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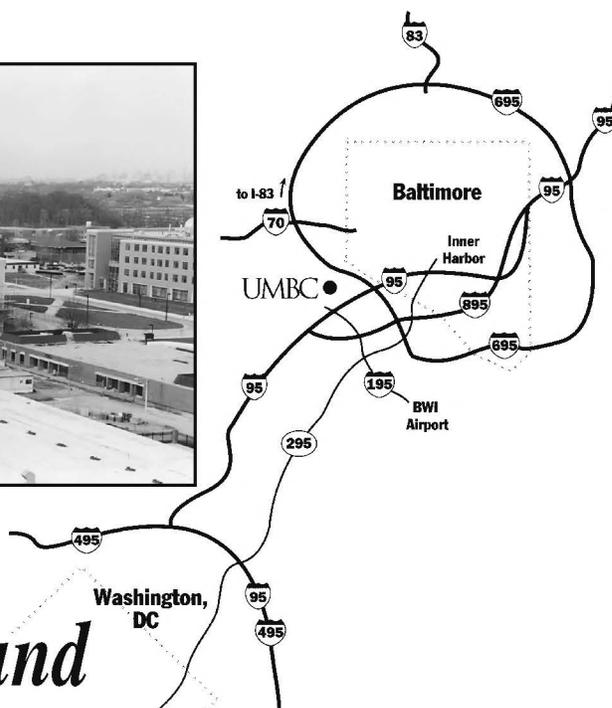
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ChE at  
*University of Maryland  
 Baltimore County*

TARYN BAYLES, DOUGLAS FREY, THERESA GOOD, MARK MARTEN, ANTONIO MOREIRA, GREGORY PAYNE, GOVIND RAO, AND JULIA ROSS

*University of Maryland Baltimore County • Baltimore, MD 21250*

**I**t all began twenty years ago. An MOU (Memorandum of Understanding) was signed in 1983 that created a satellite program in engineering at the University of Maryland Baltimore County (UMBC) campus. There was only one state-supported College of Engineering in Maryland at that time, at the University of Maryland College Park (UMCP), but in the late seventies and early eighties, sufficient economic development had taken place in the Baltimore region to draw legislative attention to the educational needs of the Baltimore region.

The original program created in 1983 envisaged the UMBC operation as a satellite campus, with an Associate Dean reporting to the Dean of Engineering at UMCP. Programs were set up in mechanical, chemical, and electrical engineering, with program directors in charge who would report to the respective department chairs at UMCP. The BS degree was approved in 1985 and the MS/PhD degree in 1986.

The founding fathers in chemical engineering wisely decided to call the UMBC program “Chemical and Biochemical Engineering” and made a strategic early decision to focus

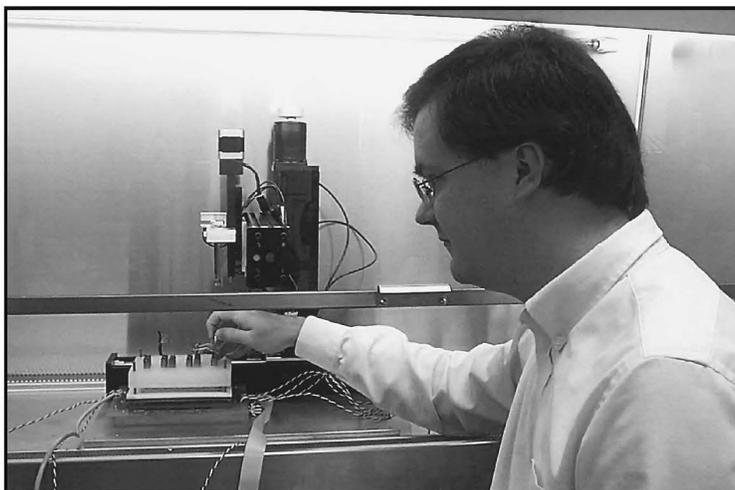
the graduate program exclusively on biochemical engineering, while offering the undergraduate degree in traditional chemical engineering. In 1986, Greg Payne joined the faculty as the first “bio” hire, followed in 1987 by Govind Rao. The program subsequently grew rapidly, with several additional hires joining the faculty (due to space limitations, only current faculty are mentioned). By 1991, engineering at UMBC had grown sufficiently to necessitate the creation of a freestanding college with its own dean, and the programs were renamed as “Departments” with corresponding “Chairs.”

