult to develop good writing skills, probably because it requires higher clarity and rigor in the thought processes. Furthermore, there is a general notion that one learns to write well in the same way that one learns to ride a bicycle, to play a musical instrument,^[7] or to swim—in an experiential manner.

When graduate students write their first manuscripts, spelling and grammatical aspects are addressed first, either by a person comfortable with the language or by a word processor. A grammatically correct document may not always read well, however. Often, advisers know that the manuscript is not written well, but cannot clearly explain why. They tend to talk about “clarity” and “style” (as distinct from that described in the Chicago or the American Chemical Society style manuals), and further confuse the student. Ultimately, the adviser might say something like, “It’s all in there—you just need to communicate it better,” and without further direction, ask the student to rewrite the paper.

Students typically rewrite their first manuscript many times, and the writing improves intuitively with each progression. Throughout this process, it is helpful if the student reads well-written scientific literature.^[8] When the adviser finally accepts the manuscript, the student knows that the final draft is written better, but is usually not aware of *why* the paper is improved. These same students later become professors/advisers, attesting to the fact that university teaching is probably the only skilled profession for which there is no formal

training (<www.ncsu.edu/felder-public/RMF.html> accessed on 3 Feb 2003), and the cycle continues.

This article presents a reasonably structured approach that faculty members can use to improve the writing skills of students. Alternatively, it also provides a direction for the not-so-experienced writers of scientific material to consciously improve their writing skills.

COHERENCE

Good communication, in either written or oral form, results from a solid knowledge of the subject, a clear awareness of the aspects that need to be communicated (and those that need to be left out), clear thinking, and good organization, assuming that the language (grammar, spelling, and pronunciation) are also addressed. For the most appropriate organization, one should be aware of how the reader/listener will perceive the information. In other words, one needs the ability to “tell a story,” or the ability to coherently present *relevant* material. In fact, many advisers ask the question, “What is your story?” when they discuss a student’s research work. The above requirements are even more critical in written communication because the communicator is not present when the receiver reads the document, unlike an oral presentation when the communicator can draw on nonverbal communication cues to bolster the material.



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A fairy tale is a good example of coherent presentation. Children can listen to a fairy tale being read and completely understand the story, even if they are sleepy at the time. If engineering students could embrace the same simplicity and coherence embodied in a fairy tale when they present scientific material, their message would be more easily understood.

This idea led to an exercise for students taking a M.Tech (graduate level) communication skills course at the Indian Institute of Technology, Bombay. They were required to narrate a fairy tale in front of the class. Many of them could not coherently narrate even a simple fairy tale such as Cinderella the first time they tried. One example: "Cinderella is that girl who wore a shoe. The Prince found her with the shoe. She went to the ball in a chariot made from a pumpkin. There was a fairy that helped her. While running away from the ball she lost one of her shoes. Cinderella had a wicked stepmother and two stepsisters...." A chronological organization of information, a crucial requirement for delivery of the tale, was completely absent.

Faculty members quite often find the same type of disorganization in a first draft of a report or manuscript written by a student. The presentation is a recital of mere facts, written in the order of recall without bothering about the relationship between them.

There is an important distinction between a fairy tale and a scientific narrative, however—the concept of external and internal times.^[9,10] External time refers to the time taken for the actual presentation and internal time refers to the duration of the sequence of events in the presentation. For example, if narrating the Cinderella story takes fifteen minutes, then the external time is fifteen minutes; the internal time is the days or months or years over which the story is set. While external time is relevant for both types of presentations, the internal time is normally absent in a scientific narrative (except, perhaps, in a background/introduction section). Instead of a chronological detailing of internal time, a logical sequence of scientific information (facts, graphs, tables, derived information, discussion, etc.) is present. Students usually develop this ability to present material in a logical sequence through experience.

TOOLS FOR COHERENCE

Students can be encouraged to develop a logical sequence of presentation, as described in a later section. Here we will consider the tools that can be used to improve coherence (see <papyr.com/hypertextbooks/engl_126/book126.htm> accessed 3 Feb 2003) and communication of the material after it is logically sequenced.

To appreciate the use of tools, consider this well-written passage by Bird,^[11] which has been slightly adapted:

In educational circles today we hear a great deal about teaching and research. However, we hear very little about the activity of book-writing, which ought to be included as a third principal activity of a university teacher since it is concerned directly with the production, evaluation, organization, and dissemination of new knowledge.

Good communication, in either written or oral form, results from a solid knowledge of the subject, a clear awareness of the aspects that need to be communicated (and those that need to be left out), clear thinking, and good organization, assuming that the language (grammar, spelling, and pronunciation) are also addressed.

Therefore, I thought it might be useful to use this lecture to focus attention on the "rites, rewards, and responsibilities" of book authorship. Since I have had the pleasure and good fortune to coauthor several books, perhaps I can offer some appropriate words of encouragement to aspiring writers and even a few helpful suggestions regarding the art of writing. Maybe I can help others avoid some of the mistakes I've made. From time to time I will cite specific personal experiences in order to avoid discussing the problems of authorship in the abstract.

What Kind of Books do Chemical Engineers Need?

A library of professional volumes includes various classes of books: (i) *edited volumes* to present very recent developments by teams of experts; (ii) *research monographs* to catalog and evaluate the research published in the preceding 5-10 years; (iii) *treatises* to give authoritative, encyclopedic coverage to one particular topic; (iv) *textbooks* to set forth the basic ideas in the field in a form suitable for students; (v) *handbooks* to summarize standard results of widespread use; and (vi) *design manuals* to provide up-to-date procedures for practicing engineers. Each of these categories has a different audience, and each requires special organizational talents. Generally speaking, there is a flow of information from (i) toward (vi) in the above listing—that is, from innovative, exploratory, and (sometimes) impractical ideas of the researcher all the way to the time-tested and reliable tools of the practitioner. Along the way many ideas and methods are inevitably discarded, and only the most useful material survives to the arena of industrial practice. But without this constant exploration of new ideas and subsequent filtration, a profession can stagnate and atrophy.

■ **Repetition** is an important tool for improving coherence. In the above example, Bird repeats the word "book(s)" in a few places to build coherence.

■ If repetition becomes boring, **synonymy** can be used; *e.g.*, Bird uses the word "volumes" to avoid a tiresome repetition of the word "books" in the first sentence of the last paragraph. Similarly, **antonymy** (using an opposite word) can improve coherence; *e.g.*, see the use of "impractical ideas" and "reliable tools" in the same sentence in the last paragraph.

■ The **pronoun** is commonly used to improve coherence between sentences; *e.g.*, the pronoun “it” is used to refer to “book-writing” in the first paragraph. Also, **parallelism**, which refers to the use of the same sentence structure in subsequent sentences, improves coherence.

■ A tool that is commonly used by engineers is **enumeration**, which refers to the use of specific markers of sequence to achieve a connection between thoughts. A good example of enumeration appears in the second paragraph in which Bird uses enumeration to link the various classes of books.

■ A tool that students learn easily is **transition**. Transitions are conjunctions or conjunctive adverbs that link sentences with specific logical relationships. They can be subcategorized according to their meaning (see <papyr.com/hypertextbooks/engl_126/book126.htm> accessed on 3 Feb 2003) as follows:

Identity • Indicates sameness (that is, in other words)

Opposition • Indicates contrast (but, yet, however, nevertheless, still, though, although, whereas, in contrast, rather)

Addition • Indicates continuation (and, too, also, furthermore, moreover, in addition, besides, in the same way, again, another, similarly, a similar, the same)

Cause and effect • (therefore, so, consequently, as a consequence, thus, as a result, hence, it follows that, because, since, for)

Indefinites • Indicates a logical connection of an unspecified type (in fact, indeed, now)

Concession • Indicates a willingness to consider the other side (admittedly, I admit, true, I grant, of course, naturally, some believe, it has been claimed that, once it was believed, there are those who would say)

Exemplification • Indicates a shift from a more general or abstract idea to a more specific or concrete idea (for example, for instance, after all, an illustration of, even, indeed, in fact, it is true, of course, specifically, to be specific, that is, to illustrate, truly)

It is easy to identify the use of transitions in the Bird example. These coherence tools can be used to improve scientific writing. While it is unlikely that Bird was aware of the coherence tools he used while writing, a faculty member should encourage a novice writer to use the tools consciously until a time when they become a subconscious part of the writing process.

STRUCTURED APPROACH FOR COHERENCE

Coherence tools can only help improve something that was initially reasonably well written. The following structured ap-

proach is one way by which well-written drafts can be achieved. It is neither a panacea nor the only way, however, since there are innumerable factors that contribute to good writing, including the writer’s own personality.

The Preliminaries

1. The writer must have the requisite knowledge/information before beginning to write. This is an absolute prerequisite.
2. If a manuscript is for journal publication, a thesis, or a report, a substantial number of discussion aspects (say, 50%) should be clear to the student before writing begins. The student should be encouraged to analyze scientific material and note the salient points for discussion, with clarity, before writing anything. Many first manuscript drafts are poor in the discussion of data/simulations.
3. The student should be relaxed; (s)he should be encouraged to drink a glass of water or to take a few deep breaths, taking care to exhale more slowly than during inhalation. Then the student should take a few blank sheets, a pencil and an eraser (or a word processor), and sit where (s)he will not be disturbed.

The Questions

Now the student should ask himself/herself the following questions and incorporate the suggestions that follow them. To illustrate, I will present an example of my own thought processes while writing a paper a few years ago.

What is the main idea that I need to communicate?

For example, we had just discovered that induced free radicals could improve the productivity of cells in bioreactors, and we were very excited about it. Therefore, the main idea that we wished to communicate was “induced free radicals can be used as a novel means to improve bioreactor productivity.” Considerable thought may be required for first-time writers to recognize the main idea to be communicated, but that is the absolute starting place.

How do I communicate the main idea?

This is fairly simple for engineers/scientists who are normally bound by the required format of a journal, the university, or a funding agency. Typically, we are required to communicate the main idea in various sections, such as Introduction, Materials and Methods, Mathematical Model, Results and Discussion, Conclusions, Nomenclature, References, Appendices, etc. Also, we rarely use anything except a linear presentation of information, which makes this aspect very simple.

Taking one section at a time, ask the question, “What do I want to communicate in this section?”

Jotting It down

Write down the points as they occur to you.

For example, what do I want to communicate in the Introduction of the manuscript on induced free radicals? We were excited about the **novelty** of the strategy—therefore I needed to communicate that. I also wanted to communicate the various **contributions** we have made in this work. In addition, I wanted to tell the readers what **motivated** us to do the work, and since the typical reader of this journal was unlikely to know much about free radicals, I needed to give the **relevant background on free radicals**. Also, to provide focus, I wanted to present the **overall aim and objectives of the work**.

If the information is given in the order above, the readers (who will most probably not be familiar with the work) will find it difficult to understand. But if the same information is presented in a logical sequence, the reader's understanding and the paper's readability would improve significantly.

Ordering

Put yourself in the reader's position and then logically order the aspects written in bold in the above section. One possible list would be

1. Relevant background on free radicals
2. Motivation for the work
3. Novelty of the strategy
4. Overall aim and objectives, along with contributions

Jotting Down: Paragraph Level

Addressing the items in the list above, I first determined what it was that I wanted to communicate to the reader and noted the points down on a piece of paper as I thought of them. They were that: 1) Free radicals can be expected to improve bioreactor productivity; 2) They mediate cell processes such as cancer, apoptosis, etc.; and 3) They are suspected mediators of the effects of temperature, osmolarity, and nutrient levels (important bioreactor variables) on cells.

Logical Ordering: Paragraph Level

If I had written the points down in the order listed above, an intelligent lay-person (the common reader) would have found my message difficult to understand. Therefore, putting myself in the reader's position showed me that I needed to reorder the points for better understanding. One possibility was: 1) Free radicals are known to mediate a number of cell processes, including apoptosis and cancer (citing references); 2) Free radicals are suspected of being mediators of the effects of temperature, osmolarity, and nutrient levels on cells (citing references), which are also important bioreactor environment variables; and 3) Free radicals can be expected to play a significant role in determining bioreactor productivity. Note that in the process, I also improved the accuracy of the information.

Linking Sentences: Paragraph Level

Next, the sentences should be linked to improve coherence,

using the various linking tools mentioned earlier:

Free radicals are known to mediate a number of significant cell processes, including apoptosis and cancer (Feig and Loeb, 1994; Feig, et al., 1994; Okuno, et al., 1998; Reid and Loeb, 1993). **Further**, free radicals are suspected of being mediators of the effects of temperature, osmolarity, and nutrient levels on cells (Nagarathnamma, et al., 1997; Osbourn, et al., 1990), which are also important bioreactor environment variables. **Therefore**, free radicals can be expected to play a significant role in determining bioreactor productivity.

Note that in addition to the transition tools indicated in bold, I also used repetition when I framed the paragraph.

Now, the first paragraph, which communicated (and not merely presented) the background, was ready.

Second Paragraph

Similarly (jotting down thoughts, ordering sentences, and linking them) motivation could be communicated in the following paragraph:

Xanthan gum is secreted by *Xanthomonas campestris* when it attacks plants (Chamnongpol, et al., 1995). The extent of xanthan gum secretion (mucoidy) is directly related to the pathogenicity of the organism on plants, which it attacks (Throne, et al., 1987; Weiss, et al., 1994). Pathogenicity is related to the induced oxy free radicals (Sutherland, 1991). **From an industrial viewpoint**, *Xanthomonas campestris* is employed for commercial bioproduction of xanthan gum, which has wide applications in food, pharmaceuticals, oil, and other industries (Lee, 1996). If the relationship between free radical induction and gum production is better understood, free radical induction may be employed as a means to improve xanthan gum productivity. **In addition**, a better understanding will help to improve cultivation strategies where oxygen is provided in situ through the liquid-phase oxygen supply strategy (Sriram, et al., 1998).

When the two "completed" paragraphs are read one after the other, the reader will notice an abrupt jump in ideas between them. The paragraphs do not seem to be linked. The first talks about free radicals and the second talks about xanthan gum. The reader, who is subconsciously expecting a link, will experience discomfort when (s)he does not find one, and this leads to a loss in communication.

Linking Paragraphs

In the example above, the relationship between free radicals and xanthan gum, especially from a production viewpoint, was unknown in the literature at that time, and therefore known information could not be used to link the two paragraphs. Given this constraint, how could the ideas be linked?

The third sentence in the second paragraph talks about free radicals and could thus be used as a connecting sentence. Bringing this sentence to the beginning of the paragraph and

suitably modifying it serves the purpose of linking both paragraphs.

Free radicals are known to mediate a number of significant cell processes, including apoptosis and cancer (Feig and Loeb, 1994; Feig, et al., 1994; Okuno, et al., 1998; Reid and Loeb, 1993). **Further**, free radicals are suspected of being mediators of the effects of temperature, osmolarity, and nutrient levels on cells (Nagarathnamma, et al., 1997; Osbourn, et al., 1990), which are also important bioreactor environment variables. **Therefore**, free radicals can be expected to play a significant role in determining bioreactor productivity.

Oxy free radicals and oxidative stress are important aspects of plant defense mechanisms against invading microorganisms (Chamnongpol, et al., 1995; Sutherland, 1991) such as *Xanthomonas campestris*, a plant pathogenic bacterium. Xanthan gum is secreted by *Xanthomonas campestris* **during its attack, and** the extent of xanthan gum secretion (mucoidity) is directly related to the pathogenicity (Throne, et al., 1987; Weiss, et al., 1994). From an industrial viewpoint, *Xanthomonas campestris* is employed for commercial bioproduction of xanthan gum, which has wide applications in food, pharmaceuticals, oil, and other industries (Lee, 1996). If the relationship between free radical induction and gum production is better understood, free radical induction may be employed as a means to improve xanthan gum productivity. In addition, a better understanding will help to improve cultivation strategies where oxygen is provided in situ through the liquid-phase oxygen supply strategy (Sriram, et al., 1998).

In a similar fashion, I could proceed to compose other paragraphs, linking them to produce a coherent document.

Summarizing the steps for improving coherence, the most important factor is that the student needs to be knowledgeable in the area and aware of the aspects that need to be communicated. Then the student needs to

- *Write down the points that (s)he needs to communicate in each section, as they come to mind.*
- *Order them logically*
- *Improve coherence (by using tools)*
- *Link paragraphs*
- *Link sections/chapters, when needed*

EFFECTIVENESS OF THE STRUCTURED APPROACH

The structured approach was presented to students taking a communication skills course at IIT Bombay. In addition, they were given exercises to practice writing (and presentation). Their writing (and presentation skills) improved significantly, and they ultimately expressed gratitude that such a course was offered to them. Some students who were comfortable with the language were initially skeptical about the utility of the course, but they learned that effective communication does not necessarily arise from an ability to write

correct grammar. At the end, these students also felt they significantly benefited from the course.

Many faculty members (15 out of 28) expressed appreciation for, and satisfaction with, the improvement in communication that they observed in the M.Tech seminar course, where students worked on a research area and presented a critical evaluation of the literature through both a written and an oral presentation. After being asked for their input, six other faculty members said the course was useful. No negative comments were received from the faculty or the students, with the exception of certain individual preferences on presentation style.

To summarize, through clear thinking and better organization of information that is based on a sensitivity to the reader's needs, better writing can be achieved. Very often, bad writing results from muddled thinking or an inability to perceive the reader's needs. Further, writing is a skill—as is swimming. One cannot expect a person who does not know how to swim to learn from a set of verbal/written instructions alone—a lot of practice is required. Similarly, good writing requires a lot of practice. The structured approach given in this article cannot obviate that requirement, but it can provide direction for practice.

ACKNOWLEDGMENT

I thank my colleagues, Professors Preeti Aghalayam, Hemant Nanavati, Kartic Khilar, and Santosh Noronha, as well as my graduate student, Susmita Sahoo, for their input.

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This new feature in CEE, "Teaching Tips," is intended to be a forum for sharing innovative teaching practices with others in the profession. These short (600 words or less) contributions should clearly state the innovation, summarize the evidence for its success, and offer guidelines for its implementation. Contributions will be reviewed for originality, general interest, and appropriateness. They should be sent to Professor Phillip C. Wankat, Chemical Engineering Department, 480 Stadium Mall Drive, Purdue University, West Lafayette, IN 47907-2100, or <wankat@ecn.purdue.edu>.

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To encourage development of collaboration skills, many classes are split into teams of students to work on projects. Common methods of selecting the team composition are

- 1) To let students form their own groups,
- 2) To have the instructor assign team members,
or
- 3) To randomly choose members.

A disadvantage to student-selected groups is that often the better students choose each other and the weakest students end up together; this approach can also hinder achieving racial and gender diversity within a group. Instructor-selection may lead to complaints of favoritism, and random-selection leaves too much to chance and is not a method that would be used in the "real world."

For several years we have used a novel approach for forming teams. We require students to bring a one-page resume to class with them. The students' names are covered with Post-It notes and the resumes are laid out on a table so all can be viewed. "Team selectors" then study them and pick up the resumes of the students to be on their team. They do not know the students' identities at that point and make their selection based solely on the skills displayed in the resume.

The team selectors could be chosen by a random method, but we prefer to have the instructor identify those with the best grades in pre-requisite subjects to

ensure there is at least one strong student per group. These selectors then randomly draw a number from a hat that will serve both as their team number and the order of selection. For example, selector #1 will form team #1 and will pick up the first resume; selector #2 will form team #2 and will have second choice; the last team selector will have last choice, but will immediately select again (*i.e.*, pick up two resumes), and then the selection sequence reverses. This process continues until all the students have been selected and teams of the desired size are formed. Identities are not revealed until all resumes have been picked up, at which point the Post-Its are removed from each resume.

An advantage of this method is that students have taken an active role in forming their team, which is similar to the approach companies use to select job applicants. We take some time to discuss the reasons students had for making their selections. This is an excellent way to illustrate the importance of a good resume.

Many students have never attempted to prepare a resume prior to this requirement, so we provide some suggestions to help them. A good starting point is the "Resume Wizard" in Microsoft Word, which takes a step-by-step approach to creating a resume. Also, most colleges have career centers that provide helpful information on this topic. An added bonus is that the self-analysis needed to construct a resume makes students aware of shortcomings in their skills and experience and provides incentive for them to work on filling those gaps as they progress through their studies.

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 fourteen double-spaced pages and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

A SIMPLE OPEN-ENDED VAPOR DIFFUSION EXPERIMENT

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The value of problem-based learning in undergraduate chemical engineering instruction is well established.^[1] But even with publication of a simple mass-transfer experiment,^[2] de Nevers' statement that, "A permanent problem in engineering education is to find simple, portable, low-cost classroom demonstrations of the principles we present to our students," remains true, and the problem appears particularly acute with respect to mass-transfer instruction.^[3]

In an attempt to enhance learning in a lecture course on mass transfer, we developed a laboratory procedure that provides an opportunity for students' experimental estimation of vapor-phase diffusion coefficients. They can also creatively expand their analyses and receive credit for their creative efforts.

Therefore, inspired by a schematic from Bird, *et al.*,^[4] we developed a mass transfer experiment requiring a simple and inexpensive laboratory procedure. Simplicity and very low cost of the laboratory procedure notwithstanding, the greatest value of the experiment lies in the breadth and depth of analyses to which students can subject the resulting data. The overall objective of the present work was to develop a simple and inexpensive mass transfer experiment suitable for open-ended analysis by undergraduates in a unit operations course on mass transfer. Specific aims of the development were simplicity and low cost, use of common equipment and supplies

that require no expertise, and certain yield of usable data suitable for open-ended analysis by undergraduate students.

MATERIALS AND METHODS

Presentation to the Class

Diffusion is the initial topic in the third lecture course in our three-course unit operations sequence. To reinforce the topic effectively, students are asked to perform a class experiment on diffusion. During the last 20 minutes of a lecture, the assignment is distributed to the class along with Lee and Wilke's paper^[5] that details an elaborate version of the same experiment. The assignment is presented as a brief dis-



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discussion of the background of the experiment and the working equations detailed below. Students are told that the “minimum base-case” analysis is to use the experimental data with the working equations to estimate the vapor diffusion coefficient for each of three pure liquids evaporating from graduated cylinders and to submit an individually prepared written report of the results.

After discussing the assignment, the class reconvenes in a lab room to become familiar with the experimental setup, which consists of an ordinary box fan, nine 100-ml graduated cylinders, hexane, acetone, distilled water, and a thermometer (see Figure 1). Students are told to use the “low” fan speed and to measure the volumetric disappearance of the three liquids from each of three graduated cylinders. Three cylinders of each liquid are included as an additional variable for students to consider; the students are given no instruction on the purpose of having more than one cylinder for each liquid. Optionally, an electronic balance can also be used for another measure of disappearance of the three liquids.

Students then organize themselves for data collection and e-mail data reporting over the ensuing two-to-three-day period required for significant evaporation of water (hexane and acetone evaporate more quickly than the water).

An Open-Ended Assignment

Since the assignment is open-ended, students are told that they may creatively expand their analysis of the experimental data and receive unlimited additional credit for their extra work. Since no particular “correct” answer is sought even in the base case, the assignment is open-ended relative to technical scope and to grading. Student ideas for analyses beyond the base case are discussed with individual students only if discussion is initiated by the student.