The bio focus has turned out to be a great boon for the department. UMBC was the first chemical engineering department in the country to have such a focus, and it continues to this day to be the country’s only chemical engineering department to focus its graduate program exclusively on the bio area. From the beginning, this specialization attracted a great deal of attention, particularly from prominent biochemical engineering faculty at other institutions. One of the most exciting moments in our young history was when Professor

Daniel Wang from MIT spent half of his first (and only!) sabbatical at UMBC (with the other half spent at CalTech). We learned a great deal from him and through similar interaction with Professors Arthur Humphrey and Michael Shuler. Interestingly, a common thread of advice from all of these distinguished visitors during our formative years was to stay the course and keep building the program, and to resist the temptation to move into non-bio areas. Everyone felt that the concentration of faculty in the bio area and the unique location of UMBC in a bio-dense region of the country would eventually result in a strong and vibrant department.

## THE PRESENT

The department's more recent history has proven that the strategy of focusing its graduate program exclusively on the bio area was a sound decision. Although the department went through its share of growing pains and tough times in the beginning, the end result is a strong and stable department with exceptional facilities and equipment and outstanding faculty, staff, and students. For example, all faculty members in the department have active research pro-



*Peter Harms (NSF Graduate Fellow) adjusts a high throughput microreactor.*

grams with substantial external funding, and every eligible junior faculty member has received an NSF CAREER award. Table 1 lists the current faculty and staff in the department, along with their interests and responsibilities.

A great asset of being a high-profile department at a relatively small institution (see UMBC profile in Table 2) is an unusually close con-

**TABLE 1**  
**Current Personnel at UMBC**

■ **Dr. Taryn Bayles • Lecturer**

BS, New Mexico State University  
MS (Petroleum), MS and PhD, University of Pittsburgh  
Undergraduate education and outreach; transport phenomena

■ **Dr. Douglas Frey • Professor**

BS, Stanford University  
MS and PhD, University of California, Berkeley  
Chromatography of biopolymers

■ **Dr. Theresa Good • Associate Professor**

BS, Bucknell University  
MS, Cornell University  
PhD, University of Wisconsin-Madison  
Cellular engineering; optimization of chemotherapy and other problems in biocomplexity

■ **Dr. Mark Marten • Assistant Professor**

BS, State University of New York, Buffalo  
MS and PhD, Purdue University  
Bioprocessing, proteomics, and genomics; microbial responses to real-life environments

■ **Dr. Antonio Moreira • Professor and Vice Provost**

BS, University of Porto, Portugal  
MS and PhD, University of Pennsylvania  
Post Doc, University of Waterloo, Canada  
Regulatory/GMP issues, scale-up; downstream processing

■ **Dr. Gregory Payne • Professor**

BS and MS, Cornell University  
PhD, University of Michigan  
Biomolecular engineering; renewable resources

■ **Dr. Govind Rao • Professor and Chair**

BS, IIT (Madras)  
PhD, Drexel University  
Fluorescence-based sensors and instrumentation; fermentation and cell culture

■ **Dr. Julia Ross • Associate Professor**

BS, Purdue University  
PhD, Rice University  
Cell and tissue engineering; cell adhesion in microbial infection and thrombosis

**Support Staff**

Mary Anderson • IT Support Associate  
Laurie Botto • Office Assistant  
Mike Frizzell • Technician  
Victor Fulda • Technician  
Denise Kedzierski • Administrative Assistant

**Research Faculty**

Dr. Yordan Kostov • Research Assistant Professor  
Dr. Nandakumar Madayiputhiya • Research Associate  
Dr. Leah Tolosa • Research Assistant Professor  
Dr. Pyon Kyun Shin • Research Associate  
Dr. Haley Kermis • Research Associate

nection with administration. Everyone from the university President on down is literally at arms reach and is tremendously responsive and supportive of departmental needs.