Working Equations

Equation (1) is used to compute the experimental diffusion flux of each species:

$$N_A = \frac{W_A}{M_A \theta S} \quad (1)$$

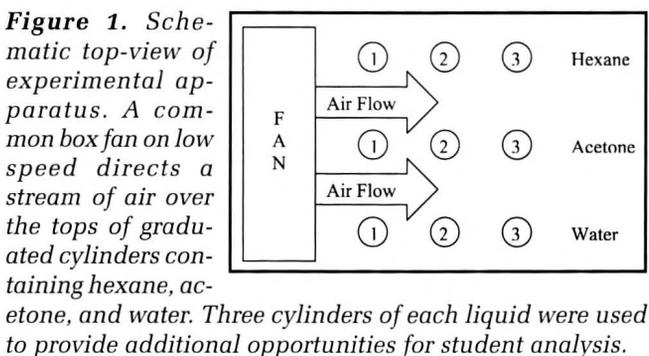


Figure 1. Schematic top-view of experimental apparatus. A common box fan on low speed directs a stream of air over the tops of graduated cylinders containing hexane, acetone, and water. Three cylinders of each liquid were used to provide additional opportunities for student analysis.

where

- N_A molar flux of A (mole/hr-cm²)
- W_A mass of component A vaporized (grams)
- M_A molecular weight of A
- θ elapsed time (hours)
- S cross-sectional area of graduated cylinder (cm²)

Based on Figure 2, a diffusion coefficient is defined using the integrated form of Fick’s law:

$$N_A = \frac{DP\Delta p}{RTp_f x} \quad (2)$$

where

- D diffusion coefficient for A (cm²/s)
- P atmospheric pressure (atm)
- Δp difference between the partial pressure of A at the liquid-gas interface and the partial pressure of A in air at the mouth of the cylinder (atm)
- R universal gas constant (cm³ atm/mole/K)
- T ambient temperature (K)
- p_f log-mean partial pressure difference (atm)
- x effective length of the diffusion path (cm)

Assuming Raoult’s-law behavior, the vapor pressure of liquid A, P_A , at the liquid-gas interface was substituted for the partial pressure of A, p_A , at the same location. Thus the log-mean partial pressure difference, p_f , becomes

$$p_f = \frac{(P - p_o) - (P - P_A)}{\ln\left(\frac{P - p_o}{P - P_A}\right)} \quad (3)$$

where

- P_A vapor pressure of A (atm)
- p_o partial pressure of A in air above the cylinder (atm)
- P total pressure of gas above the cylinder (atm)

Because an average molar diffusive flux for the period of observation was used, the average length, x_a , cm, of the diffusion path over the period of observation was also used:

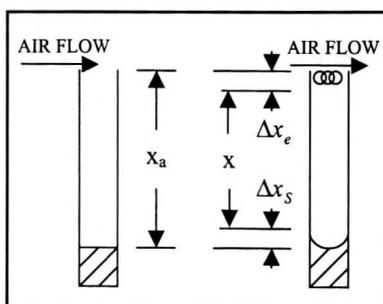


Figure 2. (Left) Schematic of air stream passing over the top of a graduated cylinder containing vaporizing liquid (cross-hatched region). (Right) Schematic of graduated cylinder with turbulence indicated at the cylinder top and a curved meniscus at the liquid surface. x_a is the apparent distance of the diffusion path. dx_e is a correction to the apparent diffusion path due to putative turbulence; dx_s is a correction to the apparent diffusion path due to curvature of the meniscus.

$$x_a = \frac{x_{\theta_{n+1}} + x_{\theta_n}}{2} \quad (4)$$

where

$x_{\theta_{n+1}}$ apparent path length at time θ_{n+1} (cm)

x_{θ_n} length at time θ_n (cm)

Because of putative turbulence at the top of the cylinder and the effect of a curved meniscus at the liquid surface (see Figure 2), the actual diffusion path length, x , is somewhat less than the apparent diffusion path length, x_a , that can be physically measured along the vertical wall of the cylinder. Thus the actual diffusion path length, x , is obtained by correcting the apparent diffusion path length, x_a :

$$x = x_a - \Delta x_s - \Delta x_e = x_a - \Delta x \quad (5)$$

where

Δx_s distance correction due to the meniscus (cm)

Δx_e distance correction due to turbulence (cm)

Δx total distance correction (cm)

Equation (2) can be rewritten to yield a value for an *apparent* diffusion coefficient based on an *apparent* diffusion path:

$$D_a = \frac{N_A RT p_f x_a}{P \Delta p} \quad (6)$$

where

D_a apparent vapor diffusion coefficient (cm²/sec)

Rearrangement of Eq. (6) gives

$$N_A = \frac{D_a P \Delta p}{RT p_f x_a} \quad (7)$$

Equating the expression for N_A in Eq. (7) with that in Eq. (2) and noting that $x = x_a - \Delta x$,

$$N_A = \frac{D_a P \Delta p}{RT p_f x_a} = \frac{D P \Delta p}{RT p_f (x_a - \Delta x)} \quad (8)$$

Rearranging Eq. (8) leads to a useful expression relating the apparent diffusion coefficient (D_a), the apparent diffusion path length (x_a), the actual diffusion coefficient (D), and the total path length correction (x),

$$\frac{1}{D_a} = \frac{-\Delta x}{D} \frac{1}{x_a} + \frac{1}{D} \quad (9)$$

The value of Eq. (9) in finding the actual diffusion coefficient should now be clear. Measurements at different times of liquid remaining in the cylinder, each associated with a measured x_a value, allows computation of D_a values from Eq. (6). According to Eq. (9), a plot of $1/D_a$ versus $1/x_a$ should yield a straight line with an intercept of $1/D$ and slope $-\Delta x/D$. Using this technique, a value for the actual diffusion coefficient along with the total path length correction (Δx) can be obtained.

RESULTS AND DISCUSSION

Students' Extra Work

Is it at steady state? • The working equations were based on steady-state diffusion, but many students never questioned the assumption of steady state relative to the experimental data. Several other students rightfully questioned the assumption of steady state using Eq. (10) from Lee and Wilke,^[5] which provides an estimate of the approach of the diffusive flux to the steady-state diffusive flux of the same system:

$$\frac{(N_A)_{\theta=\theta}}{(N_A)_{\theta=\infty}} = 1 - 2e^{-\frac{D\pi^2\theta}{x_o^2}} + 2e^{-\frac{4D\pi^2\theta}{x_o^2}} - 2e^{-\frac{9D\pi^2\theta}{x_o^2}} + 2e^{-\frac{16D\pi^2\theta}{x_o^2}} - 2e^{-\frac{25D\pi^2\theta}{x_o^2}} \quad (10)$$

where

$(N_A)_{\theta=\theta}$ flux of species A at any time θ

$(N_A)_{\theta=\infty}$ flux of species A at infinite time

x_o length of diffusion path

θ time

The estimated times required to achieve $(N_A)_{\theta=\theta}/(N_A)_{\theta=\infty} = 0.999$ were 4 minutes, 4 minutes, and 2 minutes for acetone, hexane, and water, respectively. Data acquired during the unsteady period should be excluded from analysis.

Turbulence and Δx • Most students were able to use the experimental data along with the working equations to compute an actual diffusion coefficient according to Eq. (9). An example of the type of plot dictated by Eq. (9) is shown for hexane in Figure 3. For all three liquids, however, the plots consist of two definite linear regions, *i.e.*, a value for $1/x_a$

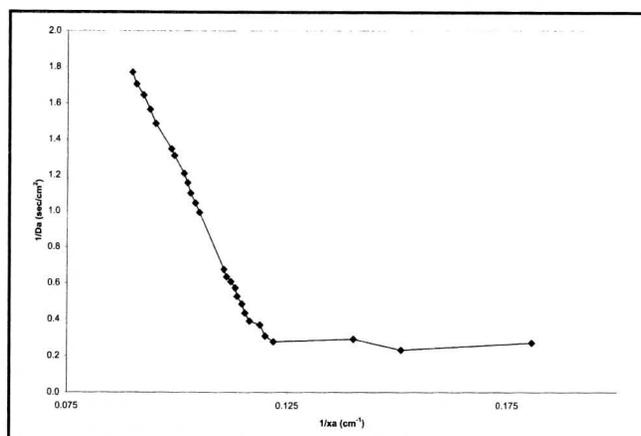


Figure 3. Plot of the inverse diffusion path (abscissa) versus the inverse of the apparent vapor diffusion coefficient (ordinate) for hexane from a single graduated cylinder. Data left of abscissa values $1/x_a = 0.125$ are used with Eq. (9) as a means to obtain a vapor diffusion coefficient value corrected for turbulence at the top of the graduated cylinder and a curved meniscus at the liquid surface.

exists that indicates transition between the two linear regions. A plurality of students simply ignored this inconsistency while others pursued its potential meaning. Students who pursued it quickly recognized that $1/x_a$ was related to Δx , and ultimately realized that some part of the Δx region estimated using Eq. (9) and Figure 3 actually included data from within the putative turbulent region at the top of the cylinder, *i.e.*, during early times, for small x_a ; mass transfer in the turbulent region is not due to simple diffusion alone and must be excluded in estimating a vapor diffusion coefficient.

Thus students were faced with using an iterative approach of estimating Δx , using Eq. (9) and Figure 3 and then repeating the estimation procedure after excluding data from within the estimated turbulent region. Iteration continued until Δx estimates stabilized at 6.51 cm, 8.68 cm, and 4.53 cm for acetone, hexane, and water, respectively, compared with the distance from the initial liquid level to the cylinder top of 5.39 cm and the total height of each cylinder of 23.7 cm. Each cylinder's inside diameter was 2.8 cm.

Although it may appear that the turbulent region varied with the liquid species, we suggest that a more likely cause of variation among the heights of the turbulent regions was cylinder placement relative to the fan and other cylinders. In an attempt to eliminate the turbulent region in the tube above the liquid, a variation of this experiment could possibly use wire gauze to fill the space between the cylinder top and the initial liquid level in the cylinder.

Ambient Partial Pressure: Does $p_o = 0$? • The partial pressure of the diffusing species in air supplied by the fan passing over the cylinders appears in Eq. (3), which provides an estimate of the diffusion driving force. Clearly, the partial pressure for organic species that vaporize relatively slowly may realistically be assumed as zero, but since water was one of the three diffusing species used in this assignment and since water can be present in ambient air due to humidity, the assumption of zero partial pressure of water was investigated (but by fewer than five students). Several students attempted to include a partial pressure value obtained from humidity data archived by the National Weather Service. Unfortunately, these humidity values were not realistic for room air in the air-conditioned lab. One student, however, included the water partial pressure as an adjustable parameter in his model in an Excel spreadsheet. He used Excel's Solver tool to perform a nonlinear least squares minimization of error on water molar flux to compute a "most likely" estimate of water partial pressure. The relative humidity thus obtained was 68%.

Pedagogical Impact

In the first year this assignment was used (Year 1, N=3), 14

students received grades of 100 or greater, while only two students did not complete the minimum base-case. The Year-1 average grade was 97.0, with standard deviation of 12.59. In Year 2 (N=19), grades bifurcated into a high grade group (n=12, avg grade = 105.0, std dev = 5.0) and a low grade group (n=5, avg grade = 60.5, std dev = 8.5), with two students not submitting a report.

The open-ended nature of the assignment motivated many students to pursue extra work beyond the minimum and sparked several students to a level of creativity not previously exhibited in their chemical engineering work.

In end-of-semester surveys, students were asked to rate their level of learning on course topics including diffusion. The levels were modeled on Bateson's three levels of learning.¹⁶ In Year 1, of students responding, six students (24%) indicated they had mastered aspects of diffusion, 17 students (68%) indicated they had some facility with diffusion, and only two students (8%) indicated they were merely familiar with diffusion. In Year 2, of students responding, six students (46%) indicated they had mastered aspects of diffusion, five students (38%) indicated they had some facility with diffusion, and again, only two students (15%) indicated they were merely familiar with diffusion.

Based on instructor evaluation of student work and students' self-assessment of learning, we were very satisfied with the utility of this assignment to enhance student learning of mass transfer. The open-ended nature of the assignment motivated many students to pursue extra work beyond the minimum and sparked several students to a level of creativity not previously exhibited in their chemical engineering work. Students' grades were determined from the same instrument from which they learned and they could receive any amount of credit for which they were willing to work; they faced no artificially imposed upper limit on credit they could accrue.

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COMPUTER EVALUATION OF EXCHANGE FACTORS IN THERMAL RADIATION

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Computer software packages that supplement traditional classroom presentations can provide opportunities in reflection and action to students.^[1-4] A key factor for successful development and use of computer packages in engineering education is identification of activities that cannot be accomplished by other means, *e.g.*, analytically. Such is the case for most thermal radiation problems.

Thermal radiation is offered as part of heat transfer courses in all chemical engineering programs, although not as intensively as in their mechanical engineering counterparts. At least two aspects are very peculiar to thermal radiation transfer compared to other modes of transport. First, the mechanism of thermal radiation has no analogy in momentum and mass transport—a very useful tool in the instruction of the different modes of transport. Second, the equations of heat transfer by radiation are strongly nonlinear, making it difficult to solve radiation problems using analytical or even numerical techniques, especially for complex geometries and/or real surfaces.

In evaluating any thermal radiation exchange, it is fundamental to calculate the view or exchange factors. Generally, the instruction of thermal radiation to chemical engineers revolves around a thorough understanding of the properties of the view factor and of the tools to evaluate it. For simple geometries, view factors have been evaluated and tabulated in catalogues.^[5,6] For moderately involved geometries, however, view factors are exceedingly difficult to evaluate analytically. Different numerical techniques, such as the finite element method, area and line integral methods, and the Romberg formula, were used to compute the view factor.^[7-9] More often than not, statistical approaches, such as the Monte Carlo (MC) technique, are the only alternative.

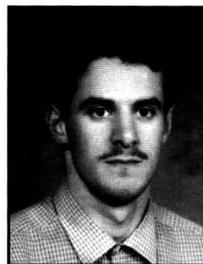
An advantage of the MC technique is its ability to tackle the most complicated problems with relative ease. It also allows for a better analysis of the design parameters that affect distribution of thermal patterns arising from thermal radiation exchange in realistic geometries in an effort, for instance, to optimize these parameters. Its disadvantage lies in the issue of accuracy of the results, although statistical errors can

be resolved through an increase in sample size and an adequate choice of a random number generator.

This paper describes a computer program that serves as an educational tool in the instruction of the notion of view factor in a nontrivial geometry using the MC technique. The concept of exchange factor, which induces the effect of multiple reflections, is also considered in detail. Thermal radiation occurs between discrete sources (both a single source and a linear succession of sources are considered) and the walls of a rectangular enclosure containing an obstructing surface. All surfaces are separated by a transparent medium and are assumed to be isothermal with uniform properties. The surfaces can be black, diffuse-grey, or diffuse-nongray. The discrete sources are black bodies emitting at a high temperature ($T = 2700\text{K}$). In order to make the problem tractable at the undergraduate level, the surfaces are assumed to be cool enough so their emission can be neglected.

MODELING

The enclosure considered is a box with six sides and obstructing surface as sketched in Figure 1a. Thermal radiation is emitted by discrete isotropic sources in the form of energy bundles that travel along straight paths through the enclosure until they are absorbed by a surface or terminated after a preset, high-enough number of reflections on the surfaces. Solving exchanged thermal radiation using the MC technique necessitates tracing the history of randomly sampled photons from their point of emission to their point of absorption or



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attenuation, after simple or multiple reflections. A photon history is tracked using a ray-tracing approach^[10] (as shown in Figure 1b) relative to enclosure and source systems of coordinates. In order to follow the history of energy bundles in a statistically sound way, the position and properties of bundles are chosen according to probability distributions. The fraction of energy emitted over wavelengths between 0 and λ is expressed by^[11]

$$R(\lambda) = \int_0^\lambda P(\lambda)d\lambda = \frac{\int_0^\lambda E_\lambda d\lambda}{\int_0^\infty E_\lambda d\lambda} \quad (1)$$

Equation (1) is then inverted to correctly model a specific bundle property. In case of a single source, the position of the latter in the enclosure is rather deterministic. For the case of a uniform linear succession of discrete sources, based on Eq.

(1) a source position (x_s, y_s, z_s) is chosen randomly along a linear segment of coordinates $(x_{sg,1}, y_{sg,1}, z_{sg,1})$ and $(x_{sg,2}, y_{sg,2}, z_{sg,2})$, as follows:

$$\begin{aligned} x_s &= (1 - R_s)x_{sg,1} + R_s x_{sg,2} \\ y_s &= (1 - R_s)y_{sg,1} + R_s y_{sg,2} \\ z_s &= (1 - R_s)z_{sg,1} + R_s z_{sg,2} \end{aligned} \quad (2)$$

where R_s is a number between 0 and 1 picked at random.

For the nongray case, the wavelength of emission from a source is determined according to the polynomial description proposed by Haji-Sheikh^[12] and given in the Appendix (Part 1).

The direction of emission or reflection of an energy bundle is defined by the direction vector R_u , whose coordinates are expressed in terms of the azimuthal, ϕ , and polar, θ , angles. The two angles are determined by

$$\theta_s = \cos^{-1}(1 - 2R_\theta) \quad \theta_{surf} = \sin^{-1}(\sqrt{R_\theta}) \quad (3)$$

$$\phi_{s,surf} = 2\pi R_\phi \quad (4)$$

θ_s is valid for bundle emission from a source (solid angle = 4π), and θ_{surf} is used for a bundle reflected from a surface. The expression for the azimuthal angle is valid for both a source and a surface.

The position of a bundle in space is defined in terms of its origin and the direction vector, R_u , by

$$x = x_s + x_u t \quad y = y_s + y_u t \quad z = z_s + z_u t \quad (5)$$

where t is a positive value.

For a bundle to hit one of the planar surfaces defined by

$$Ax + By + Cz + D = 0 \quad (6)$$

where $A, B, C,$ and D are constants, the following equation must be fulfilled:

$$A(x_s + x_u t) + B(y_s + y_u t) + C(z_s + z_u t) + D = 0 \quad (7)$$

Equation (7) is used to solve for t , which is then substituted into Eq. (5) to compute the bundle position. A bundle intersects a surface if its coordinates are within the bounds of the specified surface. Similarly, further planar surfaces with differing shapes can also be considered if their geometries are well defined.

Among the bundles impinging on a surface, a fraction α is absorbed and the rest of the bundles are reflected from the surface. Absorption of a bundle is determined by comparing the surface absorptivity at a given wavelength, α_λ , with a randomly generated number, R_α . The condition of absorption of an energy bundle by a surface is given by

$$R_\alpha \leq \alpha_\lambda \quad (8)$$

In this case, a new bundle is generated and its history is traced using Eqs. (2) through (8). If a bundle is reflected on a sur-

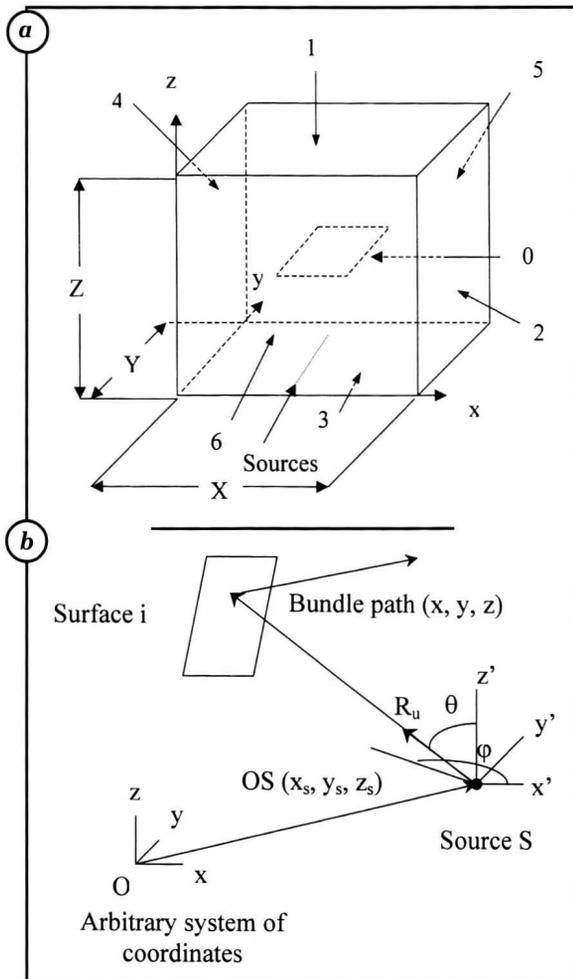


Figure 1. Schematics of enclosure geometry (a) and vector description of an energy bundle (b). The dimensionless depth and height of the enclosure are $Y/S = 1$ and $Z/X = 1$ (with $X = 20$ cm), respectively, and the dimensions of the obstructing surface are 10×10 cm².

face, a new direction for the bundle in the enclosure is chosen and the bundle history is traced using Eqs. (3) through (8).

In the present work, the exchange factor is defined as the fraction of diffuse radiation emitted by a discrete source, s , that is absorbed by a surface, i , either directly or after multiple reflections on the surfaces

$$dF_{s-i} = \frac{\text{number of photons leaving } s \rightarrow i \text{ (direct \& indirect)}}{\text{total number of photons leaving } s} \quad (9)$$

The total exchange factor F_{s-i} between a source s and a surface, i , is calculated by integrating Eq. (9) over a large number of energy bundles emitted by source s :

$$F_{s-i} = \left(\frac{NA_{s-i}}{NB} \right)_{NB \gg 1} \quad (10)$$

Finally, the total exchange factor F_{sg-i} between a linear succession of sources and any surface, i , in the enclosure is obtained by summing up all factors F_{s-i} given by Eq. (10) over the number of all sources making up the linear surface.

RESULTS AND DISCUSSION

In the following paragraphs, three cases with increasing complexity are presented and solved using the computer program. The latter serves as an exercise in an undergraduate course in heat and mass transfer. The lessons learned through each solved case include closed- and open-ended questions and require students to use thinking skills, in accordance with Bloom's Taxonomy.^[4] The dimensions of the system geometry and the values of many other parameters can be changed at will by the students through an input file (see description of the code usage in the Appendix, Part 2). The parameters pertain to enclosure, blocking surface, and heating wire dimensions; to blocking surface and heating wire locations; and to the properties of the surfaces.

In Case 1, a black enclosure without the obstructing surface is considered, and a test problem is presented. The test problem also has an analytical solution so students can verify the computations for themselves. Case 2 concerns radiative exchange in a diffuse-gray enclosure containing a diffuse-gray obstructing surface. Unless otherwise stated, all surfaces are assumed to have the same absorptivity, α , of 0.45. Case 3 is similar to Case 2, but all surfaces are treated as nongray, *i.e.*, with wavelength-dependent absorptivities. In the present study, all calculation results for Cases 2 and 3 correspond to a number of energy bundles per single source of 10^6 . Moreover, thermal radiation is emitted by a linear succession of sources, with a sample size of 500 sources, mimicking a heating wire. The sources are considered to lie between segment ends of dimensionless coordinates $(x_{sg}/X=0.5, y_{sg}/X=0.25)$ and $(x_{sg}/X=0.5, y_{sg}/X=0.75)$.

Case 1

The Monte Carlo program has been tested for the case of an enclosure whose six walls are black. For the sake of simplification, in the example presented here heat radiation is emitted from a single source placed at position $(x_s/X=0.5, y_s/X=0.5, z_s/X=0.5)$ coinciding with the center of the black enclosure. Results for this example are shown in Figures 2 and 3.

Figure 2 illustrates the calculated view factors between the source and

the six surfaces of the enclosure as a function of the size of the sample of energy bundles. By so doing, the students get a better feel for the Monte Carlo method by observing its accuracy as a function of sample size. As the total number of emitted bundles increases, the calculated values of the view factors tend directly to or oscillate about the exact solution corresponding to $F_{s-1} = F_{s-2} = F_{s-3} = F_{s-4} = F_{s-5} = F_{s-6} = 1/6$ for surface 1 through surface 6, respectively. One point worthy of notice in Figure 2 is that accuracy in the calculated view factors is improved only for a bundle sample size of 10^5 and larger. For the latter bundle sample size, the computed view factors are: $F_{s-1} = 0.1662$, $F_{s-2} = 0.1664$, $F_{s-3} = 0.1667$, $F_{s-4} = 0.1670$, $F_{s-5} = 0.1667$, $F_{s-6} = 0.1669$, for surface 1 through surface 6, re-

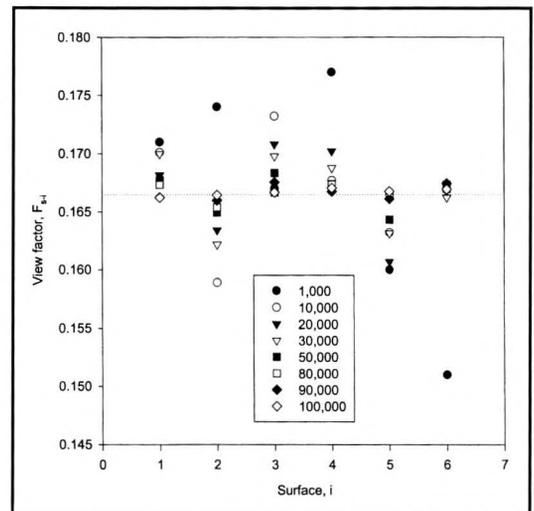


Figure 2. Calculated view factors of the different black surfaces as a function of the number of emitted bundles (in the inset). The dotted line represents the analytical solution.

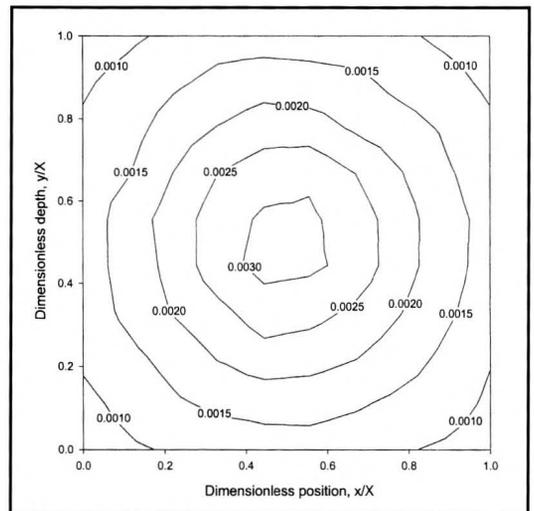


Figure 3. Contour plot of the view factor over the black surface of the bottom wall.

spectively, with a maximum relative error of 0.3%. In Figure 3, a typical contour plot depicting the distribution of the local view factor is shown for surface 3 (bottom wall). For all surfaces, the view factor reaches its largest value around the center of a surface, which is closest to the source, and decreases toward surface edges.

Case 2

In this case, the walls of the enclosure and the obstructing surface are considered diffuse and gray. The center of the obstructing surface, denoted surface 0, coincides with the center of the enclosure. A linear succession of sources is located between the bottom wall of the enclosure and the obstructing surface.

Figure 4 shows the dependence of the calculated exchange factors of the surfaces on the height, z_{sg}/X , of the linear source when all surfaces are assumed to have an absorptivity of 0.45. As the linear source is moved upward from the bottom wall, the magnitude of the exchange factor increases from ~ 0.09 to ~ 0.22 for the obstructing surface, and decreases from ~ 0.34 to ~ 0.20 for the bottom wall. This result is expected since the exchange factor is inversely proportional to the square of the distance between two interacting bodies. For the remaining surfaces, *i.e.*, the lateral surfaces and surface 1 (top wall), the value of the calculated exchange factor slightly increases as the linear source is raised to a dimensionless height of 0.3, then the exchange factor slightly decreases with increasing the height of the linear source (see Figure 4). The results also show that the exchange factors of surface 2 and surface 4 are equal in magnitude (as well as those of surfaces 5 and 6). This is because of the symmetry they exhibit relative to the obstructing surface and linear source (the same goes for surfaces 5 and 6).

The distributions of the calculated exchange factor, corresponding to a height of the linear source of 0.1, on the ob-

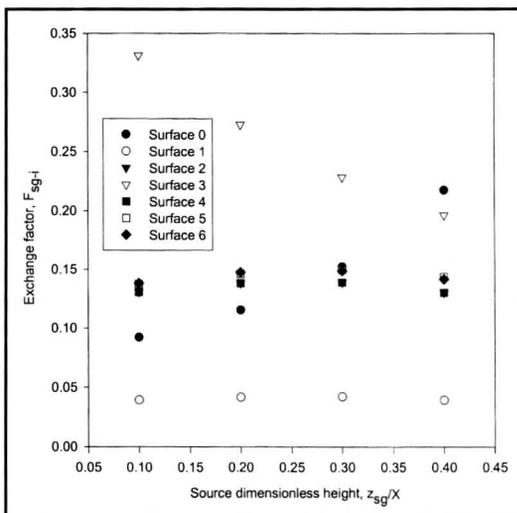


Figure 4. Dependence of exchange factors on the height of the linear source for the different surfaces (in the inset).

structing surface and surfaces 1 and 2, are presented in Figures 5a,b,c, respectively. It is interesting to note that the exchange factor was found to be at its maximum value near the center of the top surface, where the central areas do not face the source directly, as can be seen in Figure 5b. One of the reasons for this distribution pattern is that multiple bundle reflections on the surfaces were needed for the exchange factors to fulfill the summation relation. For instance, the sum of the calculated exchange factors for all surfaces is higher

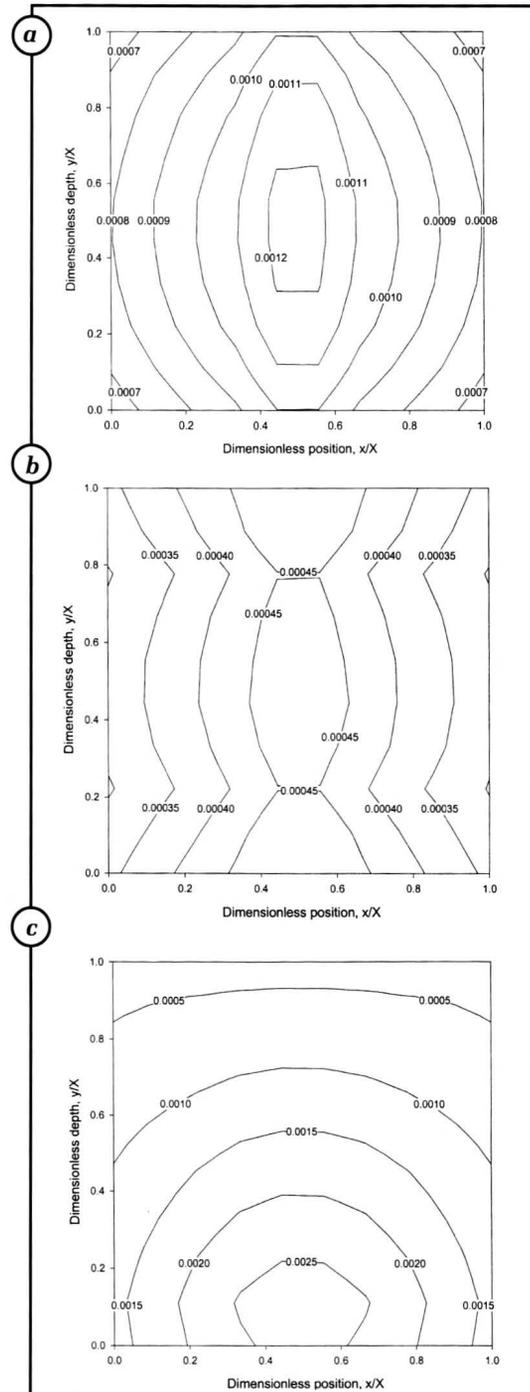


Figure 5. Contour plots of the exchange factor over surface 0 (a), surface 1 (b), and surface 2 (c).

than 99.95% only after four, six, and twelve reflections before terminating a bundle for a surface absorptivity, α , of 0.70, 0.45, and 0.20, respectively. Figure 6 illustrates the effect of surface absorptivity on the calculated exchange factors of the different surfaces. A decrease in surface absorptivity induces an increase (decrease) in the exchange factor for the top wall (bottom wall). A low surface absorptivity implies that a bundle has a good chance of being reflected upon impinging on a surface rather than being immediately absorbed. That is, a bundle can travel a long distance within the enclosure and reach remote areas before it is terminated.

Case 3

In this case, the walls of the enclosure and the obstructing surface are considered nongray and their spectral absorptivity is assumed to follow the simple distribution shown in Figure 7a (this is a good approximation for some important metals.⁽¹³⁾) The MC program has a routine to account for the wavelength dependence of surface absorptivity. Thermal radiation emission is due to a linear succession of sources with the same characteristics as those corresponding to the results of Case 2, and with $z_{sg}/X = 0.1$.

Figure 7b illustrates the calculated exchange factors of the different surfaces in the enclosure as a function of the splitting (cut-off) wavelength λ_{sp} . The magnitudes of the exchange factors vary sensibly as λ_{sp} is increased for the top wall (F_{sg-1} varies from ~ 0.08 to ~ 0.04) and bottom wall (F_{sg-1} varies from ~ 0.26 to ~ 0.33), but only slightly for the obstructing surface and lateral walls of the enclosure. As can be seen in Figure 7b, the calculated exchange factors are insensitive to λ_{sp} for values of the latter higher than $4.0 \mu\text{m}$ and become comparable in magnitude to exchange factors corresponding to the gray-body case (see Figure 6, case with $\alpha = 0.45$).

CONCLUSIONS

This paper has discussed calculation of the view/exchange

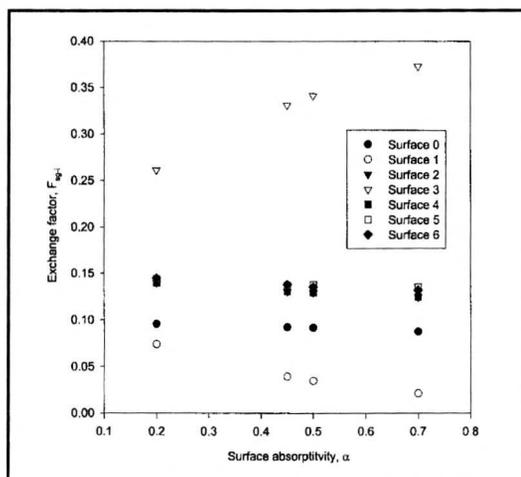


Figure 6. Calculated exchange factors as a function of surface absorptivity for $Z_{sg}/X = 0.1$. The different surfaces are indicated in the inset.

factor in an enclosure, with three problems related to different aspects of thermal radiation, using the MC method. The methodology has been presented in a simple and intuitive way so that no additional background in statistics is required. It provides new mathematical concepts that, generally, are not taught in courses on thermal radiation. The computer program is modular, very robust, and easy to use as an educational tool in the analysis of radiation problems. In the future, the author intends to make an executable JAVA version of the package available on-line to potential users.

ACKNOWLEDGMENT

The author thanks the undergraduate students who helped in implementing and testing the computer program.

NOMENCLATURE

- A,B,C,D constants defining a plane
- D_{1-5} coefficients of inverse probability function, $\mu\text{m.K}$
- E emissive power, $\text{W}/\text{m}^2/\mu\text{m}$
- F view factor; exchange factor
- NB,NA number of emitted bundles; number of absorbed bundles
- R cumulative distribution function; random number in range 0-1; direction unit vector

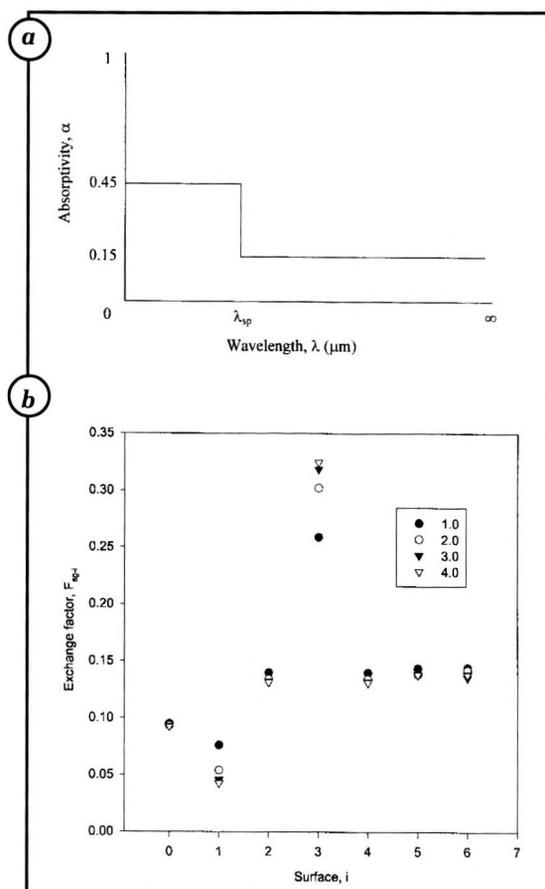


Figure 7. Distribution of the spectral absorptivity for Case 3 (a), and variation of exchange factors of the different surfaces with the splitting wavelength in the inset (b).

T, absolute temperature of emitting source, K; length of bundle
 X, Y, Z dimensions of enclosure, m
 x, y, z Cartesian system of coordinates; bundle Cartesian coordinates, m

Greek Symbols

α surface absorptivity
 θ angle to normal; polar angle
 φ azimuthal angle
 λ wavelength of emission, μm

Subscripts

i, s surface i, source s
 sp, sg splitting, segment
 surf surface
 u unit
 s-i from source s to surface i
 sg-i from segment to surface i
 λ at a given wavelength
 1, 2 end-points of linear source

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APPENDIX

Part 1. For the nongray case, the wavelength of emission from a source was determined as follows:^[12]

$$\lambda T = D_1 + D_2 R_\lambda^{1/8} + D_3 R_\lambda^{1/4} + D_4 R_\lambda^{3/8} + D_5 R_\lambda^{1/2} \quad \text{when } 0.0 < R_\lambda < 0.1$$

$$\lambda T = D_1 + D_2 R_\lambda + D_3 R_\lambda^2 + D_4 R_\lambda^3 + D_5 R_\lambda^4 \quad \text{when } 0.1 < R_\lambda < 0.9$$

$$\lambda T = \left\{ 15.2886 \times 10^{10} / \left[D_1 R_{-\lambda} + D_2 R_{-\lambda}^2 + D_3 R_{-\lambda}^3 + D_4 R_{-\lambda}^4 \right] \right\}^{1/3}$$

when $0.9 < R_\lambda < 1.0$

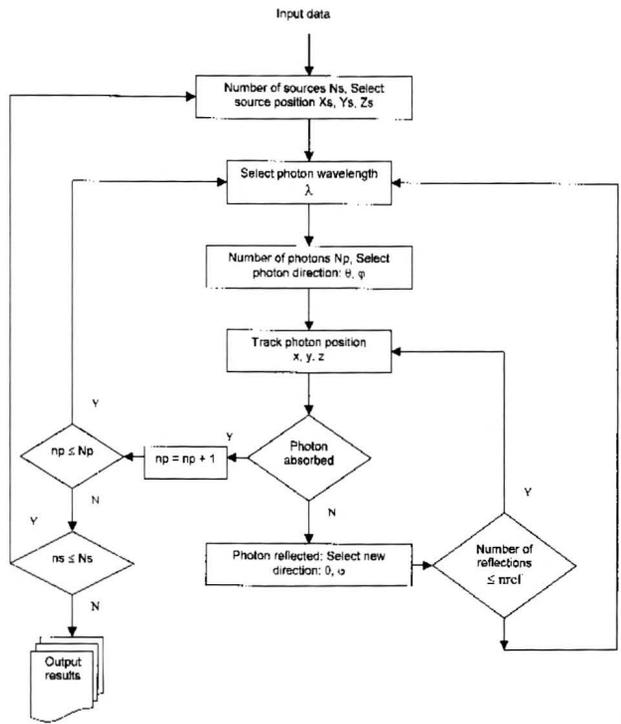
with $R_{-\lambda} = 1 - R_\lambda$, and $T =$ temperature of emitting source.

The coefficients for $\lambda T = f^{-1}(R_\lambda)$ given above are summarized in the table below (λT in $\mu\text{m.K}$)

Range of R_λ	D_1	D_2	D_3	D_4	D_5
0.0 - 0.1	503.274	230.243	5863.85	-10759.6	8723.14
0.1 - 0.4	1560.84	7603.61	-15540.1	31257.7	-20844.8
0.4 - 0.7	2846.63	-4430.38	27936.0	-41041.9	25960.9
0.7 - 0.9	345197	-1828567	3674856	-3284391	1108939
0.9 - 0.99	1.2	9.476	-44.84	156.9	-
0.99 - 1.0	1.10064	16.8148	-183.445	890.699	-

Part 2. Flowchart for MC calculation of radiation view/exchange factors. Data pertaining to the geometry and dimensions of the enclosure and obstructing surface, optical properties and temperatures of the surfaces in the enclosure, heating source location and temperature, number of bundles per photon, physical constants, and preset calculation tolerances are needed as input to the computer program. All data pertaining to length and position are expressed in absolute quantities. The input file interfaces between the user and the computer package, and several output files are

obtained upon execution of the code. The program was written in C++ using Microsoft Visual Studio, and the output files, in .txt format, are readily transferable to SigmaPlot, a statistics and graphics software from SPSS, Inc., for further processing.



EXPERIMENTS AND OTHER LEARNING ACTIVITIES USING NATURAL DYE MATERIALS

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Ever-increasing concerns and constraints regarding student safety and health, waste disposal, and liability can significantly hamper development of interesting and relevant laboratory experiences in a chemical engineering program. Using chemical reagents is likely the most problematic of the possible safety and health concerns faced by chemical educators. While placing the highest priority on the safety of our students, we still wish to provide learning experiences that prepare them for their careers, meet our learning objectives, and are (we hope) inherently interesting. Approaches that can be taken to provide especially safe laboratory experiences are many; some of them include

- *Avoiding chemical reagents (other than water and air) altogether*
- *Using microquantities of chemical reagents*
- *Investing in ultrasafe equipment, facilities, and specialized training*
- *Using simulations and/or remote laboratory experiences*

Each of these approaches has some significant advantages, but each also has its disadvantages: avoiding chemical reagents altogether is impractical when learning objectives involve chemical reaction kinetics, for example, and using only microquantities is impractical when learning objectives involve experience with pilot or industrial-scale unit operations.

In recent years, an additional personal concern of the author has been that chemical engineering students have little exposure to or opportunity to work with materials in “raw” form. Laboratory materials nearly always comprise highly processed and purified reagents. This, despite the fact that a very large fraction of the top production chemicals produced in the United States^[1] are commodities produced from basic raw materials, including petroleum, mined goods, agricul-

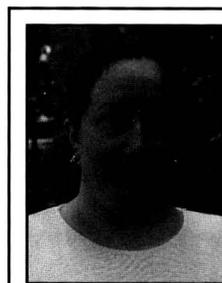
tural products, surface and ocean waters, and air.

A description of an experimental approach designed to support a particular chemical engineering technical topic, but that can be adapted to other chemical topics and other uses, is presented in this paper. The hope is that it can serve as a guide to others contemplating incorporating raw and natural materials into chemical engineering laboratory experiences.

MOTIVATION

In addition to the learning goals common to any laboratory experiment in any chemical engineering laboratory course, an additional cognitive^[2] learning goal desired by the author was that students achieve knowledge of some differences between raw and highly processed materials when incorporated into a chemical process. Some additional elements motivating the use of natural dyestuffs include

- *Safety* Natural dyestuffs have been in use for many centuries; many of them are extremely well characterized, and the ones we chose have no safety warnings associated with them. We insist on the best laboratory and safety practice at all times, but the safety of these materials was a valuable aspect of their performance.
- *Environmental Friendliness* As a result of their low hazard, disposal of wastes generated when using



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natural dyestuffs is simple—dye extracts pose no problems to municipal water treatment systems, and spent dyestuffs can be disposed of in general waste. (The author prefers to collect the dyestuffs for garden composting.)

- **Cost** Commercially available dyestuffs range in price from very expensive (indigo and carmine, up to \$50/lb) to modest (logwood, \$8/lb), while some usable materials are nearly free (onion skins).
- **Aesthetics** Natural dyestuffs and their extracts are low-odor and generally pleasant-smelling, and the colors of the extracts can be quite vivid, which is of additional appeal to students.
- **Topical Richness and Complexity** Students often become bored when working with materials and processes that are extremely well-characterized—“Why should I bother studying this when I know the answer already?” is a common complaint. Although there is a very large amount of information available on the production of natural dyes, it is mostly in the form of recipes and “folk wisdom.” This makes an engineering approach to their processing both interesting and useful. I have had more than a few students speculate that application of chemical engineering principles could possibly lead to profitable commercial production of natural dyes.

NATURAL DYESTUFFS

Forty-seven plants are listed in *Dye Plants and Dyeing*.^[3] A selection of plants for each major color group is given in Table 1. In addition to plant sources, there are some animal sources (cochineal, for example, is extracted from the carapaces of scale insects that live on cactus plants) and mineral sources (for example, ochre, from a type of iron ore). A variety of sources for some of the more readily available dyestuffs can be found with minimal search on the World Wide Web. Prices for logwood chips, a moderately expensive material, are about \$30 per pound retail; fifty grams of chips is enough for 15 or more small-volume (50 ml or less) experi-

mental extractions. Less expensive dyestuffs include alkanet root (about \$4 per pound), madder root (about \$4-\$10 per pound), and osage orange sawdust (about \$10 per pound). In addition to a wealth of material available through the World Wide Web, there are many text references available detailing dye plants,^[3] dyeing recipes and approaches,^[4,5] and world dyestuff production.^[6]

Experiment for Using Statistical Design of Experiments to Screen Processing Factors

This laboratory experiment is conducted in the junior-level chemical engineering laboratory course at Arizona State University. The course is designed to meet six learning objectives:

1. *Students will be able to design experimental runs to achieve a specified experimental goal and perform the experiments in a safe, ethical, and professional manner.*
2. *Students will be able to record and analyze experimental data, and to interpret analyzed results using appropriate theory and models.*
3. *Students will be able to effectively communicate all aspects of their experimental work and analyses in oral and written form.*
4. *Students will be able to make appropriate use of a computer in data analysis and in oral and written communication of their experimental work.*
5. *Students will be able to perform technical work in teams.*
6. *Students will have demonstrated the above skills in the context of chemical engineering knowledge acquired in earlier courses.*

The natural dye extraction experiment is implemented to introduce students to statistical design of experiments (DoE). The experiment is framed in the context of performing DoE on a variety of processing factors for dye extraction as if for eventual development of a full commercial process.