Another unusual aspect is the close ties our department has with the Biology and Chemistry Departments as a result of many common faculty research interests. At its inception, our department occupied research space and facilities generously loaned to it by the Chemistry Department, and it also received strong support from the Biology Department. All of our faculty members also participate in the Molecular and Cell Biology and in the Chemistry-Biology Interface Programs at UMBC. These two programs have resulted in biology graduate students working in chemical/biochemical engineering laboratories and vice versa, leading to a creative interdisciplinary mix in our laboratories.

## HIGHLIGHTS

We are fortunate to be at the leading edge of a revolution. Biotechnology has become a dominant aspect of the US economy. Indeed, just as the previous century witnessed enormous strides in chemistry- and physics-based technologies, this century is poised to herald advances based on biology. The human genome has been sequenced, and unprecedented opportunities are opening up in the biotech/pharma world. We plan to exploit these opportunities with a vigorous research and education program that targets its bioprocess aspects, and through bioengineering applications that focus on cellular interactions in disease-causing states.

Our current undergraduate curriculum (see Table 3, Column 1) has little to differentiate it from other departments across the country that offer the chemical engineering major. This is changing, however. Our bio-focused graduate research program, coupled with enormous growth in the pharma/biotech industry, provided the inspiration for a new biotechnology/bioengineering track at the undergraduate level that we began in 2001 (Table 3, Column 2). While we plan to offer both the traditional track and the new track within the chemical engineering major for the next few years, we anticipate that the new track will ultimately emerge as a new major, depending on enrollment and acceptance of its graduates by employers and graduate/medical schools.

An unusual aspect of UMBC's graduate offerings, developed by Tony Moreira, is the four-course sequence in Biochemical Regulatory Engineering.

- *Regulatory Issues in Biotechnology*

**TABLE 2**  
**UMBC Facts, 2002-2003**

■ **President** • Freeman A. Hrabowski, III

■ **Faculty** • 680 full time and 350 part-time

■ **Students, Fall 2002**

- 11,711 enrolled
  - Undergraduate, 9,549
  - Graduate, 2,162
  - Full-time, 8,779
  - Part-time, 2,932
- Freshman Class 2002
  - First-time freshmen, 1,370
  - Living on campus (74%), 1,007
  - SAT percentiles
    - 25th - 1120
    - 75th - 1290
  - Average SAT
    - Top Quartile - 1374

■ **Chemical and Biochemical Engineering Statistics**

- Undergraduate, 100
- Graduate, 34
- Faculty, 10 FTE

■ **Academic Programs**

UMBC offers 37 majors and 32 minors or certificate programs in the physical and biological sciences, social and behavioral sciences, engineering, mathematics, information technology, humanities, and visual and performing arts. New degree programs include environmental science, financial economics, and a B.F.A. in acting.

UMBC's Graduate School offers 27 master's degree programs, 21 doctoral degree programs, and seven graduate certificate programs. Programs are offered in education, engineering, imaging and digital arts, information technology, life sciences, psychology, public policy, and a host of other areas of interest. A new gerontology PhD program is one of only six in the United States.

■ **Achievements**

- Ranked in top tier of nation's research universities—Doctoral/Research Universities-Extensive—by the Carnegie Foundation
- Six-time Pan-American Intercollegiate Team Chess champions
- National Science Foundation ranking for federally funded research in science and engineering jumped by nearly 50 places (from 200 to 153) in less than five years
- Named a "Hot School" by the 2003 *Kaplan/Newsweek College Guide*
- Only Maryland university rated a "Best Value" by the 2001 *Kaplan/Newsweek College Guide*
- Ranked 16th nationwide in NASA funding
- Named "Chess College of the Year" by *Chess Life* magazine in 2000
- Won the NCAA Northeast Conference Commissioner's Cup in 1999, 2000, 2001, and 2002
- Recognized as a college that builds character by *The Templeton Guide*
- Awarded Phi Beta Kappa chapter in 1997
- Only Howard Hughes Medical Institute Investigator at a Maryland public university
- Two-time recipient of U.S. Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring
- Consistently ranked among the top five research universities nationally in production of bachelor's degrees in Information Technology
- Designated a Center of Academic Excellence in Information Assurance by the National Security Agency