Students are provided with the following context statement

TABLE 1
Some Plant Sources of Natural Dyes for Various Colors^[3-5]

<u>Yellows</u>	<u>Blues</u>	<u>Reds</u>	<u>Greens</u>	<u>Purples</u>	<u>Oranges</u>	<u>Browns</u>	<u>Greys/Blacks</u>
Black Oak Bark	Logwood	Madder	Ivy Berries	Logwood	Annatto	Cutch	Black Walnut
Fustic	Indigo	Brazilwood	Wallflower	Blackberry	Coreopsis	Black Walnut Hulls	Logwood
Osage Orange	Woad	Bloodroot	Lily of the Valley	Alkanet	Silver Birch	Elderberry	Mountain Laurel
Turmeric	Red Cabbage	Munjeet	Plantain Roots	Grapes	Turmeric	Henna	Sumac
Saffron		Pokeweed	Nettle	Red Cedar Root		Onion	Iris Root
Weld		Strawberries				Yew	
		Cherries				Sumac Leaves	
		Raspberries				Juniper Berries	
		Beets				Coffee Grounds	

and experiment-specific learning objectives:

“Natural” or naturally based consumer products currently have a limited, but growing (and devoted!), customer base. This is especially true for clothing and in cosmetics and personal care products, where “organically grown” fibers or a “naturally derived” specialty chemical (to be used in a cosmetic, a shampoo, fragrance, or nutraceutical), having the same functionality and performance as a “non-natural” fiber or chemical might sell for ten-or-more times the price.

A challenge in using “natural” feedstocks in chemical processes is that they have properties that can be quite variable—consider, for example, indigo (the leaves, stems, and flowers of which contain the familiar blue dye of blue jeans). The **productivity** (bushels of plant matter/acre) of land planted in indigo will depend on all the usual agricultural factors (climate factors, water factors, soil-type factors, farming-practice factors). The **quality of the plants** themselves will also depend on most of these agricultural factors—the ‘quality’ including concentration of the dye chemicals of interest, their ease of processing, and the types and kinds of impurities. The **quality and quantity of extracted dye** will depend on the plant quality as well as on a host of processing factors—extraction pH, oxygen concentration in extraction bath, extraction time, temperature, degree and types of mixing, extraction co-solvents, etc.

For this experiment, you will be assigned a particular dyestuff (brazilwood, logwood, or madder) and perform a statistically designed (“DoE”) experiment with the intent of testing possible dye processing factors for significance. You should perform this experiment in the context of the development of a commercially viable process for extracting natural dyes, with a view to tapping into the growing market for ‘natural’ materials. You will generate an appropriate statistical hypothesis, design the experiments required to test the hypothesis, conduct the experiments, analyze the results, and either falsify or support the proposed hypothesis.

The learning objectives for this experiment are that you

1. Achieve and demonstrate Comprehension Level of Learning for generation and testing of DoE screening-type hypotheses.

2. Achieve and demonstrate Application (Analysis) Level of Learning for planning experiments, in particular, full-factorial DoE screening experiments.

3. Achieve and demonstrate Application (Analysis) Level of Learning when applying principles from

earlier ChE and core courses to analysis of experimental data.

Pre-Lab Expectations • Students are assigned a particular dyestuff (brazilwood, logwood, or madder) and are required to do some background research on natural dyes in general and on their assigned dyestuff in particular. From this background research they generate a set of possible “measures of goodness” or outcomes that can be used to characterize their experimental outcome. From this set, they choose one (normally, dye concentration or strength). They also generate a large set of possible processing factors influencing the output variable. They narrow these down to four to be tested in a full-factorial two-level screening type experiment and develop the details of the experimental runs in consultation with the instructor (issues: safety, practicality, available processing, analytical equipment, etc.). After being signed off by the instructor, they conduct the experiment.

Conduct of the Experiment • Supplies must be provided to allow students to test processing factors:

- Temperature: hot plates and/or temperature baths, temperature measurement
- Extraction time: timers
- Agitation: Stirrers, shakers, or agitators
- Solvent composition: reagents and chemicals, balances and/or graduated cylinders, pipettes, etc.
- Pre-extraction dyestuff soaking: reagents, timers, etc.
- Dyestuff particle size: mortar and pestle, grinder, size screens, etc.

It is important to either provide students with a comprehensive list of available equipment and supplies in the laboratory or require them to specify required supplies at a pre-

TABLE 2
Typical Student Choices for High and Low Factor Levels for Statistical DoE Experiment

Process Factor	Temperature	Solvent ^a	Pre-soak	Extraction time	Agitation	Dyestuff particle size ^b
Typical ‘high’ factor value	100°C	ethanol	24 hours 20°C	20-50 minutes	high speed	as received
Typical ‘low’ factor value	20°C	water	none	1-5 minutes	none	reduced

^a Students were permitted to choose water, ethanol, or with justification from the literature, to choose other “safe” solvents or solvent systems (e.g., aqueous acetic acid, saline solution)

^b As-received particle size varied significantly for different dyestuffs: madder was received as roots with an average root piece of 4x40 mm, while brazilwood was received as roughly 300 μm particles. Reduction was accomplished via laboratory blender or by mortar and pestle.

lab meeting to assure that necessary supplies are adequate for the testing of their chosen factors. Table 2 gives typical low and high values chosen by students in the conduct of their DoE experiments.

Dyebath Analysis • There are several approaches that can be taken to analyze dye concentration—a colorimetric approach, where samples of extract from each run are compared to a wide set of known standards; a spectroscopic approach where samples of extract from each run are analyzed using UV-vis spectroscopy and Beer's law; or an analytical chemistry approach where extracts are further treated to purify (and weigh) the pure dye. In both colorimetric and spectroscopic approaches, a significant challenge is that the range of dye concentrations in the extracts might span three or even four orders of magnitude. In this case, neither the eye nor the spectrometer will have enough dynamic range to fully accommodate all samples, so a stronger sample might have to be pre-diluted to fit into a narrower 'instrumental' range.

Data Analysis • The experimental data set will comprise a matrix of data that is analyzed using DoE algorithms, normally via computer programs such as Minitab, JMP, Design-Expert, Fusion Pro, or add-on statistical software for MS-Excel such as XLSTAT.^[7] Depending upon the students' statistics background, required analysis can be as simple as a significance test for each of the factors, or as complex as response surface analysis. In this course, students were only required to complete a significance test.

LEARNING EFFECTIVENESS

Students tended to rather easily develop a competent DoE experimental design, but they often exhibited confusion between experimental design in the statistical sense and experimental planning—they often did not adequately imagine the actions they would be taking in the laboratory, and as a result they underestimated the time required or did not adequately

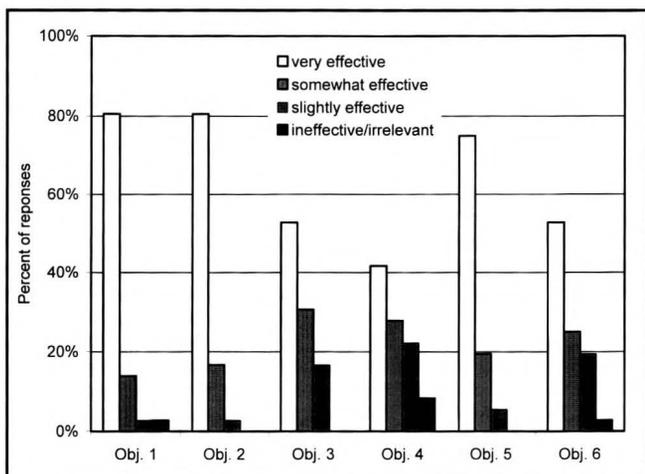


Figure 1. Student ratings of the effectiveness of the dye-extraction experiment in meeting each of the course learning objectives (listed in the text).

plan for the complexity of simultaneous runs. In this implementation, we used colorimetric analysis of dyebaths to ascertain extraction effectiveness. We plan on implementing spectrophotometric analysis in the next implementation, both as additional training for students in modern experimental methods and to enhance the precision of the experimental results.

Students were asked to rate the effectiveness of the dye extraction experiment and report-writing experience on their achievement of each of the course's learning objectives. Results are shown in Figure 1 for the Spring 2003 semester, the first implementation of this experiment.

On average, students rated the dye extraction experiment as a very effective activity toward the achievement of three of the course learning objectives (ability to design and perform experiments, ability to record and analyze data, and working in teams), somewhat-to-very effective for two objectives (ability to communicate effectively and apply skills in a chemical engineering context), and somewhat effective for one (ability to effectively use computers). These data indicate that the students viewed the learning experience as integrative within the course, which was certainly the intention of the instructor.

Positive comments about this experience included

- *I think the lab was the most important assignment of the course because it encompasses all of the learning objectives and seemed to be the climax of the course...I think more emphasis should be placed on it.*
- *Out of the tasks completed in this course, the design of experiments was the most useful in achieving the course learning objectives.*

Student suggestions for how to improve the experience mostly referred to a wish for more training in appropriate software for statistical analysis of their results. For example,

- *...require students to have more computer interaction*
- *...have an in-class tutorial on how to use available software*

MASS TRANSFER EXPERIMENTS

These are described for sophomore- or junior-level work after students have been introduced to simple mass transfer concepts. Simple estimation of an overall mass transfer coefficient can be obtained by looking at the driving force for extraction. If C represents the concentration of the dye in the extract, and C_{eq} represents the equilibrium (or saturation) concentration of dye in the solvent, then assuming that the mass transfer coefficient is dominated by resistance at the dyestuff/solvent interface, the relation

$$\frac{\partial C}{\partial t} = k(C_{eq} - C) \quad (1)$$

Continued on page 141.

INCORPORATING NONIDEAL REACTORS IN A JUNIOR-LEVEL COURSE

Using Computational Fluid Dynamics (CFD)

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Within the last few decades, there has been a significant increase in technological and computational tools that are available to students—using simulation packages to design process flow diagrams is now the norm in academia. Despite the advancement of computational tools, however, there is still growth potential for implementation of these tools in the chemical engineering undergraduate curriculum. Such tools can be beneficial for teaching advanced topics to undergraduate students in beginning courses. For example, analysis of nonideal reactors can be implemented in a junior-level chemical reaction engineering course using computational fluid dynamics (CFD).

This paper describes the incorporation of CFD in a junior-level chemical reaction engineering course at Oklahoma State University in which students use CFD to predict the single-reaction conversion of a species in a nonideal reactor. The last few weeks of the course are dedicated to teaching the students about nonideal reactors—specifically, obtaining and using residence time distribution (RTD) functions to assess the reactor. The students are assigned to teams of two-to-four students in which each team completes one CFD project to obtain the RTD for a given geometry and flow conditions. The students use the RTD, along with a given chemical reaction, to predict the conversion of a reactant at the exit of the reactor. Two classes of CFD demonstrations are provided on how to predict an RTD. An example for predicting the RTD in a straight tube, followed by predicting the conversion of a reactant, is described below.

In many undergraduate chemical reaction engineering courses, the content includes in-depth analyses of ideal reactors, such as batch, semi-batch, plug-flow (PFR), and continuous-stirred tanks (CSTR), for single or multiple isothermal or nonisothermal reactions. For the batch, semi-batch, and CSTR, the ideal assumptions include instantaneous and complete mixing (no spatial variations in concentration, temperature, or reaction rate). The ideal assumptions for a PFR

include no radial variation in temperature and concentration and no mixing in the axial direction (spatial variations occur only in the axial direction). Nonideal reactor analysis is a subject that is covered near the end of most textbooks^[1,2] and may not always be covered in a beginning course. Since students enrolled in transport phenomena or fluid mechanics courses at the undergraduate level learn about nonideal flow conditions, implementation of the nonideal flow concepts in reactor design would be beneficial for connecting the two courses and exposing students to reactor design that is more applicable to industrial settings.

NONIDEAL REACTORS

Several methods, ranging from combinations of hypothetical ideal reactors to detailed mathematical modeling, are used to characterize nonideal reactors.^[2-4] One method involves incorporating the residence time distribution (RTD) with models to predict the conversion of a species following passage through a chemical reactor. The RTD is a characteristic of the mixing that occurs in a chemical reactor and is informative about how long species reside in the reactor. The RTD of

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a reactor is not dependent on the chemical reaction. A major focus of this paper describes how to obtain an RTD and then apply the RTD to a model that combines a chemical reaction to predict the reactant conversion.

Experimentally, the RTD is determined by injecting a *tracer* into the reactor and measuring the tracer concentration in the exit stream as a function of time. The tracer should be a nonreactive species, be easily detectable, should have physical properties similar to those of the reacting mixture, and should not absorb on the walls or other surfaces in the reactor. These requirements are necessary so that the tracer's behavior reflects the flow properties of the reactants and products. In reaction engineering textbooks, the RTD is usually given in homework problems and examples.^[2] The advantage of incorporating CFD into the curriculum is that students can simulate an RTD for any reactor geometry rather than performing time-intensive experiments or having the RTD provided. Students can then model the conversion occurring in any nonideal reactor geometry using the simulated RTD. We introduced the CFD program (CFX, AEA Technologies, Pittsburgh, PA) in the transport phenomena course, which is taught in the semester prior to the reaction engineering course.

To demonstrate the use of CFD in analyzing nonideal reactors as part of a junior-level chemical reaction engineering course, a tubular reactor with laminar flow is provided as an example. The RTD is obtained for the tubular reactor by applying a step change in the concentration of a tracer flowing into the reactor (represented as C_0) and evaluating the temporal mixing cup tracer concentration at the reactor outlet. As stated before, the RTD is independent of the chemical reaction so the chemical reaction is not integrated into the CFD modeling. The dimensionless mixing cup (or volumetric flow-averaged) tracer concentration (C_{mix}/C_0) as a function of time is defined for a cylindrical reactor exit as

$$\frac{C_{\text{mix}}}{C_0}(t) = \frac{\int_0^R [C(r)/C_0] V(r) r dr}{\int_0^R V(r) r dr} \quad (1)$$

where $[C(r)/C_0]$ is the dimensionless tracer concentration and $V(r)$ is the axial velocity for a given radial position, r , at the reactor exit. R is the radius of the tube. When performing experiments, $C_{\text{mix}}(t)$ is the measured tracer concentration at a given time when collecting samples at the reactor exit. In the absence of experiments, CFD can be used to predict $C(r)$ and $V(r)$ as a function of time, then (C_{mix}/C_0) can be obtained as a function of time from Eq. (1).

Once (C_{mix}/C_0) is determined, the RTD function $[E(t)]$ is determined for use in models (described later) to predict the conversion of a species for a given reactor geometry. For a positive step change in the tracer concentration, $E(t)$ is evaluated from (C_{mix}/C_0) according to

$$E(t) = \frac{d[C_{\text{mix}}/C_0]}{dt} \quad (2)$$

$E(t)$ has several characteristics, such as the integral from $t = 0$ to t represents the fraction of effluent that has been in the reactor for less than time, t , and the integral of $E(t)$ from $t = 0$ to ∞ is one.

METHOD FOR OBTAINING RTD FUNCTION USING CFD

Example of a Tubular Reactor

Geometry • The tubular reactor is 30 cm long with a 2.5-cm internal diameter. Laminar flow through the reactor provides a parabolic velocity profile. For this example

$$V(\text{cm/sec}) = V_{\text{max}} \left(1 - \left(\frac{r}{R} \right)^2 \right) \quad (3)$$

with $V_{\text{max}} = 2$ cm/s. The reactor geometry was created in CFX with the required dimensions; first, a 2.5-cm-diameter circle was drawn, then the circle was extruded 30 cm and properly trimmed to obtain a solid vessel (using CFX terminology, the solid represents a fluid domain—in this case the fluid domain is the liquid inside the reactor).

Fluid Domain • A fluid domain must be established that describes the fluids that will exist within the geometry during the simulation. For the RTD predictions, two fluids are selected when creating the fluid domain—water and tracer. The water properties at room temperature and pressure are already in the CFX database. The fluids editor is used to create a new fluid called “tracer” that has the same physical properties as water, with the addition of an aqueous tracer diffusivity of 2×10^{-5} cm²s⁻¹. In the domain options, a transient problem with 0.1-second timesteps and a total simulation time of 40 seconds is specified. The specified time step and the maximum number of iterations for a time step is important for an accurate solution; decreasing the time step until the solution no longer changes demonstrates an appropriate time step. The reference pressure is atmospheric. Isothermal laminar flow is also specified.

Boundary Conditions and Initial Values • The inlet and outlet boundary conditions in CFX may be described using the normal speed, pressure, Cartesian velocity components, or the mass flow rate. The inlet boundary was specified using the 1-D velocity profile according to Eq. (3). The velocity equation can be input into CFX using an expression editor. The tracer mass fraction at the inlet was specified at 10% ($C_0 = 2170$ mol/m³). Any tracer mass fraction could be specified, however, since the tracer has the same properties as the water. The outlet boundary condition was specified as atmospheric pressure. For the initial values within the reactor at $t = 0$, the velocity components were chosen according to Eq. (3) and the mass fraction of tracer was specified as zero.

Mesh Parameters and Solving • Prior to using CFX, a mesh was automatically generated. To assess the accuracy of the solution, however, the mesh should be refined until the solution no longer changes. Following mesh generation, convergence criteria were selected and a transient-results file was established for input of the transient results once the solution was obtained. The velocity and tracer mass fraction were chosen for the output. CFX then solved the transient problem using the continuity and momentum equations that are already built into the software. Following the solution, a file was generated giving the spatial velocity and tracer mass fraction with time at all spatial points within the reactor. Obviously, the velocity components should not change with time (Eq. 3 can be used to calculate the axial velocity component as a function of radius) since the laminar flow profile was established as an initial condition and the inlet laminar velocity profile should not affect the established profile. For this example, the velocity profile from the CFX solution confirmed that the initial velocity profile remained constant throughout the simulation. A nonchanging flow profile is imperative for evaluating the RTD since the tracer is used to characterize the species movement in a steady-state flow regime. The spatial tracer mass fraction will change with time, however, due to the introduction of tracer at the inlet.

Once temporal velocity and tracer mass fraction profiles were obtained as a function of spatial position, the profiles at the tube exit were used to calculate (C_{mix}/C_0) as a function of time according to Eq. (1). Rectangular coordinates were given in the output file so the radius was calculated according to

$$r = \sqrt{x^2 + y^2}$$

The RTD function $[E(t)]$ was then calculated from the time derivative of (C_{mix}/C_0) according to Eq. (2).

RTD RESULTS

After solving the transient problem, CFX Visualize was used to run a transient animation of the tracer mass fraction within the tubular reactor. Figure 1 shows snapshots of the 10% tracer solution (black) as it travels through the reactor initially filled with pure water (white). The intermediate gray colors representing less than 10% tracer are also shown and demonstrate dispersion of the tracer as it travels through the reactor. A plug-flow reactor would show a solid black area upstream of a solid white area changing with time. The parabolic velocity effects on the tracer profile due to laminar flow are also evident, as demonstrated by the radial gradients in the tracer composition. The visual animation is an excellent tool for demonstrating nonideal reactor characteristics such as radial composition gradients and dispersion.

Figure 2 shows an example calculation for the dimensionless “mixing cup” tracer concentration using the CFX output data at 30 seconds. Using the data at the reactor outlet, the product of the dimensionless tracer concentration (C/C_0) , velocity (V) , and radius (r) was plotted as a function of the radius. The area under the curve represents the numerator of Eq. (1). Similarly, the product of the velocity and the radius (r) was plotted as a function of the radius, with the area under the curve representing the denominator of Eq. (1). Thus, the

ratio of the two areas represents the dimensionless “mixing cup” tracer concentration (C_{mix}/C_0) at 30 seconds. C_{mix}/C_0 was similarly calculated for all other times.

Figure 3 shows the calculated (C_{mix}/C_0) as a function of time. (C_{mix}/C_0) obtains steady state at around 40 seconds and approaches unity. Figure 4 shows $E(t)$ versus time as obtained from Eq. (2). The area under the $E(t)$ curve is approximately 1.03, which is consistent with the theoretical value of one. The $E(t)$ curve can also be used to calculate the residence time according to

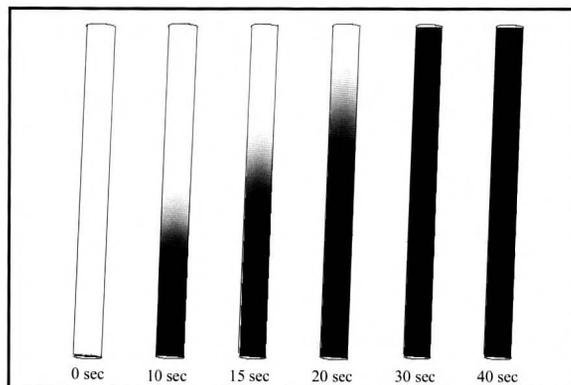


Figure 1. CFX flow profiles for a step tracer input in a tubular reactor. Snapshots of the 10% tracer solution (black) as it travels through a tubular reactor initially filled with pure water (white) are shown. Intermediate gray colors representing less than 10% tracer are also shown. The tubular reactor is 30 cm long with a 2.5-cm internal diameter.

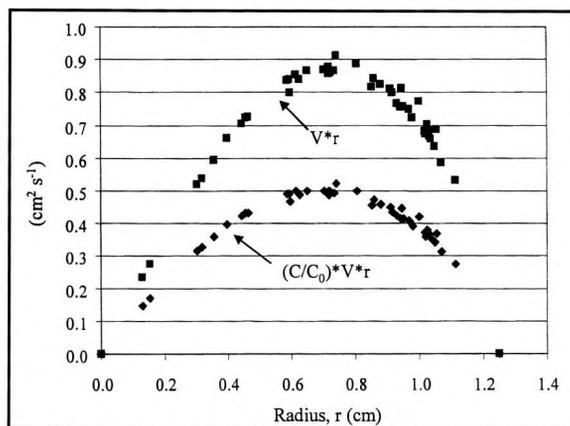


Figure 2. Dimensionless mixing cup (C_{mix}/C_0) tracer concentration analysis. At the reactor outlet, the product of the dimensionless tracer concentration (C/C_0) , velocity (V) , and radius (r) was plotted as a function of the radius at 30 seconds. The area under the curve represents the numerator of Eq. (1). Similarly, the product of V and r at the reactor outlet was plotted as a function of the radius with the area under the curve representing the denominator of Eq. (1). The ratio of the two areas represents the dimensionless mixing cup tracer concentration (C_{mix}/C_0) at 30 seconds.

$$t_{\text{res}} = \int_0^{\infty} tE(t)dt \quad (4)$$

A value of $t_{\text{res}} = 29.5$ seconds was obtained from the data, which is in agreement with the theoretical residence time of 30 seconds [reactor length (30 cm) divided by the radial-averaged velocity (1 cm/s)]. For a plug-flow reactor, $E(t)$ would be a spike at t_{res} . Deviation from plug flow (nonideality) would result in spreading of the spike, as demonstrated in Figure 4. As deviation from plug flow becomes greater (and approaches a well-stirred reactor), the spread becomes wider and more asymmetrical. The $F(t)$ curve, which is the same as the (C_{mix}/C_0) curve shown in Figure 3, was calculated according to

$$F(t) = \int_0^t E(t)dt \quad (5)$$

Both $E(t)$ and $F(t)$ are used to calculate the conversion limits for a nonideal reactor, as described below.