- *Good Manufacturing Processes for Bioprocess*
- *Quality Control and Quality Assurance for Biotechnology Products*
- *Biotechnology GMP Facility Design, Construction, and Validation*

This course sequence is also available as a stand-alone certificate program that is highly sought after by biotechnology industry professionals. Graduate students who complete this certificate program are highly attractive to industry—these issues are of critical importance to industry and programs of

this type are not generally available at most institutions.

While the primary focus of our graduate program is on PhD students, we are also mindful of industry's need for trained Master's students. This, coupled with an attractive integrated BS/MS option available to undergraduates, will result in significantly more MS degrees being granted over the next few years. Ultimately, this is primarily a resource issue, as the majority of the faculty is involved in long-term research

**TABLE 3**  
**BS Degree in Chemical Engineering: Traditional (left) and Bio (right) Tracks**

<i>Freshman Year</i>	
CHEM 101 Principles of Chemistry I (4)	CHEM 101 Principles of Chemistry I (4)
MATH 151 Calculus and Analytic Geometry I (4)	MATH 151 Calculus and Analytic Geometry I (4)
ENES 101 Introductory Engineering Science (3)	ENES 101 Introductory Engineering Science (3)
GFR electives (6)	GFR electives (6)
CHEM 102 Principles of Chemistry II (3)	CHEM 102 Principles of Chemistry II (3)
CHEM 102L Introductory Chemistry Lab (2)	CHEM 102L Introductory Chemistry Lab (2)
PHYS 121 Introductory Physics I (4)	PHYS 121 Introductory Physics I (4)
MATH 152 Calculus and Analytic Geometry II (4)	MATH 152 Calculus and Analytic Geometry II (4)
ENES 110 Statics (3)	<b>BIOL 100 Concepts of Biology (4)</b>
GFR electives (3)	GFR electives (3)
<i>Sophomore Year</i>	
CHEM 351 Organic Chemistry I (3)	CHEM 351 Organic Chemistry I (3)
ENCH 215 Chemical Engineering Analysis (3)	ENCH 215 Chemical Engineering Analysis (3)
MATH 251 Multivariable Calculus (4)	MATH 251 Multivariable Calculus (4)
PHYS 122 Introductory Physics II (4)	<b>BIOL 302 Molecular and General Genetics (4)</b>
CHEM 351L Organic Chemistry Lab I (2)	<b>BIOL 303 Cell Biology (3)</b>
MATH 225 Introduction to Differential Equations (3)	<b>BIOL 303L Cell Biology Laboratory (2)</b>
Advanced Science elective (3)	<b>CHEM 352 Organic Chemistry II (3)</b>
ENES 230 Introduction to Materials (3)	MATH 225 Introduction to Differential Equations (3)
GFR electives (6)	GFR electives (6)
<i>Junior Year</i>	
CHEM 301 Physical Chemistry I (4)	CHEM 301 Physical Chemistry I (4)
CHEM 311 Advanced Laboratory I (3)	<b>CHEM 437 Comprehensive Biochemistry I (4)</b>
ENCH 300 Chemical Process Thermodynamics (3)	ENCH 300 Chemical Process Thermodynamics (3)
ENCH 425 Transport Processes I (3)	ENCH 425 Transport Processes I (3)
GFR electives (3)	GFR elective (3)
CHEM 302 Physical Chemistry II (3)	<b>CHEM 438 Comprehensive Biochemistry II (4)</b>
ENCH 427 Transport Processes II (3)	ENCH 427 Transport Processes II (3)
ENCH 440 Chemical Engineering Kinetics (3)	ENCH 440 Chemical Engineering Kinetics (3)
ENCH 442 Chemical Engineering Systems Analysis (3)	ENCH 442 Chemical Engineering Systems Analysis (3)
ENGL 393 Technical Writing (3)	ENGL 393 Technical Writing (3)
<i>Senior Year</i>	
ENCH 437 Chemical Engineering Laboratory (3)	ENCH 444 Process Engineering Economics and Design I (3)
ENCH 444 Process Engineering Economics and Design I (3)	ENCH 445 Equilibrium Stage Computations (3)
ENCH 445 Equilibrium Stage Computations (3)	<b>ENCH XXX Bioengineering elective (3)</b>
ENCH XXX Chemical Engineering elective (3)	<b>ENCH XXX Bioengineering elective (3)</b>
GFR electives (3)	GFR elective (3)
ENCH 446 Process Engineering Economics and Design II (3)	ENCH 446 Process Engineering Economics and Design II (3)
ENCH XXX Chemical Engineering elective (3)	<b>ECH 485L Bioengineering Laboratory (3)</b>
ENCH XXX Chemical Engineering elective (3)	<b>ENCH XX Bioengineering elective (3)</b>
GFR electives (6)	GFR electives (6)