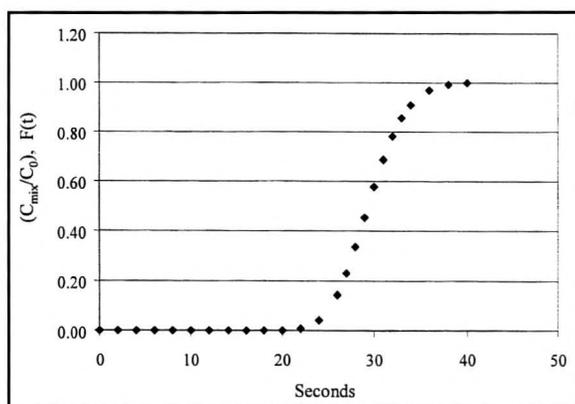


Figure 3. The dimensionless mixing cup tracer concentration (C_{mix}/C_0) was calculated using Eq. (1) and is shown as a function of time. The inlet tracer concentration (C_0) is 2170 mol/m^3 . As defined by Eq. (5), $F(t)$ was obtained from the $E(t)$ curve (see Figure 4).

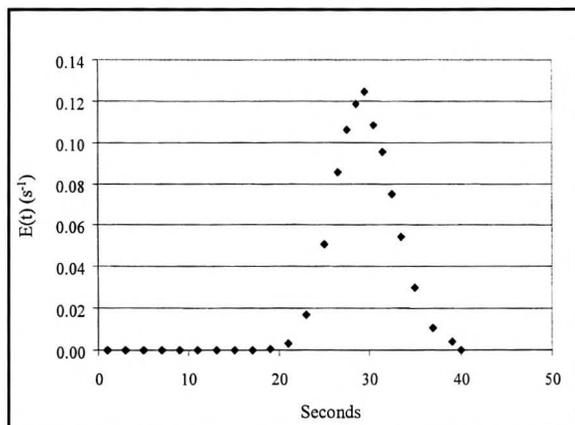


Figure 4. The RTD function $[E(t)]$ obtained from Eq. (2) is shown as a function of time.

APPLICATION OF RTD FOR NONIDEAL REACTOR MODELING

To demonstrate the application of using $E(t)$ and $F(t)$ to model the conversion in nonideal reactors, the nonelementary liquid-phase reaction $A \rightarrow D$ was chosen for the reaction in the tubular reactor with a rate law of

$$-R_A = \frac{kC_A}{(1 + K_M C_A)} = \frac{kC_{A0}(1 - x_A)}{[1 + K_M C_{A0}(1 - x_A)]} \quad (6)$$

For the constant volumetric flow conditions, the conversion (x_A) definition of $C_A = C_{A0}(1 - x_A)$ was included in Eq. (6). Parameters of $C_{A0} = 1.0 \text{ M}$, $k = 0.05 \text{ s}^{-1}$, and $K_M = 1.0 \text{ M}^{-1}$ were used.

The simplest method for predicting x_A exiting the nonideal reactor is using the rate law together with the $E(t)$ and $F(t)$ curves to estimate bounds for x_A . This method uses two zero-adjustable parameter models; a segregation model and a maximum-mixedness model. The segregation model assumes that molecules of the same residence time (or “age” in the reactor) travel in groups and each group acts as a batch reactor. The maximum-mixedness model assumes that molecules of different “age” are completely mixed as they enter the reactor. For a more detailed explanation, see reference 2 (pp. 838-851).

To obtain one bounded prediction for conversion $(x_{A,\text{seg}})$, the segregation model uses the predicted conversion for a constant-volume batch reactor $[(x_A)_{\text{batch}}]$ together with the $E(t)$ curve according to

$$x_{A,\text{seg}} = \int_0^{\infty} (x_A)_{\text{batch}} E(t)dt \quad (7)$$

For a constant-volume batch reactor, the batch conversion is obtained by integrating the following equation using the reaction rate given in Eq. (6):

$$-C_{A0} \frac{d(x_A)_{\text{batch}}}{dt} = R_A = -\frac{kC_{A0}[1 - (x_A)_{\text{batch}}]}{\{1 + K_M C_{A0}[1 - (x_A)_{\text{batch}}]\}} \quad (8)$$

Following integration of Eq. (8) to obtain an $(x_A)_{\text{batch}}$ curve as a function of time, a new curve is generated by plotting the product of $(x_A)_{\text{batch}}$ and $E(t)$ versus time. According to Eq. (7), the area under the curve represents $x_{A,\text{seg}}$. For this example, $x_{A,\text{seg}}$ is 0.59.

To obtain the other bounded prediction for conversion $(x_{A,\text{maxmix}})$, the maximum-mixedness model uses both the $E(t)$ and $F(t)$ curves, along with R_A . As noted by Fogler,^[2] the conversion is predicted by

$$x_{i+1} = x_i + (\Delta\lambda) \left[\frac{E(\lambda_i)}{1 - F(\lambda_i)} x_i + \frac{R_A(x_i)}{C_{A0}} \right] \quad (9)$$

where λ is the time and $\Delta\lambda$ is the time step. To apply Eq. (9), λ_1 is chosen to represent the latest time of the $E(t)$ curve in which E approaches zero ($\lambda_1 = 40$ seconds for this example), x_1 is zero, and negative time step is chosen ($\Delta\lambda = -2$ seconds for this example). R_A (Eq. 6) is evaluated using x_1 and the values of E and F are obtained at λ_1 . Using Eq. (9), a value for x_2 is obtained. R_A is then evaluated using x_2 and the values of E and F are obtained at $\lambda_2 = \lambda_1 + \Delta\lambda = 38$ seconds to obtain x_3 from Eq. (9). The process is repeated until $\lambda_n = 0$ seconds,

wherein x_n is the bounded conversion $x_{A,\text{maxmix}}$. For this example, $x_{A,\text{maxmix}}$ is 0.60.

The above values $x_{A,\text{seg}} = 0.59$ and $x_{A,\text{maxmix}} = 0.60$ signify that the conversion of A in the nonideal tubular reactor is between 0.59 and 0.60 for the given reaction rate. Since the E(t) curve showed only a small deviation from plug flow, the predicted conversion should be close to the conversion predicted with a PFR model. For this example, x_A is 0.60 for plug flow, demonstrating that the nonideal tubular reactor has a conversion only slightly less than plug flow. More complex reactor geometries are likely to show greater conversion deviations from plug flow, however, as the flow regime becomes more nonideal.

NONIDEAL ANALYSIS OF COMPLEX REACTOR GEOMETRIES

The power of using CFD to obtain the RTD function is that more complex reactor geometries, rather than simple tubular geometries, can also be evaluated. Thus, students can be given any reactor geometry to obtain an RTD function as well as visualize the nonideal flow patterns in the reactor. In addition, CFD can be used directly with kinetic models to design reactors.^[5] To demonstrate the nonideal flow patterns in a more complex geometry, a tank reactor (2.25" tall, 3.5" diameter) is shown in Figure 5 with a perpendicular inlet (0.50" diameter) entering the top side of the reactor (0.5" from top) and an outlet (0.25" diameter) directly at the bottom center of the reactor.

With more complex reactor geometries, the steady-state velocity flow profile within the reactor is not known *a priori* (like the tubular reactor represented by Eq. 3). As previously mentioned, the steady-state flow profile is used as an initial condition when using CFD to predict the RTD from a step tracer input. A steady-state flow profile is necessary since experimental tracer studies rely on the flow profile being established and not changing prior to the step tracer input. Therefore, before applying a step tracer input to predict the RTD, the steady-state flow profile must be determined so the profile can be used as an initial condition.

The steady-state velocity profile is obtained using CFX by defining the fluid domain with a single fluid, such as water. For this example, the inlet boundary condition was chosen as the velocity profile given in Eq. (3). The outlet boundary condition was atmospheric pressure. Upon solving, the steady-state profile is obtained throughout the geometry and is stored in a results file.

The transient tracer mass fraction following a step tracer input is obtained using the same procedure described for the tubular reactor. The initial velocity profile is read from the above results file, however, rather than being typed in, as was the case for the tubular reactor. The tracer mass fraction is still specified as zero for the initial condition. The output file will give the temporal and spatial velocity and tracer mass

fractions at the outlet that can then be used to obtain E(t) and F(t) curves for predictions of conversion.

Although for brevity of this paper, the E(t) and F(t) profiles and x_A bounded predictions were not obtained for the tank reactor, CFX Visualize was used to run a transient animation of the tracer mass fraction within the tank reactor. Figure 5 shows snapshots of the 10% tracer solution as it travels through the reactor initially filled with pure water. Intermediate shades of gray represent less than 10% tracer. The nonideality of flow is strongly evident as there are wide variations of the tracer mass fraction within the reactor. Evidence of stagnant areas can also be observed. A well-mixed reactor would show the same color throughout the reactor and would change from black to white. Again, the visual animation is an excellent tool for demonstrating nonideal reactor characteristics such as stagnant regions and large concentration gradients.

CONCLUSIONS

This work describes the incorporation of CFD in a junior-level chemical reaction engineering course to demonstrate nonideal reactor principles, as well as to model nonideal reactors. Important concepts of nonideal reactors such as concentration gradients, stagnation, dispersion, and conversion can be visualized and modeled using CFD to enhance a student's understanding of nonideal reactors. In addition, transport concepts are also emphasized. An advantage of using CFD is that an RTD profile can be predicted for any reactor geometry without performing an experiment.

Applications include changing the flow profiles and reactor configurations that allow a student to understand the role of mixing in reactor kinetics. Only two examples are shown in this paper, but there are numerous possibilities for developing problems specific to other reactor geometries. Current plans are to extend the simulation to include stirrers, pressure drops, and nonisothermal conditions to make the prob-

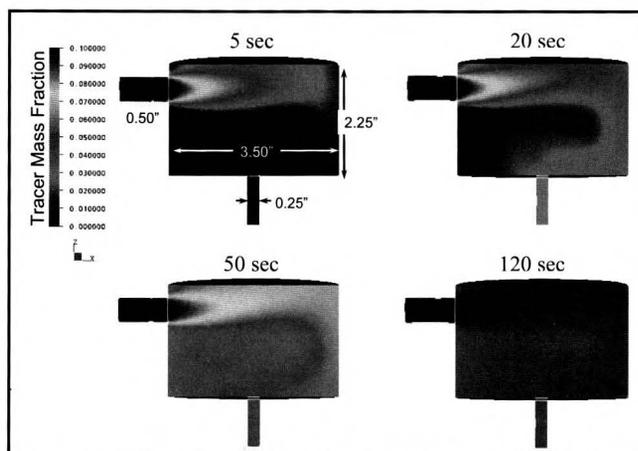


Figure 5. Snapshots of the 10% tracer solution as it travels through a tank reactor initially filled with pure water. Diameter and height dimensions are shown.

lems more realistic. In addition, the RTD can be applied to other models, including a one-parameter dispersion model, to characterize nonideal reactors. The validity of model assumptions must be checked before applying any model, however.

The nonideal reactor analysis using CFX was implemented in the junior-level chemical reaction engineering course in the spring of 2002. Student feedback led to the importance of considering some issues when implementing CFD into the curriculum. First, since students were only exposed to CFX the prior semester, assigning the project for a group, rather than an individual, enabled students to spend more time on the analysis. Second, students were often frustrated when drawing the geometry in CFX. Perhaps an instructor should consider developing a geometry database so students can spend more time analyzing reactor geometries and understanding nonideal concepts rather than drawing the geometries. In conclusion, the use of CFD programs such as CFX will enable students to be more prepared to enter today's workforce and to solve the difficult problems that arise with nonideal reactors.

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Experiments Using Natural Dye Materials

Continued from page 135.

is a reasonable starting approximation. After experimental determination of C_{eq} (either from the asymptote of the concentration/time results or from a separate experiment), concentration vs. time data at constant processing conditions (temperature, stirring, dyestuff particle size, etc.) can be analyzed graphically or analytically to determine the mass transfer coefficient from the time dependence of the concentration

$$C_{eq} - C = kC_{eq} \exp(-kt) \quad (2)$$

Further experiments can be designed to readily examine the effects of solvent, temperature, stirring, dyestuff particle size, and soaking on C_{eq} and on k .

ADDITIONAL OPPORTUNITIES

Aspects of this approach that were listed at the start of this

article suggest some further opportunities in using natural dyestuffs:

• Other ChE Experiments

This paper describes implementation for supporting the learning of statistical design of experiments relevant to early-stage process development. Variations of this experiment could support other ChE topic areas and concepts, including thermodynamics (dye solubility with temperature, solvent), unit operations (post-extraction filtration, operation costs as a function of dyebath concentration and production rate, countercurrent stage-wise extraction), and reaction engineering (for dyestuffs requiring some chemical reaction as part of the processing, such as indigo).

• Distance Experiment

A kit for the conduct of this experiment or something like it could be generated for a true distance experiment; the safety of the materials makes it possible to perform an aqueous extraction experiment in a home kitchen—analysis could be performed by color comparison to a printed standard sheet.

• Hands-On Recruiting Activity/Contest

Students could be challenged to most-closely match a target color using the smallest amounts of materials. They could be supplied with samples of a variety of dyestuffs, water, vinegar, baking soda, and perhaps some nontoxic metal salts. Materials could be price-labeled and students required to complete their work within a budget.

SUMMARY

The main purpose of this article is to spark interest in the use of natural raw materials in a variety of chemical engineering educational contexts, especially laboratory experiences. We have found that students respond positively to the laboratory use of these materials in the form of natural dyestuffs. Such materials can provide safe, environmentally friendly, aesthetically engaging hands-on experiences to support a variety of learning goals in the chemical engineering context.

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USE OF DYNAMIC SIMULATION TO CONVERGE COMPLEX PROCESS FLOWSHEETS

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Commercial process simulators are widely used for designing new processes and for analysis of existing processes. Most senior design courses contain a significant component of computer simulation of process flowsheets using these tools. The most widely used commercial process simulation software is that developed by Aspen Technology—AspenPlus for steady-state simulation and AspenDynamics for dynamic simulation—and these tools are used in the examples in this paper. The standard Aspen notation is used. For example, distillation column stages are counted from the top of the column: the condenser is Stage 1 and the reboiler is the last stage.

The simulators contain models of most common unit operations, which can be connected into a process flowsheet. If the units operate in series, with upstream units feeding downstream units, the simulation is usually reasonably straightforward. If the flowsheet contains recycle streams, however, the simultaneous solution of the typically very large number of simultaneous nonlinear algebraic equations that make up the steady-state model can be quite challenging. There is no guarantee that any algorithm will find a solution. In addition, there are sometimes multiple solutions in these nonlinear systems. The convergence of these recycle loops (or “tear” streams) is a major challenge in steady-state process simulation.

Energy integration can also produce complications because of “energy recycle” between different units. These difficulties can sometimes be avoided by using the plant utility system to break the energy linkage.

Commercial steady-state simulators contain a variety of algorithms. For example, the user of AspenPlus can try such methods as Wegstein, Broyden, and Newton. Convergence tolerances and the maximum number of iterations can also be adjusted.

The experience of many users, particularly students, has been that the convergence of recycle loops is the most diffi-

cult part of steady-state simulation. The normal procedure is to assume some conditions of a recycle stream (flow, temperature, pressure, and composition) and work down through the flowsheet until the calculated values of the recycle stream are available. If the assumed and calculated values are not sufficiently close, new guesses must somehow be made. The process is repeated until convergence between the assumed and calculated values has been attained. Often, however, convergence does not occur.

One would think that this convergence should be fairly easily achieved if the user has adjusted the design and operating parameters so the assumed and calculated conditions of the recycle stream are fairly close, but this all too frequently does not occur. For example, in one of the cases discussed later, an assumed recycle stream had a composition 98 mol% methanol and 2 mol% water, while the calculated stream is only slightly different (0.4 mol% dimethyl ether; 97.2 mol% methanol; 2.4 mol% water). The assumed flowrate is 72 kmol/hr, while the calculated flowrate is 72.9 kmol/hr. The temperature and pressures are identical. After connecting the recycle stream and defining it as a “tear” stream in the “Convergence” section of the “Data Browser” in AspenPlus, the recycle loop does not converge when using any of the algorithms.

This paper illustrates that recycle loops can be easily converged if the steady-state AspenPlus simulation (with the re-



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cycle loops not connected) is “exported” into the dynamic simulator AspenDynamics and the recycle connections are made on the dynamic model. The steps in going from a steady-state simulation to a dynamic simulation are discussed in the next section.

It should be noted that the issue of requiring good initial guesses of plant conditions in order to converge is not a problem since all the units have been converged individually in AspenPlus before going into dynamics. The “guessed” and the “calculated” values of the tear streams have also been adjusted to be fairly close to each other.

TRANSITION FROM STEADY STATE TO DYNAMIC SIMULATION

There are several items that must be taken care of to convert a steady-state simulation into a dynamic simulation: all equipment must be sized and a control structure must be developed. Luyben^[1] presents many details of these necessary steps, which are summarized below. Not all of the units that are available in steady-state AspenPlus are supported in AspenDynamics, so this limitation must be kept in mind. For example, neither the “separator” (a fictitious component splitter) nor a liquid-liquid extractor is supported in the current version (Version 11.1) of AspenDynamics.

When the steady-state simulation in AspenPlus is exported into AspenDynamics, a “pressure-driven” dynamic simulation should be used. This requires that all the “plumbing” must be specified in the flowsheet. Pumps and compressors must be inserted where needed to provide the required pressure drop for material flow. Control valves must be installed where needed, and their pressure drops selected.

This is one of the more important educational aspects of the procedure since most students have a poor grasp of plumbing. Common errors include inserting two valves into a liquid-filled line, inserting a valve in the suction of pumps, or inserting a valve at the discharge of compressors (compressor speed or its equivalent compressor work should be manipulated).

Equipment Sizing • For steady-state simulation, the size of the equipment is not needed, except for reactors. For dynamic simulation, the inventories of material contained in all the pieces of equipment affect the dynamic response, so the physical dimensions of all units must be known.

In distillation columns, the diameter of the column, the weir height, and the sizes of the reflux drum and the column base must be specified. Of course, before these can be calculated, the number of stages and the feed stage location must be set by some heuristic or rigorous optimization method. Perhaps

the easiest heuristic approach is to fix the distillate and bottoms specifications (using the *Design Spec* and *Vary* tools in AspenPlus) and keep increasing the number of stages until the required reflux ratio stops decreasing—this gives the minimum reflux ratio. Then the actual reflux ratio is set at 1.2 times this minimum. Finally, the optimum feed stage can be determined by varying the feed stage until the minimum reboiler energy consumption is found.

The *Tray Sizing* section of a distillation column block in AspenPlus can be easily used to provide the column diameter. The default weir height of 0.05 m can be used. The volumetric flowrates of liquid into the reflux drum (Stage 1, the “condenser” in Aspen terminology) and the liquid into the base of the column (the last stage, or “sump” in Aspen terminology) can be used to size the two vessels by using the heuristic of a 10-minute holdup time. These volumetric flowrates are given in the *Hydraulics* page tab of the *Profiles* section of the column block. To have these results made available, you must go to the *Report* section of the column block, select the *Property Options* page tab and click the *Include Hydraulic Parameters* box before running the program.

For example, the liquid holdup in the reflux drum of a column with a total condenser is calculated from the volumetric flowrate of liquid leaving the drum (distillate plus reflux).

$$[\text{Drum volume (m}^3\text{)}]$$

$$= [\text{Liquid volumetric flowrate (m}^3\text{/min)}][10 \text{ minutes}]$$

If an aspect ratio (length to diameter, L/D) of 2 is used, the diameter of the drum is

$$D = [2(\text{Volume})/\pi]^{1/3}$$

The same procedure can be used for flash tanks and vaporizers. Flash tank vapor velocity should also be checked.^[2]

Heat exchanger tube-and-shell volumes can be calculated from the heat-transfer area, which is known from the steady-state design, if a tube diameter D (typically 0.0245 m) is selected.

$$\text{Area} = [\text{number of tubes}][\pi D][\text{tube length } L] = N_{\text{tube}}(\pi DL)$$

$$\begin{aligned} [\text{Volume of tubes}] &= [\pi D^2/4][L][N_{\text{tube}}] \\ &= [\pi D^2/4][L][\text{Area}]/[\pi DL] = D[\text{Area}]/4 \end{aligned}$$

Shell volume is approximately equal to tube volume in most tube-in-shell heat exchangers. If the process streams in the heat exchanger are gases, the dynamics are very fast and can usually be ignored (specify *Instantaneous* in the Dynamic section of the heat-exchanger block).

Plantwide Control • When the file containing the flowsheet is opened in AspenDynamic, a default control scheme is al-

The convergence of steady-state simulations of flowsheets with recycle streams is frequently very difficult. An alternative is suggested in this paper and an example illustrates the proposed method.

ready installed on some loops. For example, level and pressure controllers are inserted on all distillation columns and reactors in the flowsheet. This default control must be modified and supplemented with other control loops to incorporate a stable basic regulatory control structure.

- **Plantwide Control Structure** A simple heuristic method for development of an effective plantwide control structure is presented by Luyben, *et al.*^[3] General principles and many examples are given in great detail. The proposed nine-step procedure has been successfully applied to a large number of realistically complex industrial processes. Some of the key concepts are: (1) the control structure should guarantee that all chemical components fed into the system are either reacted or can leave in some exiting stream; (2) a flow controller should be installed somewhere in all liquid recycle loops; and (3) all liquid levels must be controlled and pressures in gas systems, which can be multiple units connected together, must be controlled.

- **Controller Tuning** Most of the controllers are easily tuned by simply using heuristics. All liquid levels should use proportional-only controllers with a gain of 2. All flow controllers should use a gain of 0.5 and an integral time of 0.3 minutes (also enable filtering with a filter time of 0.1 minutes).

The default values in AspenDynamics for most pressure controllers seem to work reasonably well. Temperature controllers often need some adjustments. The default transmitter ranges are usually too large, and spans should be set at about 10% of the absolute temperature level (typically a span of 100 K for moderate-temperature processes).

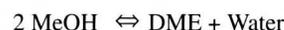
Distillation columns are typically controlled by manipulating reboiler heat input to control the temperature on some selected tray. The heuristic procedure of finding a tray where the temperature changes from tray to tray are large is easy to use and provides effective composition control in most cases. Direct composition measurements can be used if temperature changes are too small. If very large temperature changes occur in the column (over 100 K), an average temperature can be used (measuring the temperatures at three or four trays, calculating the average, and using this for control).

It should be kept in mind that the objective at this point is not to come up with the “best” control structure or the optimum controller tuning. We only need a structure and tunings that drive the simulation to a steady state.

EXAMPLE (“DME” PROCESS)

To illustrate the use of a dynamic simulator to converge a flowsheet, we select the dimethyl ether (DME) process discussed by Turton, *et al.*^[4] This design text gives a flowsheet and some preliminary design param-

eters. The chemistry is the exothermic reversible decomposition of methanol to form DME and water in an adiabatic, tubular, gas-phase reactor.