***UMBC was the first chemical engineering department in the country to have such a focus, and it continues to this day to be this country's only chemical engineering department to focus its graduate program exclusively in the bio area.***

projects that require the continuity and time investment of longer-term PhD students. At the present time, financial assistance is primarily directed at incoming PhD students (with some exceptions).

How does a small department handle so much? Part of the answer is Taryn Bayles, a full-time faculty member devoted to education and outreach. Her infectious enthusiasm and energy are largely responsible for the high profile enjoyed by the department. An example of her creative talents is demonstrated by teaching innovations incorporated into her courses, such as a design project where freshman engineering students had to build and operate a water-balloon-launching trebuchet that featured her as the target! In addition, Taryn's outreach efforts extend to several local schools and have served to increase both UMBC's visibility and the community's awareness of engineering.

In addition, several faculty members are involved in electronic instructional media development. For example, Doug Frey has developed a highly useful separations course web page that is available to anyone (found at <[www.research.umbc.edu/~dfrey1/ench445/](http://www.research.umbc.edu/~dfrey1/ench445/)>), and Julie Ross, in collaboration with faculty in the medical school, is developing innovative XML-based teaching modules.

We have close ties to industry—several faculty members have research interactions with a number of pharmaceutical/biotechnology companies. In addition, UMBC's location puts us within an hour's drive of top-notch Federal facilities including NIH, ONR, NIST, USDA, FDA, and DOD. Several of our faculty members and students have benefitted by using these unique research facilities.

## MEYERHOFF PROGRAM

UMBC is home to the nationally recognized Meyerhoff program, which has a strong track record for graduating mi-

**TABLE 4**  
**Former Chemical/Biochemical Engineering Meyerhoff Scholars**

*“\*” indicates non-minority student.*  
*“( )” indicates currently working on graduate degree requirements*

Stephanie Bates - Clemson University • MS
Christy Butler - Case Western Reserve • (MD/PhD)
Adetokunbo Eniola - Penn • (PhD)
Andre Johnson - Employed
Ray Onley - Georgia Tech • (MS)
Bradley Peterson - MIT • (PhD)*
Lee Pitts - Johns Hopkins • (PhD)
Simone Stalling - Penn • (MD/PhD)
Kendra Sarratt - Penn • (PhD)
Jeremiah Tabb - Georgia Tech (PhD)
Felicia Boone - Employed
Kafui Dzirasa - Duke • (MD/PhD)
Alexis Hillock - Georgia Tech (PhD)
Michael Johnson - UMBC • (PhD)
Camelia Owens - Delaware • (PhD)
Jason Pinnix - Penn • (PhD)
Natasha Powell - Unknown • (MD/PhD)
Marc Price - Employed
Frederick Scott - UMBC • (MD)
Jason Thorpe - Georgia Tech • (PhD)

nority students and sending them on to top-ranked PhD programs. The program was started in 1994 by President Freeman Hrabowski with a grant from the Meyerhoff Foundation and has since attracted national recognition.

To date, the Meyerhoff Scholarship Program has produced 296 graduates (the first degrees were awarded in 1993). One-hundred and forty-eight students (148) are currently enrolled in PhD, MD/PhD, or other graduate or professional degree programs at institutions ranging from Yale, Harvard, and Stanford to MIT, Johns Hopkins, Carnegie Mellon, and Berkeley. An additional 107 students have already completed graduate-degree requirements and are working as researchers and teachers at some of the finest institutions and companies in the world. Research studies have demonstrated that when compared to a sample of high-achieving non-Meyerhoff African-American students, Meyerhoff scholars have a significantly higher incidence of attending medical school or graduate school in the sciences, engineering, or math.

These findings have been substantiated by the fact that the National Science Foundation and the National Institutes of Health have identified UMBC, a predominantly white institution, as having one of the most effective programs contributing to minority-student success in science in the nation. Table 4 lists the Meyerhoff students from Chemical & Biochemical Engineering.

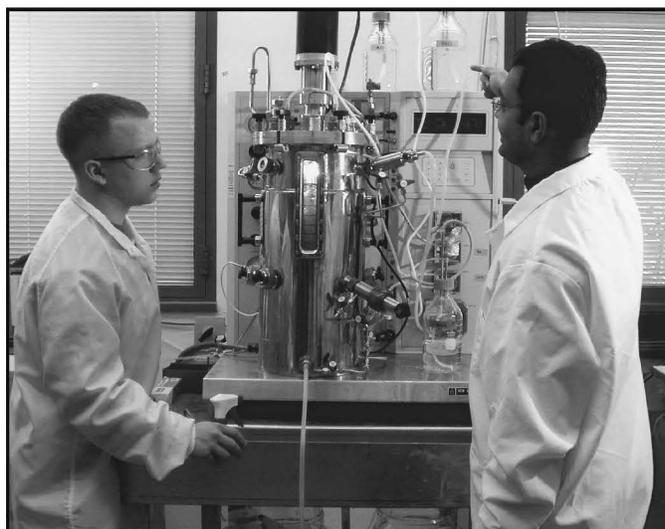
## LUMPKIN MEMORIAL LECTURE

Janice Antoine Lumpkin was one of the first African-American female faculty members in the chemical engineering field in this country. She graduated from MIT and Penn with BS and PhD degrees, respectively, and joined UMBC in 1989, initially as a part-time faculty member. She later converted to a full-time position and brought her catalysis skills to bear on understanding the mechanisms and kinetics of protein



◀ *Sungmun Lee (left), Theresa Good (center), and Wanida Wattanakaroon (right) purifying and testing photoimmuno conjugates for T-cell cancer treatment.*

*Graduate student Swapnil Bhargava (right) instructs undergraduate Seth Miller (left) on the operation of a 20-liter fermentor in Mark Marten's lab. ▼*



oxidation. Tragically, she passed away in 1997 after the birth of her fourth child. The department has honored her memory in the form of a high-profile memorial lecture that is part of UMBC's annual Life Sciences Day celebration. An eminent person is invited to deliver the Lumpkin Memorial Lecture for this celebration. Past Lumpkin lecturers include Arthur Humphrey, Daniel Wang, Douglas Lauffenberger, Sangtae Kim, and Barry Buckland. AIChE has also instituted a travel award in her name for attendance at its annual national meeting.

## THE FUTURE

We share a sense of excitement and anticipation about the future. Biotechnology is transforming life as its early promise is maturing. There is an unusual atmosphere shared by all members of this department—indeed, the feeling one gets is more like being in a small biotech company than in a traditional university setting. Our strengths and the challenges we face as we look into the future are

### Strengths

- **Focus on Biotechnology and Bioengineering:** this is a major factor in our ability to achieve excellence. A traditional chemical engineering department faces competition for resources from other subspecialties such as catalysis, polymers, etc. This is never an issue for us.
- **Outstanding Faculty:** Our faculty members are as productive as those at higher-ranked peer institutions. We are a young group and are aggressive and passionate about both research and teaching. Furthermore, the environment is extremely collegial and friendly.
- **Well-Equipped Laboratories:** Our research areas are well supported with state-of-the-art equipment, and we truly have unmatched equipment resources

compared to our much higher-ranked peers. Again, this is partly due to our focus on one area.