The reaction is exothermic, and the adiabatic temperature

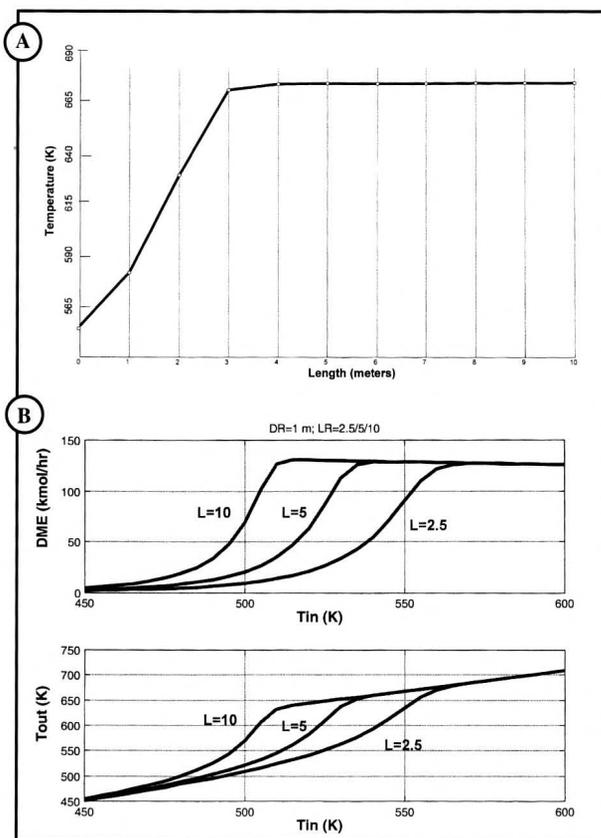


Figure 1. (A) Adiabatic reactor temperature profile (10 meters length). (B) Effect of inlet temperature for different reactor lengths.

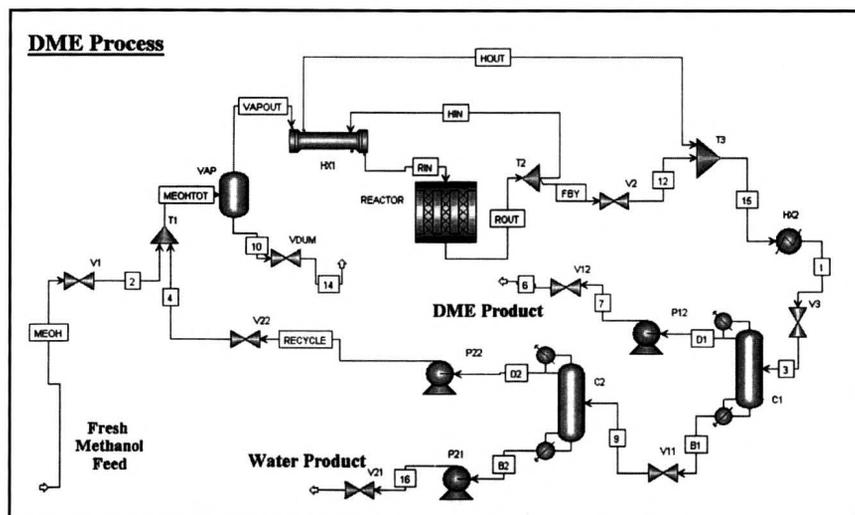


Figure 2. DME flowsheet.

rise is about 120 K. The temperature profile is shown in Figure 1A for a reactor that has a diameter of 0.72 m and is 10 m long. Figure 1B shows how reactor inlet temperature T_{in} affects the production of DME and the reactor exit temperature T_{out} for three different reactor lengths. The inlet temperature required to achieve maximum conversion decreases as the reactor is made bigger. Since the reaction is exothermic, the maximum conversion decreases slowly as temperatures increase.

The equilibrium constant is about 6 at a reactor temperature of about 600 K, so the per-pass conversion is about 80%. This requires a recycle of methanol back to the reactor from the separation section. Figure 2 gives the AspenPlus flowsheet, and Figure 3 gives stream conditions. The NRTL physical property package is used in the simulation.

Fresh methanol and recycle methanol are vaporized and heated to 555 K. The vapor-phase reaction occurs at about 15 atm. Reactor effluent is cooled and fed into a two-column separation section. The low-boiling DME is the distillate product in the first column C1, which operates at a pressure of 10 atm so that cooling water can be used in the condenser (reflux-drum temperature is 318 K with 99.9 mol% DME purity). The column has 32 stages, is fed on Stage 15, and is operated with a reflux ratio of 0.5.

The bottoms of Column C1 is fed to the second column C2 in which water is removed from the bottom and recycled methanol is removed from the top. This column operates at 1.1 atm and has a reflux-drum temperature of 340 K. It has 22 stages and a reflux ratio of 1.5.

Reaction Kinetics • One of the most difficult parts of developing a flowsheet is getting the reaction kinetic parameters correctly specified. Any errors in unit conversions are

amplified by the exponential expressions.

Since the reaction is reversible, both the forward and the reverse reaction rates must be specified. Thurton, *et al.*,^[2] provide a kinetic expression for the forward reaction rate

$$R_F (\text{kmol} / \text{hr} / \text{m}^3) = 1.21 \times 10^6 e^{-80,480/RT} P_{\text{MEOH}} \quad (1)$$

where P_{MEOH} has units of kPa and the activation energy has units of kJ/kmol. Aspen insists on expressing reaction rates in kmol/sec/m³, so we must divide by 3600. More seriously, Aspen also insists that partial pressure be in Pa, not in kPa. A common error is to multiply by 1000 to convert the pressure in Eq. (1) from kPa to Pa. This is incorrect. The pressure in Eq. (1) is in kPa, and Aspen uses Pa, so the pre-exponential factor must be divided by 1000.

$$\begin{aligned} R_F (\text{kmol} / \text{sec} / \text{m}^3) &= 1.21 \times 10^6 e^{-80,480/RT} [P^{\text{kPa}}] / 3600 \\ &= 1.21 \times 10^6 e^{-80,480/RT} \left[\frac{P^{\text{Pa}}}{1000} \right] / 3600 \\ &= 0.3361 e^{-80,480/RT} P^{\text{Pa}} \end{aligned} \quad (2)$$

Turton, *et al.*,^[4] also give information about the equilibrium constant, but state that the published data does not seem to match the calculations using free energies. This was confirmed by running an *R-Gibbs* reactor in AspenPlus, which gave a much lower reactor conversion than would be predicted by the published data.

The heat of reaction is $\lambda = -11,770$ kJ/kmol, so we can estimate the activation energy of the reverse reaction from that of the forward reaction.

$$E_F - E_R = \lambda \Rightarrow E_R = 80,480 - (-11,770) = 92,250 \text{ kJ} / \text{kmol} \quad (3)$$

	MEOH	RECYCLE	RIN	ROUT	D1	B1	B2	FBY	1
Substream: MIXED									
Mole Flow kmol/hr									
DIMET-01	0.0	5.26672E-9	5.26566E-9	130.8673	130.8673	5.26672E-9	3.8486E-23	52.34693	130.8673
MEOH	262.0000	73.02976	335.0264	73.29178	130.9983	73.16076	130.9980	29.31671	73.29176
WATER	0.0	.5078546	.5078378	131.3752	6.7731E-13	131.3751	130.8672	52.55007	131.3751
Mole Frac									
DIMET-01	0.0	7.1619E-11	1.5693E-11	.3900267	.9990000	2.5750E-11	2.9379E-25	.3900267	.3900268
MEOH	1.000000	.9930939	.9984865	.2184331	1.00000E-3	.3576916	9.99998E-4	.2184331	.2184331
WATER	0.0	6.90605E-3	1.51352E-3	.3915402	5.1703E-15	.6423084	.9990000	.3915402	.3915401
Total Flow kmol/hr	262.0000	73.53782	335.5343	335.5343	130.9983	204.5358	130.9982	134.2137	335.5342
Total Flow kg/hr	8395.046	2349.180	10744.12	10744.12	6033.130	4710.988	2361.807	4297.648	10744.12
Total Flow l/min	175.3164	52.67718	17092.40	21437.16	162.4282	108.3552	43.21094	8574.864	243.3503
Temperature K	298.1500	342.2560	555.0000	672.7188	318.1082	424.6567	379.1812	672.7186	325.0000
Pressure atm	17.00000	17.00000	14.90000	14.40000	10.00000	10.21094	1.242897	14.40000	12.00000
Vapor Frac	0.0	0.0	1.000000	1.000000	0.0	0.0	0.0	1.000000	0.0
Liquid Frac	1.000000	1.000000	0.0	0.0	1.000000	1.000000	1.000000	0.0	1.000000

Figure 3. DME stream data.

Wegstein is used (with a limit of 30 iterations), the source of the *RECYCLE* stream is specified to be the discharge of pump P22 and it is specified as a *Tear* under the *Convergence Section* of the *Data Browser*. The program is run.

The convergence loop fails to converge.

This is a typical result in many cases. It should be noted that *Design Specs* and *Vary* features are used on both distillation columns. In Column C1, the distillate DME product purity is specified to be 99.9 mol% DME, and the distillate flowrate is varied. In Column C2, the bottoms water product purity is specified to be 99.9 mol% water, and the bottoms flowrate is varied. The reflux ratio is fixed in both columns.

Increasing the maximum iterations does not achieve convergence. Switching to the Broyden algorithm is equally unsuccessful.

This failure to converge certainly does not occur in all cases for all flowsheets, but it does occur in many cases. Senior students spend many frustrating hours trying to get recycle loops to converge.

Converting to Dynamic Simulation • The diameters of the two columns are calculated in the *Tray Sizing* section: 0.61 m for C1 and 0.94 m for C2. The liquid flowrates into the reflux drums of C1 and C2 are 0.242 and 0.131 m³/min, respectively, as found in the *Hydraulics* page tab. Reflux drum sizes (D x L) in the two columns are set at 1.2 x 2.4 m and 1 x 2 m, respectively, using an aspect ratio of 2. The liquid flowrates into the base (to the sump from the next-to-last stage in the column) of C1 and C2 are 0.213 and 0.0853 m³ min, respectively. Reboiler sizes in the two columns are set at 1.1 x 2.2 m and 0.82 x 1.64 m, respectively.

The heat exchangers are assumed to be “instantaneous” since they are gas phase. Reactor size is already specified for the steady-state simulation. The only other dynamic unit in the flowsheet is the vaporizer. Its liquid feed is 10,700 kg/hr with a density of

785 kg/m³, which gives a diameter of 1.1 m and a length of 2.2 m to provide ten minutes of holdup.

The file is pressure checked and exported into AspenDynamics. The default control scheme is shown in Figure 6. Note that each column has pressure and level controllers, some of which are fully connected and others without the controller output signal (OP) connected to a valve. This default control scheme must be modified to provide an effective regulatory control scheme.

Before doing anything, an *Initialization* run and a short *Dynamic* run should be made to confirm that all the plumbing is okay and the process is correctly configured.

Closing the Recycle Loop • The procedure for changing the process structure in AspenDynamics is the same as in AspenPlus. The stream *RECYCLE* is deleted. The destination of the stream *RCALC* is made the inlet to valve V22. Another set of *Initialization* and *Dynamic* runs should be made. Now the default control structure can be modified. It is a good idea to perform *Initialization* and *Dynamic* runs after each new change in the control structure so that any error in controller installation can be detected individually. The most common error is to have the wrong action in the controller (for example, specifying reverse action when it should be direct action).

An obvious alternative to deleting *RECYCLE* and reattaching *RCALC* is to delete *RCALC* and reattach *RECYCLE*. If this is attempted, the little green box at the bottom of the AspenDynamics screen turns red, indicating that something is wrong. Double-clicking the red box opens the window shown at the top of Figure 7, which states that the problem is overspecified. Clicking the *Analyze* button opens the window shown at the bottom of Figure 7, which says that the temperature and pressure of the *RECYCLE* stream must be changed from fixed to variable. Clicking the *ACCEPT* button turns the box green again. Then *Initiation* and *Dynamic* are again run to make sure all is okay. Now the default control scheme can be modified.

Plantwide Control Structure • Using the method proposed in Luyben, *et al.*,^[3] a plantwide control scheme is developed that features the following loops:

- The feed flow to the first column is flow controlled. This puts a flow controller in the liquid recycle loop. It also has the advantage of keeping a fixed steady flow to the column. Since the final DME product is produced in this column, product quality variability is minimized by not permitting disturbances to enter this column.
- The vaporizer level is controlled by manipulating the fresh methanol feed. This guarantees that only the amount of methanol that is being consumed in the reactor will be fed into the process. If more DME production is required, the setpoint of the flow controller on Column C1 feed can be increased. Using reactor inlet temperature to change production is not effective because of the reversibility of the reaction. For example, sometimes increasing reactor inlet

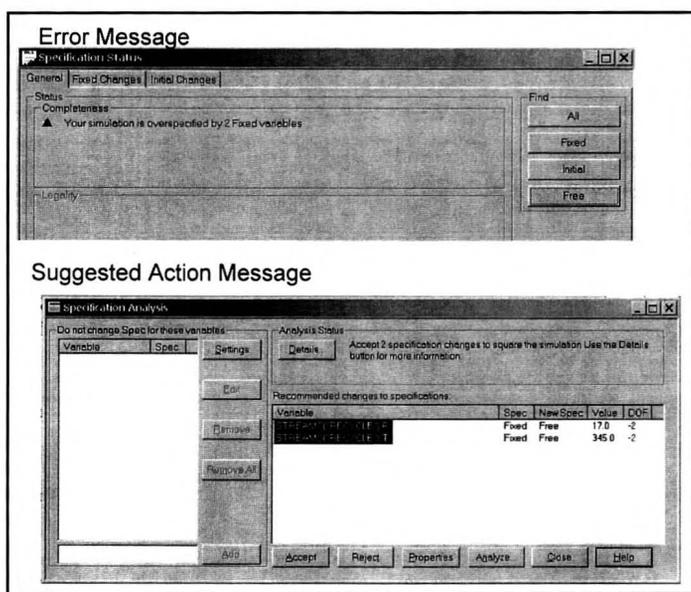


Figure 7. Error message and suggested action message.

temperature produces a decrease in the production of DME.

- Vaporizer pressure is controlled by manipulating steam (heat input Q) to the vaporizer.
- Reactor inlet temperature is controlled by the HX1 heat exchanger bypass flow (valve V2).
- Condenser HX2 exit temperature is controlled by manipulating cooling water (heat removal Q).
- The pressure in each column is controlled by condenser heat removal.
- The reflux-drum level in each column is controlled by manipulating distillate flow.
- The base level in each column is controlled by manipulating bottoms product flow.
- A temperature in each column is controlled by manipulating reboiler heat input. The steep part of the temperature profile in C1 is at Stage 17 and in C2 at Stage 19, so these tray locations are selected. The temperature setpoint in C1 is 380 K and in C2 is 370 K.
- The reflux ratio in each column is controlled. The distillate flowrate is measured, multiplied by the desired reflux ratio (0.5 in C1 and 1.5 in C2) and this signal sets the flowrate of reflux.

Figure 8 gives the

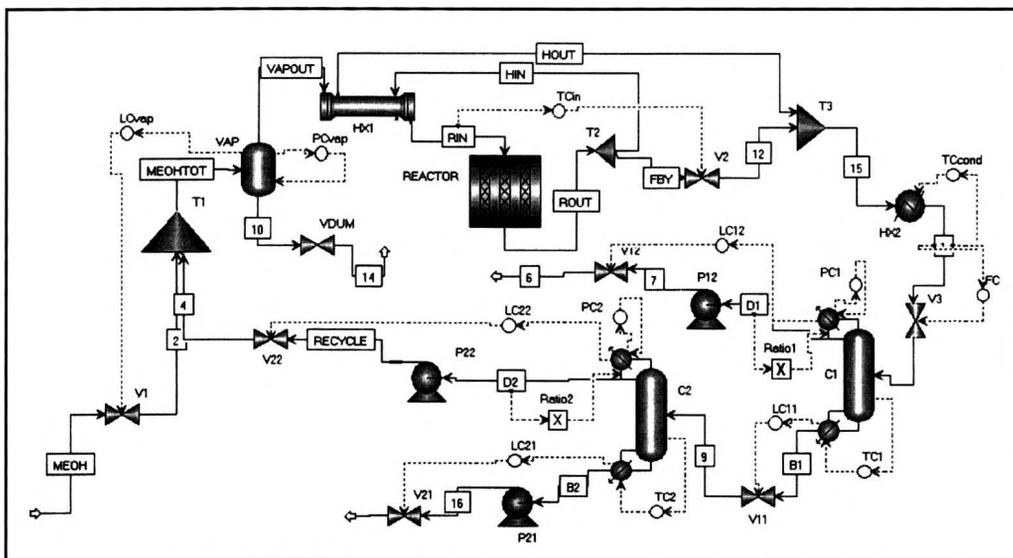


Figure 8. Plantwide control structure: DME process.

TABLE 1
DME Controller Parameters

Controller (Action)	Transmitter Range min/max (units)	Valve Range min/max (Units)	Integral Time K_c τ_I (min)
FC (Rev)	0/663 (kmol/hr)	0/100 (%)	0.5 0.3
TCin (Dir)	500/600 (K)	0/100 (%)	2 5
LCvap (Rev)	0/3.26 (m)	0/100 (%)	2
TCcond (Rev)	300/400 (K)	-2030/0 (kcal.sec)	2 20
PCvap (Rev)	10/20 (atm)	0/1910 (kcal/sec)	5 12
TC1 (Rev)	300/400 (K)	0/690 (kcal/sec)	1 20
LC11 (Dir)	0/2.5 (m)	0/100 (%)	2
LC12 (Dir)	0/3.4 (m)	0/100 (%)	2
PC1 (Dir)	5/15 (atm)	-442/0 (kcal/sec)	5 12
TC2 (Rev)	300/400 (K)	0/688 (kcal/sec)	1 20
LC21 (Dir)	0/2 (m)	0/100 (%)	2
LC22 (Dir)	0/2.52 (m)	0/100 (%)	2
PC2 (Dir)	0/2.2 (atm)	-860/0 (kcal/sec)	20 5

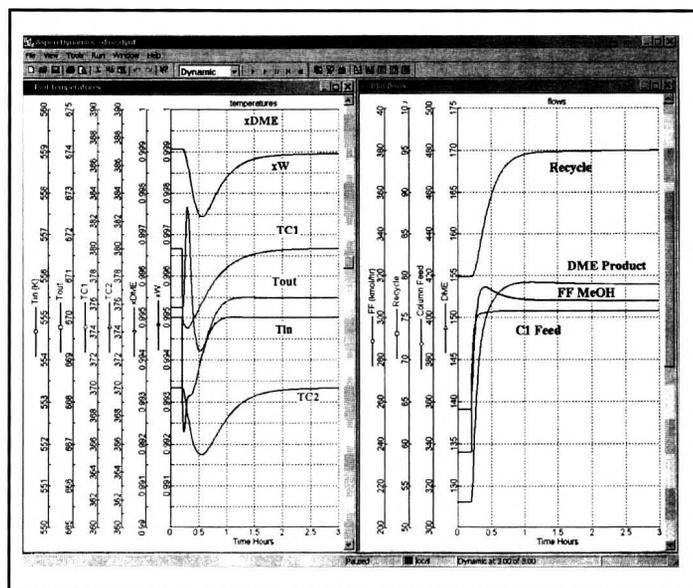


Figure 9. Dynamic responses to 20% increase in feed to column C1.

AspenDynamics flowsheet with this control structure installed. All level controllers are proportional with $K_c = 2$. Table 1 gives controller tuning parameters and transmitter spans. The dynamic simulation is run until it reaches a steady-state condition. This may take several “process hours” (several minutes of computer time), depending on the complexity of the flowsheet. When running the dynamic simulation out to a steady state, valve V22 in the recycle line went wide open and the reflux-drum level in Column C2 began to rise. The power to the pump P22 was increased to solve this valve saturation problem. The details of how this is done are given in Luyben.^[1]

The same valve saturation problem occurred in V12 when the

setpoint of the C1 column feed flow controller was increased 20% (from 236 to 402 kmol/hr). The power to pump P12 was increased. Notice that the steady-state signals to valves V22 and V12 are 20% and 29%, respectively, instead of the normal 50%, because of the higher valve pressure drops.

Figure 9 shows the dynamic response of the system to a 20% increase in column C1 feed. The initial condition is the steady-state condition. The fresh feed of methanol increases from 262 to 308 kmol/hr and DME product increased from 131 to 154 kmol/hr (17.5% increase in production rate). The purities of both the DME and the water products are maintained for this large disturbance. The system takes about two process hours to come to the new steady state.

The one-recycle process illustrates how easily the flowsheet can be converged by using dynamic simulation. Figures 10 and 11 give an example of a process with two recycles. The methyl acetate and butanol reactants not consumed in the reactor are separated in a three-column separation section and recycled in two different streams. More details of this example are available from the author.

CONCLUSION

The convergence of steady-state simulations of flowsheets with

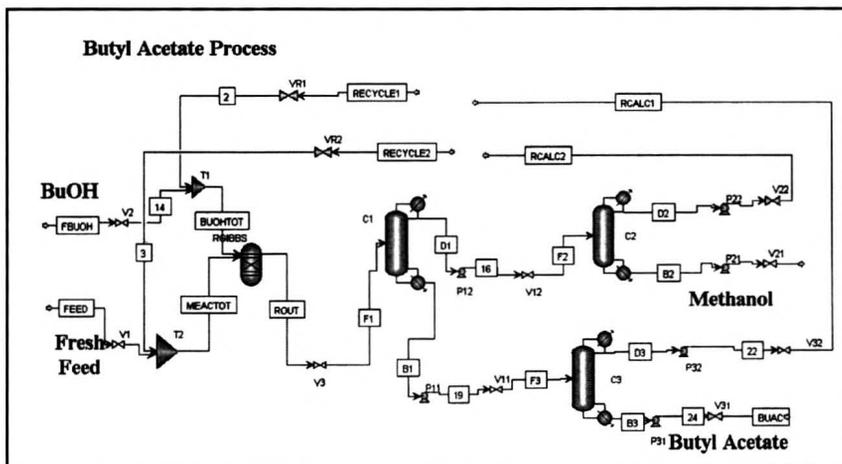


Figure 10. Flowsheet for two-recycle butyl acetate process.

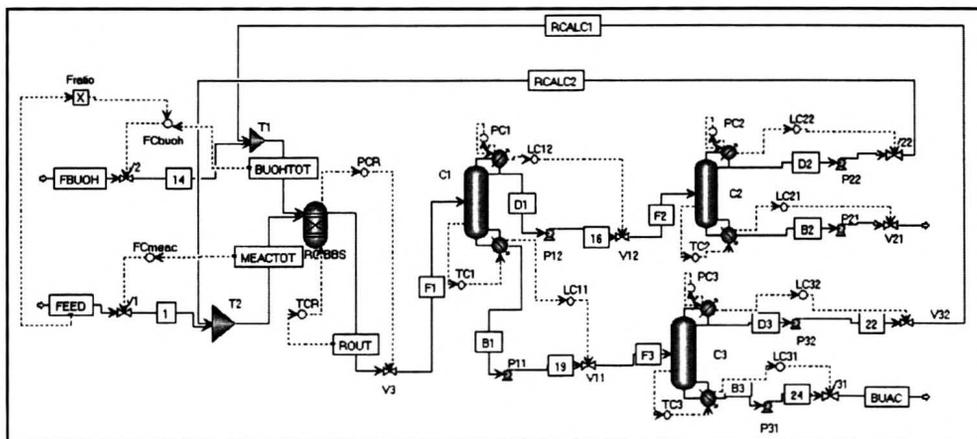


Figure 11. Plantwide control structure for two-recycle process.

recycle streams is frequently very difficult. An alternative is suggested in this paper and an example illustrates the proposed method. The steady-state simulation is converted into a dynamic simulation, and the recycle loops are converged by letting the dynamic simulation run to steady-state conditions.

The method depends on the development of a base-level regulatory plantwide control structure, which can be obtained by following a simple heuristic design procedure. Simple controller tuning rules can be applied to eliminate detailed and lengthy controller tuning efforts.

There is, of course, an additional benefit for this approach. The dynamic simulation can also be used to look at the dynamic effects of alternative design conditions (flowsheet structure, operating conditions, equipment sizes, etc.). This approach, which is called "simultaneous design," is a design philosophy in which both the steady state and the dynamic performances of a process are considered at all stages of the development of a process. The book by Seider, *et al.*,^[5] discusses this approach in more detail.

NOMENCLATURE

- D diameter
- DME dimethyl ether
- E activation energy
- FF fresh feed
- K_c controller gain
- L length
- P_j partial pressure of component j
- TCn tray temperature controller in column n
- T_{in} reactor inlet temperature
- T_{out} reactor exit temperature
- τ_I integral time constant in PI controller (minutes)
- λ heat of reaction

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USING SMALL BLOCKS OF TIME FOR ACTIVE LEARNING AND CRITICAL THINKING

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During lecture periods, five- or ten-minute time slots sometimes arise that do not warrant introducing new topics in a course but do afford the opportunity for learning. I use these short periods of time with two types of learning exercises: “Estimation Problems” and the “Top 10 Chemicals.” Both are active learning activities that involve critical thinking.^[1-7] In addition, they help maintain student interest and motivation, and they also can serve to provide a break in the class period.

Because both of these activities are used in an introductory thermodynamics course, the estimation problems are slanted to reinforce principles of thermodynamics. They also include, however, problems that touch on subject matter found in other engineering and physical science courses. The Top-10-Chemicals exercise reinforces both principles of chemical engineering and process chemistry more typically covered in chemistry courses, or (possibly) not at all in the curriculum.

ESTIMATION PROBLEMS

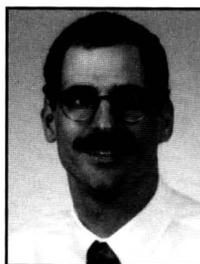
The short estimation problems are used to improve the ability of students to use limited information to quickly find approximate order-of-magnitude solutions. These problems are typically presented to the students as short statements on the chalkboard; the students then spend 2-5 minutes working together in small groups to develop a problem-solving strategy and an order-of-magnitude solution estimate. I ask the students to volunteer at the blackboard to present their answer to the other students, and very often students are willing to do this. I take this as an important indicator that they feel comfortable and confident in demonstrating their knowledge in front of their peers and me. This type of problem solving, where students teach each other, also serves to reinforce their own intellectual capabilities and combats the per-

ception that only the professor can solve problems.

Table 1 is a partial list of the estimation problem statements used so far, and the solutions to two of them (#13 and #2) are presented in more detail below. The first estimation problem, “Estimate the power usage of a home microwave oven,” reinforces principles of thermodynamics. For this problem, the students invariably choose to heat a cup of water from room temperature to the boiling point. This leads to an energy, which can be computed from the enthalpy change of water, $\Delta H = mC_p \Delta T$, which is then converted to power by dividing ΔH by a heating time of 3-5 minutes. With this “seat of the pants” approach, the students determine a power usage of several hundred watts, which is certainly a valid estimate for small microwave ovens and is within an order of magnitude of the power for large units.

At this point, the student who has presented the answer sits down to a well-deserved round of applause from the instructor and the other students; the applause is certainly well-deserved, not only for presenting in front of the class but also for presenting extemporaneously.

Because we are in a thermodynamics class, I then lead a discussion of how the result can be formally obtained from the First Law of Thermodynamics for a closed system ap-



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TABLE 1
Problem Statements for Estimation Problems

Estimate...

1. ...the number of BS chemical engineers graduated each year in the USA
2. ...the annual residential energy use in the United States
3. ...the number of cars sold per year in the United States
4. ...the concentration of atoms in the surface of a solid
5. ...the annual gross domestic product of the United States
6. ...the motor size of a garage door opener
7. ...the energy required to climb two flights of stairs
8. ...the power output of the human heart
9. ...the water pressure in town
10. ...the distance an auto skids during braking from high speed
11. ...the tons of cooling an air conditioner must supply for a residential home
12. ...the carbon dioxide production from automobile exhaust per day in town
13. ...the power usage of a home microwave oven
14. ...the number of toothbrushes sold per year in the United States
15. ...the entropy production of a student while sitting in class
16. ...the energy obtained from a windmill
17. ...the cost to produce a gallon of gasoline in a refinery

plied to the initial and final states of water in the cup (see Figure 1). For this problem, the terms for changes in kinetic and potential energies are taken as zero, and the heat transfer, Q , and the work, W , are also taken as zero. The type of microwave (mw) energy that crosses the system boundary, however, is added to the First Law as Q_{mw} . This aspect of the problem reinforces the principle that when we use the First Law as a bookkeeping tool to conserve energy, we may need to add terms to account for the process under consideration. Although the First Law of Thermodynamics for a closed system is most often formulated in terms of the internal energy, for liquids the constant volume and constant pressure heat capacities are approximately equal, and thus the internal energy and enthalpy changes are approximately equal as well.

At this point, after the students realize how their “estimated” solution is, in fact, well grounded in fundamental aspects of thermodynamics, it is instructive to define the system as the magnetron or, alternatively, as the microwave oven itself. Figure 1 demonstrates the application of the First Law of Thermodynamics for these cases as well. If the magnetron is taken as the system, the First Law reduces to a form where values to calculate the electrical work into the magnetron, W_{elec} , or the microwave energy emanating from the magnetron, Q_{mw} , are not readily available. Thus, it is not possible to obtain a numerical value for the energy use with this approach from the given problem statement.

If the entire microwave oven is taken as the system, then again we cannot immediately estimate the power input; equating the internal energy change of the microwave with the internal energy change of the contents of the cup, however, leads to the same solution presented earlier. Thus, the students can observe how judicious selection of the system as the contents of the cup facilitates quickly achieving a solution estimate. These other forms of the First Law also naturally lead to a discussion of where thermal heat losses or storage may occur (the cup, the magnetron, the power cord) and how these influence the energy efficiency of the device. At the end of this exercise, which examines a common process in simplified terms, the utility of estimation and the ramifications of process simplification are reinforced for the students.

A second type of estimation problem, determining the annual residential energy use in the United States, is not directly related to course content. Here, students typically elect to use their monthly electrical energy bill and an estimate of the cost of electricity of 5-10 cents per kW-h to arrive at an order-of-magnitude answer (see Figure 2).

Often, for this problem some students can conceptually

Estimate the power usage of a home microwave oven.

1) First Law with cup contents as system:

$$\Delta U_{liquid} + \Delta E_k + \Delta E_p = Q + W + Q_{mw}$$

$$\Delta U_{liquid} \approx \Delta H = m \int C_p dt = 0.3 \times 4.18(100-20) = 100 \text{ kJ}$$

Power Required:

$$P_{elec} = \frac{Q_{mw}}{\text{Time}} = \frac{100,000 \text{ J}}{3 \text{ min} \times 60 \text{ s/min}} \approx 500 \text{ Watts}$$

2) First Law with magnetron as system ($\Delta U_{magnetron} \approx 0$):

$$W_{elec} = -Q_{mw}$$

\therefore Unless we have electrical values, we cannot proceed.

3) First Law with microwave as system:

$$W_{elec} = \Delta U_{microwave} \approx \Delta U_{liquid} \approx m \int C_p dt$$

\therefore same as approach 1) above

Figure 1. Representation of the chalkboard for estimating the power usage of a home microwave oven.

alize the solution strategy but lack specific values for the U.S. population, for the number of U.S. households, or for the energy cost per kW-h. Collectively, however, the class typically knows one or more of these values, and thus an estimate can be computed and presented to the other students. To conclude this problem, we often use a simple error analysis to assess how certain we are of specific numbers and thus the overall estimate. We may know the population or number of households to within 10%, the cost of energy to within a factor of two, the number of months per year exactly, and the monthly dollar usage to within a factor of five. Taken together, these uncertainties allow us to bound the error in the overall estimate. For this particular problem, the estimate of annual residential energy consumption of 10^{12} kW-h is within 25% of the reported value.^[8] I usually conclude this particular problem by mentioning that the total U.S. electricity usage is approximately 1/3 residential, 1/3 industrial, and 1/3 commercial.

For some of the estimation problems, no student is willing to present a solution strategy at the chalkboard. In these cases, I usually draw the solution from the students by asking a sequence of questions that steps them through the thought process necessary to arrive at an estimate. Often, the students actually do know the solution strategy, but are not 100% certain. After observing the "estimation" methodology a few times, additional students then develop the confidence to share their solution with the rest of the class.

THE TOP 10 CHEMICALS

The discussion of each top-10 chemical is initiated by having the students guess what is the next chemical on the running list. Usually, the students know about 3-5 of the chemicals, but generally not in order. The top 10 chemicals on a mass basis produced per year in the United States are listed in Table 2.^[9] A discussion of each chemical is conducted first by querying the students for the source of raw materials for the chemical. For sulfuric acid, the source of sulfur is either mined sulfur, spent sulfur, or sulfur obtained as hydrogen

sulfide gas from hydrodesulfurization units in refineries.

The students are next queried as to the sequence of likely reactions to convert the raw material to the desired product. The reactions to convert sulfur or hydrogen sulfide to sulfur dioxide, then to sulfur trioxide, and then to sulfuric acid are thus obtained from the students, who use their knowledge of general chemistry to ascertain what might be likely reactions based solely on chemical formulas. A representation of the appearance of the chalkboard for the reactions leading to sulfuric acid is shown in Figure 3.

The uses of sulfuric acid are next discussed. The main use is to digest phosphate-containing rock to produce phosphate fertilizer. I tell the students that it is comforting to know that the main use for the number-one chemical produced is ultimately so that we can feed ourselves.

Each time we cover one of the top 10 chemicals, the list is augmented, and as the semester progresses, knowledge gained from previous chemicals can be applied to subsequent ones; the parallels between ethylene (#3) and propylene (#7), for example, are obviously quite pronounced. The fact that sulfuric acid is the number-one chemical, primarily used to digest phosphate-containing rock, should make it no surprise that phosphoric acid, used in phosphate-based fertilizer production, also appears in the top ten.

In a similar analogy, polyethylene, the sixth most-produced chemical, is derived from ethylene, the third most-produced chemical and the number-one organic chemical. Other commonalities among the

TABLE 2
Top 10 Chemicals Produced in the United States in 2001^[9,10]

1. Sulfuric acid	6. Polyethylene
2. Nitrogen	7. Propylene
3. Ethylene	8. Ammonia
4. Oxygen	9. Chlorine
5. Lime	10. Phosphoric acid

Estimate the annual residential energy usage in the United States.

of US households \approx 100 million

Average household monthly electrical bill \approx \$100

Cost of energy per KW-h \approx \$0.07

$$\text{Total electricity usage} \approx \frac{10^8 \text{ household} \times \$100/\text{month-household} \times 12 \text{ months}}{\$0.07/\text{KW-h}}$$

$$\approx 10^{12} \text{ KW-h}$$

Figure 2. Representation of the chalkboard for estimating the annual residential energy use in the United States.

top ten chemicals also become apparent during the course of the semester. For example, three of the top ten (sulfuric acid, ammonia, and phosphoric acid) are used in the manufacture of fertilizers for growing food.

At the end of the semester, the students are given a copy of the Top 100 Chemicals.^[9] We briefly examine it to glean some long-term trends. For example, thirty years ago, nitrogen was

not in the top ten.

Methyl-t-butyl ether (MTBE) is another interesting example to consider. Its emergence as a top 10 chemical can be linked to its role as an octane enhancer as lead—a known carcinogen in gasoline—was phased out. Now, MTBE is a suspected carcinogen, and its production can be expected to decline as new octane enhancers are introduced into fuels. Two pairs of chemicals—nitrogen and oxygen, and caustic and chlorine—which are often produced in tandem, afford an opportunity to bring in some economic considerations related to pricing and the imbalance of product supply and demand.

SUMMARY

Two activities, “Estimation Problems” and the “Top 10 Chemicals,” are used as active learning and critical thinking exercises to use small blocks of class time. Although each exercise addresses different aspects of chemical engineering, they have a common basis in delivery in that both involve extensive class participation, which helps to maintain student attention. In addition, these two learning opportunities can serve an important educational role by expanding the knowledge base of the students. Probably even more important—the students enjoy both interactive exercises and more than half of them comment favorably on one or both of these exercises in their end-of-year course evaluations; some selected comments are listed in Table 3. Finally, because of the participatory nature of these exercises, they help build a strong rapport between the students and the instructor.

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Top 10 Chemicals

1. Sulfuric Acid (H₂SO₄) ~ 80 billion lbs produced per year

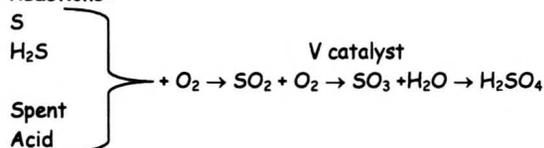
Source of Raw Materials:

S from sulfur mines

H₂S from petroleum refineries and natural gas

Spent sulfuric acid (contaminated and diluted)

Reactions:



Major Uses:

~ 2/3 to digest phosphate-containing rock to produce phosphate fertilizers for agricultural uses

~ 1/3 miscellaneous uses

- metal/ore processing
- petroleum refining
- pulp and paper manufacturing

Figure 3. Representation of the chalkboard for discussing the number-one Top-10-Chemical, sulfuric acid.

TABLE 3

Selected Student Comments from End-of-Year Evaluation

- I liked the Top 10 Chemicals, estimation problems, etc. They are a nice way of “taking a break” while still learning.
- Instructor was very enthusiastic, encouraged involvement in problems and estimation.
- Changing the topic several times a class helps us to remain focused and to continue to learn. Has done a wonderful job.
- I liked the Estimation Problems and Top 10 Chemicals. I felt this course related well to real-life problems.
- Other non-lecture based activities are especially good.
- Top 10 Chemicals and Estimations are good teaching parts of this course.
- I like the fact that the Top 10 Chemicals and the Estimation Problems...get the class communicating and thinking.
- Top 10 Chemicals and Estimation Problems keep us interested and force us to think like engineers (problem solvers).
- The Estimation Problems show us that we know and can accomplish a lot more than we think we can.

TEACHING NONIDEAL REACTORS WITH CFD TOOLS

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Behavior of nonideal reactors and their flow pattern characterization are issues taught in a majority of chemical reaction engineering (CRE) courses^[1-4] (depending on the curriculum structure, usually at the undergraduate level) and therefore they are addressed in most CRE textbooks.^[6,8-8] In this respect, the classical stimulus-response tracer experiments^[9] are essential to obtain theoretical functions such as the residence time distribution (RTD), which are crucial for diagnosis of equipment operation, reactor modeling, and prediction of conversion. Comprehension of the involved concepts, which are not easily grasped by students, can be improved with laboratory sessions—but this is not always feasible. This disadvantage can be overcome, however, by implementing computer simulation of tracer experiments,^[10] particularly with a commercial computational fluid dynamics (CFD) tool.^[11-13]

CFD codes have been widely used for simulating flow pattern in real systems, and their use in a chemical engineering undergraduate course has several advantages, as pointed out by Sinclair.^[14] Among those advantages are: first, the use of color in CFD plots allows students to visualize flow behavior, and this visualization of the flow phenomenon can significantly facilitate and enhance the learning process. Second, students can explore the effects of change in the system geometry, system properties, or operation conditions. All these advantages, apart from the fact that students *like* to experience software tools used in industry (which are usually user-friendly), justify implementation of CFD codes in CRE courses, particularly when teaching RTD theory.

Such tools have some disadvantages and/or limitations, however. Commercially available codes may be extremely powerful, but their operation requires a high level of skill and understanding to obtain meaningful results. In addition, CFD cannot be adequately used without continued reference to experimental and/or analytical validation of numerical results.^[13]

The case study described here can be implemented as homework for students taking a CRE course dealing with nonideal reactors. Simulations can be performed using a commercial

package such as Fluent, but it is advisable that a brief tutorial be provided so students can quickly familiarize themselves with the program. In this tutorial, the essential steps that must be followed for any simulation should be outlined. Different reservoir/reactor geometries can be provided for different groups of two-to-three students, but each group should perform its own parametric study (*e.g.*, evaluate the effect of space-time, or Reynolds number, in flow pattern characterization, or Damköhler number in reaction simulations). Finally, the students should compile the results obtained by other colleagues and discuss them in a final written report.

Using 2-D reservoirs/reactors with laminar flow (described in detail in the next section), students should perform the following tasks, which are also the objectives of this paper:

1. Characterize the hydrodynamics in the vessel(s).
2. Determine the RTD from tracer experiments, which includes diagnosis of reservoir/reactor operation.
3. Predict the conversion in a continuous-flow system.

CASE STUDY FORMULATION AND SIMULATION WITH FLUENT

It is well known that the mean residence time (\bar{t}_r) has an important effect on the performance of some large natural

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conversion systems, such as biological lagoons, since it affects the biological conversion of biodegradable matter. Moreover, the geometry of the reservoirs seems to affect the RTD, and thus \bar{t}_r . It is therefore very important to perform tracer experiments in these systems (or try to estimate the RTD function) in order to better design such wastewater treatment plants. The mean residence times in these large reservoirs or lagoons are extremely high (ranging from one day up to several months^[15,16]), however, so tracer experiments are impractical.

Possible strategies to overcome this problem involve obtaining the RTD on pilot-scale setups with various geometries, where tracer experiments are easily conducted, and performing a scale-up analysis, or deriving the RTD by solving the Navier-Stokes and diffusion-convection equations that students learned in the fluid mechanics curricula.^[e.g.,16] Commercially available CFD packages (*e.g.*, Fluent, CFX, Fidap, Phoenix, STAR-CD, FLOW3D, etc.) can readily solve the balance equations for reactor operation coupled with the Navier-Stokes equations. Thus, we adopted the second approach.

The case study considers a 2-D reservoir with dimensions L (length) and H (height) in laminar flow and isothermal conditions (see Figure 1). Reservoirs with different aspect ratios (L/H) were considered, varying between 0.5 and 20 (with $H = 0.1$ m). Both the inlet and the outlet boundaries of the reservoirs have a height of 0.01 m, with distances from the bottom of the reservoir of 0 and 0.02 m, respectively. A fully developed parabolic velocity profile is imposed at the inlet boundary

$$u_x = U_{\max} \left[1 - \left(\frac{y - H/20}{H/20} \right)^2 \right] \quad (1)$$

where U_{\max} is the fluid velocity at the center of the inlet boundary, $U_{\max} = 1.5 U_{\text{mean}}$. A constant species concentration profile is assumed at the inlet boundary. On the walls (see Figure 1), no-slip conditions are assumed ($u_x = u_y = 0$) and a null flux (zero gradient) of species concentration is imposed. At the outflow boundary condition, the CFD code extrapolates the required information from the interior cells (a zero diffusion flux is assumed for all flow variables in the direction normal to the exit plane). In the simulations, the Reynolds number,

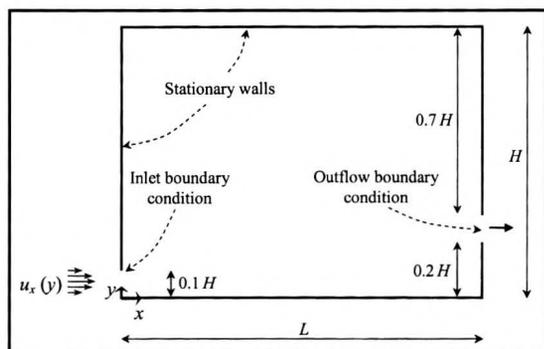


Figure 1. Sketch of reservoir geometry.

here defined based on inlet conditions, ranged from 1 to 100. Changing Re for a given fluid and reservoir is equivalent to changing the fluid velocity (and thus the residence time).

The governing equations to be solved are (for an incompressible fluid)

Continuity

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0 \quad (2)$$

Momentum

$$\rho \frac{\partial u_x}{\partial t} + \rho \left[\frac{\partial(u_x^2)}{\partial x} + \frac{\partial(u_x u_y)}{\partial y} \right] = -\frac{\partial P}{\partial x} + \mu \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} \right) \quad (3)$$

$$\rho \frac{\partial u_y}{\partial t} + \rho \left[\frac{\partial(u_x u_y)}{\partial x} + \frac{\partial(u_y^2)}{\partial y} \right] = -\frac{\partial P}{\partial y} + \mu \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} \right) \quad (4)$$

Species Transport

$$\frac{\partial C}{\partial t} + \frac{\partial(u_x C)}{\partial x} + \frac{\partial(u_y C)}{\partial y} = D \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right) + S(C) \quad (5)$$

In Eq. (5), $S(C)$ is a source term. For the transport of an inert tracer, by convection-diffusion, $S(C) = 0$, while for the transport of a reagent species, $S(C) = -kC$ (assuming a first-order irreversible reaction).

Simulations were run with the commercial package Fluent 6.0. The fluid considered is water ($\nu = \mu/\rho = 10^{-6} \text{ m}^2\text{s}^{-1}$), and a tracer solution was created in Fluent's database with identical properties of water, so that it does not affect reactor hydrodynamics. A molecular diffusivity of $5 \times 10^{-10} \text{ m}^2\text{s}^{-1}$ was considered, which is a typical value for liquids.^[17] A tracer step input was used, with uniform concentration across the entrance section, together with the parabolic velocity profile defined in Eq. (1).

Fluent can simulate both the hydrodynamics and chemical reaction processes, and therefore the reservoirs previously considered can be used for modeling continuous-flow reactors (*e.g.*, biological lagoons). In this case, simulations were run by defining a reactant and a product, both with properties identical to water. The reactor is initially full of water (inert), the laminar flow is established; after that (time $t = 0$) the reactant is fed to the reactor, similarly to the tracer step input. Conversion of reactant is calculated based on the time evolution of species concentration at the reactor exit, obtained from a mass-weighted average formulation.

We must point out that to achieve a high level of accuracy, all the simulation results presented in this paper involved a detailed analysis of the numerical algorithms, the mesh employed, and the time step adopted (in transient simulations). For instance, the QUICK scheme of Leonard^[18] was selected for discretization of the convective terms, a second-order

implicit formulation was used during unsteady stimulation, and the computational grid contained typically 100x100 elements (note that for reservoirs with $L/H \gg 1$, it is convenient to use a larger number of cells in the x-direction). It is always a good practice to perform the calculations on several meshes with different levels of refinement in order to obtain mesh-independent results. A similar procedure should be adopted regarding the time step used in transient calculations. A control-volume approach is used by Fluent to numerically solve the governing equations.^[11]

RESULTS AND DISCUSSION

► *Hydrodynamic Characterization*

Figure 2 shows contour plots of the stream function within the reservoir, with $L/H = 1$, which illustrates the trajectories of the fluid elements (streamlines). For a given inlet velocity (or more broadly speaking, a given Reynolds number), the formation of a recirculation zone above the entrance of the reservoir, where velocity is small, is evident, thus suggesting formation of a stagnant region. It is noteworthy that the importance of such a region increases with Re , becoming particularly large for Re values around 100 where fluid trajectories are almost linear. Lower Re numbers lead to a smaller stagnant region and more curved streamlines. For $Re < 1$, inertia is negligible and the trajectories obtained are equivalent to creeping-flow conditions.

For longer reservoirs, the conclusions are similar, but now the importance of the recirculation zone decreases (for the same fluid inlet velocity). Indeed, the steady state streamlines shown in Figure 3, obtained for a reservoir with $L/H = 5$, show formation of a stagnant zone above the entrance, where the size increases with the Reynolds number. Comparison with the stream function contours of Figure 2, however, shows that for the same Re , the fraction of dead volume decreases when the geometric ratio L/H increases.

► *RTD Determination from Tracer Experiments*

After performing steady state simulations, students can proceed to transient runs, but they must first define a tracer step input at the inlet boundary condition. They must also be aware that for $t = 0$, no tracer exists within the reservoir and that the laminar flow is already established. They must first initialize the entire domain with a null tracer concentration and wait until the laminar regime is established before introducing the tracer step change at the inlet. After that, the CFD code solves the convection-diffusion equation that describes the tracer transport in the reservoir and the concentration field of tracer under transient regime is obtained. Particularly interesting is its concentration at the outflow boundary, $C_{out}(t)$. The contours of tracer concentration throughout the reservoir along time are also very interesting because they provide a good perspective on the evolution of concentration fronts. For a reservoir with $L/H = 1$, some frames were recorded at different times and are shown in Figure 4. They

show that only for $\theta = t/\tau$ around 0.22 can one start to 'see' tracer at the reservoir exit. In addition, even for a very long time of operation (about five times the residence time), the reservoir is not completely full of tracer, due to the stagnant zone previously identified. To better illustrate this transient behavior, it is possible to create an animation sequence with Fluent, using several frames obtained from the previous simulation. This was done and is available at <http://www.fe.up.pt/~mmalves/cfd/reactor/index.htm>.

With the data of transient tracer concentration at the outlet of the reservoir, which can be exported to an ASCII file, students can then compute the so-called Danckwerts' F curve, the normalized response of the reactor to a step input,

$$F(t) = \frac{C_{out}(t)}{C_{in}} \quad (6)$$

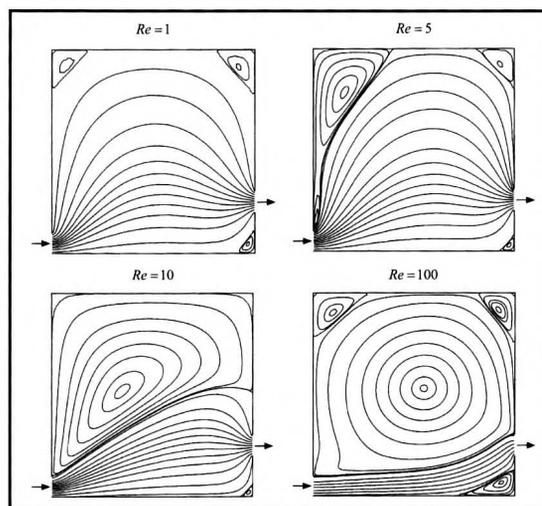


Figure 2. Steady state contours of the stream function for the reservoir with $L/H = 1$ as a function of the Reynolds number.

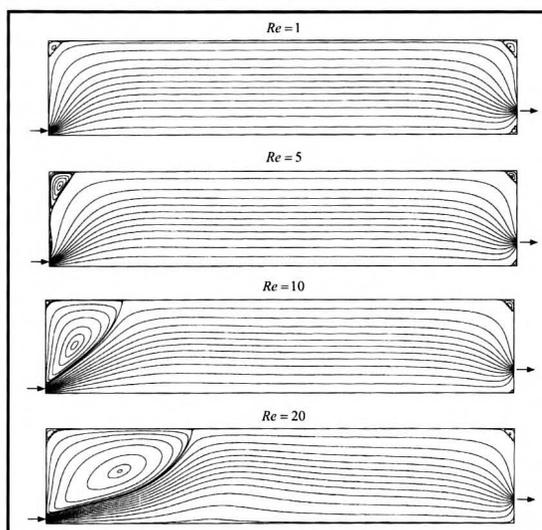


Figure 3. Steady state contours of the stream function for the reservoir with $L/H = 5$ as a function of the Reynolds number.

Data can then be manipulated with a spreadsheet program such as Microsoft Excel. Results shown in Figure 5 show the expected F curve, which only reaches the asymptotic value of 1 for very long times. It is worth mentioning the use of a logarithmic time scale, showing that tracer starts to exit the reservoir at around $\theta = t/\tau = 0.22$ due to its transport by convection, while fluid elements that enter the stagnant region only come out (by diffusion) much later (see detail of Figure 5).

With the response to a step input, the RTD function can now be computed by

$$E(t) = \frac{dF(t)}{dt} \quad (7)$$

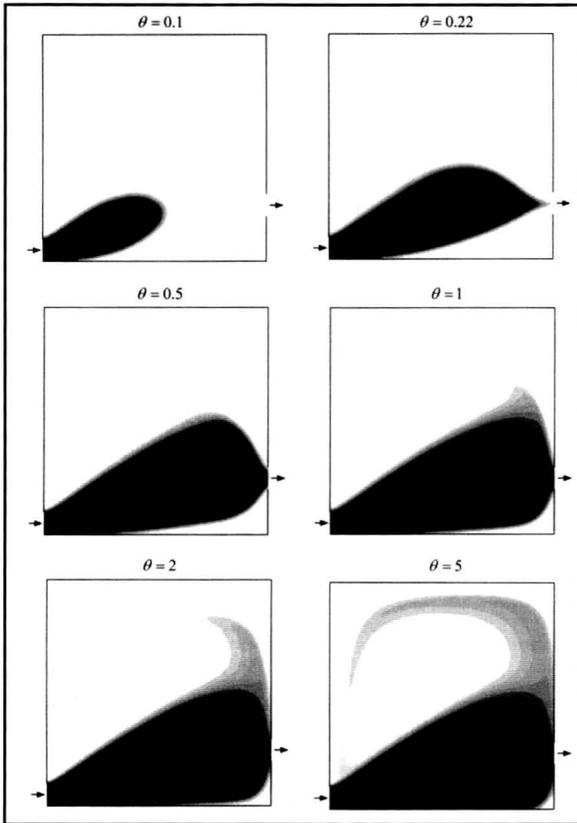


Figure 4. Transient tracer concentration contours for the reservoir with $L/H = 1$ ($Re = 10$).

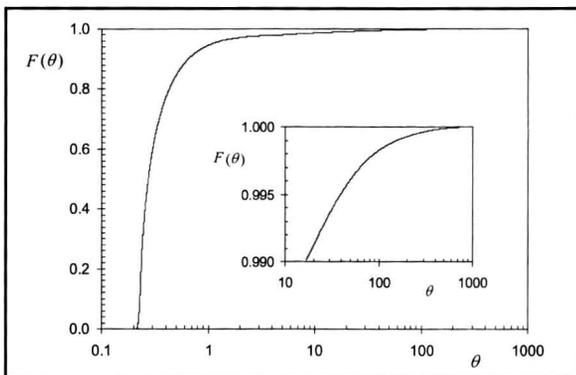


Figure 5. Danckwerts' F curve for the reservoir, with $L/H = 1$ ($Re = 10$).

or, in terms of reduced time θ ,

$$E(\theta) = \frac{dF(\theta)}{d\theta} = \tau E(t) \quad (8)$$

Figure 6 shows the RTD curves as a function of the Reynolds number, which gives an idea (for a given fluid) how space-time affects the RTD function. In all cases, the RTD curves evidence a very long tail and that a large fraction of fluid elements exits the reservoir with ages younger than the space-time, τ . Both features are indicative of the existence of large stagnant regions, together with slow recirculating flows near the inlet, as can be seen in Figure 2. The fact that Re affects the RTD curve is also visible in Figure 6. Higher Reynolds numbers imply that the fluid elements start to leave the reactor sooner and a higher fraction of fluid elements has a smaller residence time.

The effect of the reservoir geometry on the RTD is shown in Figure 7. It can be seen that when L/H increases, the curves are shifted to the right, *i.e.*, the mean residence time seems to increase because the importance of the recirculating zone decreases. This was previously found in the steady state streamlines shown in Figures 2 and 3. It is particularly noteworthy that for very long reservoirs, one tends toward an asymptotic $E(\theta)$ curve, also shown in Figure 7. This curve corresponds to the case of laminar flow between parallel plates, given by^[19]

$$E(\theta) = \begin{cases} \frac{1}{3\theta^3} & \theta \geq \frac{2}{3} \\ \sqrt{1 - \frac{2}{3\theta}} & \theta < \frac{2}{3} \\ 0 & \theta < \frac{2}{3} \end{cases} \quad (9)$$

It must be stressed that for this situation, *i.e.*, laminar flow between parallel plates, the parabolic profile is characterized by a maximum velocity at the center that is 1.5 times the average velocity, while for flow in pipes this ratio is 2.

The RTD functions can then be used to calculate the mean residence time, defined as

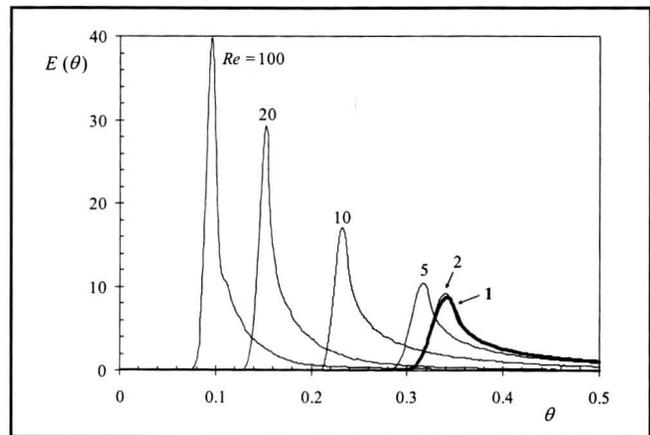


Figure 6. Effect of the Reynolds number on the residence time distribution (reservoir with $L/H = 1$).

$$\bar{t}_r = \int_0^{\infty} tE(t)dt \quad (10)$$

or

$$\bar{\theta}_r = \frac{\bar{t}_r}{\tau} = \int_0^{\infty} \theta E(\theta)d\theta \quad (11)$$

For a closed-closed system (*i.e.*, with no dispersion) and if no bypass or stagnant regions exist, it is well known that the mean residence time and space-time are equal.^[7,20] Due to the very long tail of the RTD function, however, this is only verified if simulations are run up to very high times, typically θ of $0(10^3)$. Otherwise, the normalization condition

$$\int_0^{\infty} E(t)dt = \int_0^{\infty} E(\theta)d\theta = 1$$

is not satisfied and the computed mean residence time is smaller than the real space-time.

Calculation of the mean residence time is very important for evaluation of malfunctions during the reactor's operation. Indeed, a straightforward way to diagnose the reactor's flow performance consists of comparing the computed value of the mean residence time from Eq. (10) with the space-time ($\tau = V/Q$, where V is the total volume of the reactor and Q is the volumetric flow rate), which is equivalent to comparing $\bar{\theta}_r$ with 1. Disagreement between these two values may indicate the existence of bypasses, dead volumes, etc. For instance, as indicated by Froment,^[5] if a region of the vessel retains a portion of the fluid for an order of magnitude greater than the mean residence time of the total fluid, then for all practical purposes, that portion is essentially at rest and the region is wasted space in the vessel.

The values obtained for the mean residence time shown in Tables 1 and 2 were calculated by integration of the RTD curves up to $\theta = 10$. It is evident that they strongly depend on both the Reynolds number and the geometry of the reservoir. As Re decreases, the mean residence time increases (Table 1). As expected, when L/H increases, the mean residence time approaches the space-time value (Table 2).

Because in all cases, $\bar{t}_r < \tau$ or $\bar{\theta}_r < 1$, we can conclude that a stagnant region exists, which in practice would be a dead volume, leading to a lower reactor performance. The fraction of the reactor volume occupied by the dead region is given by^[6,20]

$$\frac{V_d}{V} = 1 - \frac{\bar{t}_r}{\tau} \quad (12)$$

The dead volume fractions obtained, shown in Tables 1 and 2, indicate that for high Re

values (or high fluid velocities) and for geometries where L/H approaches 1, or even smaller, a large fraction of the reservoir will not be efficiently used for reaction purposes.

► Prediction of Conversion in the Continuous-Flow Reactor

In a real reactor, the RTD function can be used to predict the limiting values of conversion under the two extremes of micromixing, using the well-known total segregation or maximum mixedness models.^[21] For first-order reactions (linear systems), however, the state of mixing does not affect conversion,^[20] and therefore the easy-to-use segregation approach can be applied to predict reactor performance. The total segregation model assumes that all fluid elements having the same age (residence time) "travel together" in the reactor and do not mix with elements of different ages until they exit the reactor.^[7] Because there is no interchange of matter between fluid elements, each one acts as a batch reactor, so the mean steady-state conversion (\bar{X}) in the real reactor is given by

$$\bar{X} \int_0^{\infty} X_{\text{batch}}(t) = E(t)dt = \int_0^{\infty} X_{\text{batch}}(\theta) E(\theta)d\theta \quad (13)$$

where $X_{\text{batch}}(t)$, for a first-order reaction, is given by

$$X_{\text{batch}} = 1 - e^{-kt} = 1 - e^{-Da\theta} \quad (14)$$

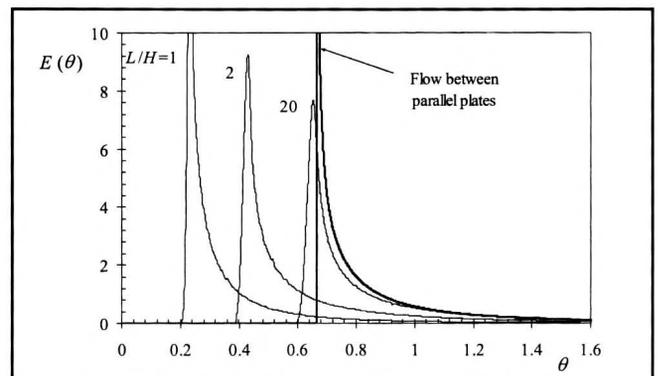


Figure 7. Effect of the geometric ratio L/H on the residence time distribution ($Re = 10$).

TABLE 1
Influence of the Reynolds Number on the Mean Residence Time and Fraction of Dead Volume (Reservoir with $L/H = 1$)

Values calculated from RTD curves up to $\theta = 10$.

Re	Mean Residence Time	Fraction of Dead Volume
	$\bar{\theta}_r = \bar{t}_r / \tau$	V_d / V
1	0.778	0.222
5	0.724	0.276
10	0.412	0.588
20	0.318	0.682
100	0.261	0.739

TABLE 2
Influence of Reservoir Geometry on the Mean Residence Time and Fraction of Dead Volume (for $Re = 10$)

Values calculated from RTD curves up to $\theta = 10$.

L/H	Mean Residence Time	Fraction of Dead Volume
	$\bar{\theta}_r = \bar{t}_r / \tau$	V_d / V
0.5	0.300	0.700
1	0.412	0.588
2	0.752	0.248
5	0.935	0.065
10	0.992	0.008
20	0.997	0.003

and $Da = k\tau$ is the Damköhler number.

Steady-state conversion is then computed by using Eq. (13), with the RTD function previously determined. It is important to remark that the segregation model can also be used for prediction of the reactor transient behavior. In this case, the upper integration limit in Eq. (13) must be set to t (or θ). This was done for our case study and the results, shown in Figure 8, illustrate the reactant conversion in transient conditions, up to steady state, for different Damköhler values. One must take care that the RTD used for prediction of reactor performance depends on its geometry and on the Reynolds number. In addition, because of the very long tail of the RTD function (as shown in Figure 5 for the $F(\theta)$ curve), prediction of steady-state conversion requires RTD data up to very large times (note the logarithmic time scale). This interesting feature is also evident in Figure 8—a non-negligible contribution to the overall reactor performance (in terms of fractional conversion), which is noticed at very long times. Such behavior can be attributed to the stagnant region and to the different time scales for the involved phenomena: reaction, convection, and molecular diffusion.

As mentioned above, Fluent can also be used to simulate the system in the presence of a reaction, and so the data shown in Figure 8 can be obtained either through the total segrega-

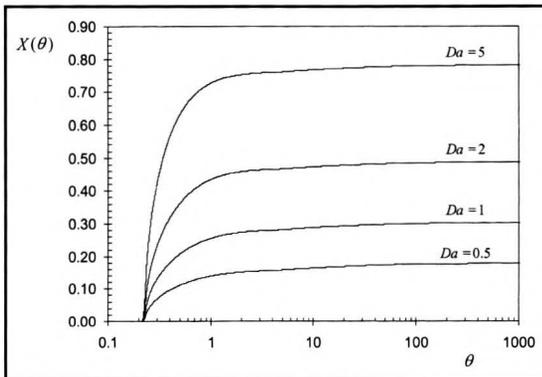


Figure 8. Unsteady-state conversion obtained for the reactor with $L/H = 1$, predicted from the segregation model ($Re = 10$).

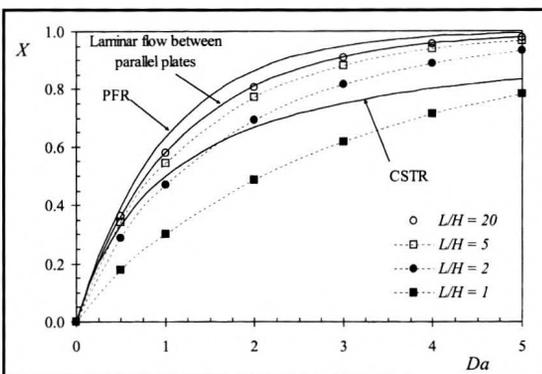


Figure 9. Steady-state conversion versus Damköhler number for reactors with different geometries ($Re = 10$).

tion model or directly from CFD simulations (obtained curves coincide). Asking students to compare results from both approaches is important because they feel more confident about the simulation results and calculations.

Simulation of the continuous-flow reactor via CFD can also be used to evidence the contours of species concentration throughout the reactor, for instance at steady state. Some color pictures can be seen on our web site at <http://www.fe.up.pt/~mmalves/cfd/reactor/index.htm>. The color gradient inside the reactor is particularly interesting to observe.

Finally, it is convenient to ask students to compare the steady-state conversion attained in the real reactor with those achieved with the ideal reactors that they learned in previous CRE courses: continuous stirred tank and plug flow reactors. For a first-order reaction, performance achieved by these reactors is given by^[e.g.,7,8]

$$X_{\text{CSTR}} = \frac{Da}{1 + Da} \quad (15)$$

$$X_{\text{PFR}} = 1 - e^{-Da} \quad (16)$$

Data shown in Figure 9 indicate that when dead regions or stagnant zones are negligible, *i.e.*, for geometries where L/H is higher than about 5 (for $Re = 10$), the performance of the real reactor lies between that of the CSTR and PFR. When L/H is close to 1, or even smaller, such anomaly (dead volume) leads to a much lower performance of the nonideal reactor—even lower than that achieved with a perfectly mixed reactor. It is also noteworthy that for very long reactors (*i.e.*, high L/H ratios), one approaches the theoretical behavior of a laminar flow reactor (flow between parallel plates) computed using the RTD function given in Eq. (9) and the segregation model.

CONCLUDING REMARKS

Concepts dealing with the RTD theory and nonideal reactors are not very familiar to undergraduate students, and thus it is not an easy task to teach these matters in CRE courses. Explanation of how stimulus-response tracer experiments provide the theoretical functions that are crucial for a reactor's diagnosis, prediction of conversion, etc., becomes clearer through experimentation, which is not always feasible. For such purposes, the use of CFD packages has been particularly advantageous. Besides, CFD tools provide a graphical portrait of flow throughout the reservoir/reactor, thus allowing going beyond simply predicting what will come out of the reactor to predicting all of the properties of interest within the reactor. Some of the concepts involved are more easily understood, such as the progression of the tracer concentration front, the formation of dead volumes, or the existence of a concentration profile along the reactor. Therefore, implementation of a CFD code has a considerable pedagogical content.

The case study we have described, a 2-D lagoon with laminar flow, was solved with the commercial package Fluent.

Using reservoirs/reactors with different geometries and/or different operating conditions, students may be asked to

- Characterize the hydrodynamics
- Determine the residence time distribution from tracer experiments, which provides diagnosis of reactor operation
- Predict conversion in a continuous-flow reactor (both steady state and transient behavior)

Our experience shows that use of the CFD code allows students to more easily understand some of the basic concepts taught in CRE curricula. Finally, comparison of numerical with analytical solutions known for laminar flow between parallel plates (*i.e.*, for geometries with high L/H ratios) improves their self-reliance regarding CFD results.

In a survey sent a few years ago to chemical engineering departments spread all over the world, two of the main points addressed by the departments to a question relating to the future of CRE courses were:^[2] the increasing importance of computer applications and software packages, and putting more emphasis on nonideal reactors. With the case study herein proposed, both issues are dealt with. In addition, students learn the potential of CFD codes, which have been successfully used in practice to design commercial-size reactors, usually with complex flow processes.^[22]

NOMENCLATURE

C	concentration of tracer, reactant, or product (mol.m ⁻³ or kg.m ⁻³)
D	diffusivity (m ² s)
Da	Damköhler number, dimensionless
E(t)	resident-time distribution function (s ⁻¹)
E(θ)	normalized RTD function, dimensionless
F(t)	Danckwerts' F curve, dimensionless
H	height of the reservoir/reactor (m)
k	reaction rate constant of the first-order reaction (s ⁻¹)
L	length of the reservoir/reactor (m)
P	pressure (Pa)
S	source term (mol m ⁻³ s ⁻¹ or kg m ⁻³ s ⁻¹)
Q	volumetric flow rate (m ³ s ⁻¹)
Re	Reynolds number, dimensionless
t	time (s)
\bar{t}_r	mean residence time (s)
U _{max}	fluid velocity at the center of the inlet boundary (ms ⁻¹)
U _{mean}	mean fluid velocity at the inlet boundary (ms ⁻¹)
u _x	x-velocity (ms ⁻¹)
u _y	y-velocity (ms ⁻¹)
V̇	volume of reservoir/reactor (m ³)
V _d	dead volume in the reservoir/reactor (m ³)
X	conversion, dimensionless
x	horizontal coordinate (m)
y	vertical coordinate (m)

Subscripts

batch	refers to batch reactor
CSTR	continuous stirred tank reactor
in	inlet conditions
PFR	plug flow reactor

out outflow conditions

Greek Symbols

$\theta = t/\tau$	reduced time, dimensionless
$\bar{\theta}_r = \bar{t}_r / \tau$	reduced mean residence time, dimensionless
μ	viscosity of the fluid (kg m ⁻¹ s ⁻¹)
ν	kinematic viscosity of the fluid (m ² s ⁻¹)
ρ	density of the fluid (kg m ⁻³)
τ	space-time (s)

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