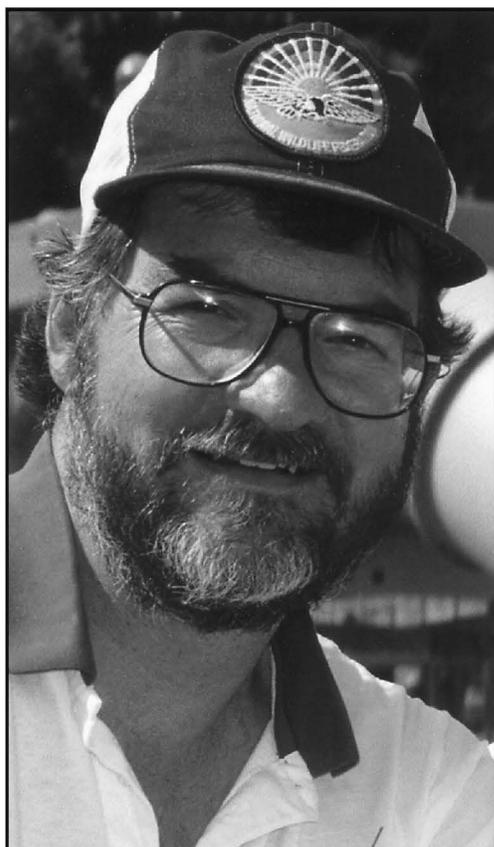
- **Outstanding Geographical Location:** We are located in an area where biotech-driven growth is inevitable, given our proximity to leading biomedical and biotechnology companies. Maryland ranks third in the nation for the number of biotech companies located in a state.
- **Outstanding Foreign Graduate Students:** UMBC is just about the only chemical engineering department that can guarantee an incoming graduate student that he or she will work on a bio-related project. This gives us a significant competitive edge in attracting students.

### Challenges

- Obtaining greater resources for building on our base in a tough budget environment.
- Few domestic graduate students—a situation that is not unique to us and that is slowly changing
- Growth in the number of faculty members. We would like to do more!

## ACKNOWLEDGMENTS

We thank Tim Ford for the photographs and Greg Simmons for the Meyerhoff Program statistics. □



# *Robert H. (Rob) Davis*

*... of the  
University of Colorado*

CHRISTOPHER BOWMAN

*University of Colorado • Boulder, CO 80309-0424*

As engineering faculty, each one of us is asked to perform at an exceptional level in research, education, and service to our universities and to our profession. These tasks often seem to be in conflict, and time pressures often force each of us to focus on one aspect at the expense of the others. For the eleven years that I have been at the University of Colorado, however, I have witnessed and worked with one faculty member who personifies those ideals—one who is committed to research at the highest level, to educating undergraduate and graduate students in the classroom and through the discovery process, and to serving his colleagues, his university, and his profession.

That person is Professor Robert H. Davis, Dean of the College of Engineering and Applied Science and Patten Professor of Chemical Engineering at the University of Colorado. He has been a prototype for what a faculty member should

be during his twenty years on the faculty. In fact, he is the only faculty member in the 110-year history of the College of Engineering and Applied Science at the University of Colorado who has received all three College awards for Outstanding Research, Teaching, and Service. He has not only demonstrated exceptional performance in each of those individual areas, but he has also focused on the synergistic interaction that exists between them.

As a hallmark of his career, Rob has worked tirelessly to develop programs that use research to assist educational efforts and to develop educational programs that impact research efforts. In addition to numerous research, teaching, and service awards within the University of Colorado, he has also been recognized with several national awards, including (most recently) the American Society for Engineering Education's Dow Lectureship Award.



◀  
Two of his favorite faculty  
from U.C. Davis, Ruben  
Carbonell (left) and  
Steve Whitaker (right)  
relaxing on a 1978  
road trip with  
Rob.

Rob and his  
PhD  
advisor,  
Andy Acrivos,  
in Cesaria, Israel,  
in 1984.  
▼

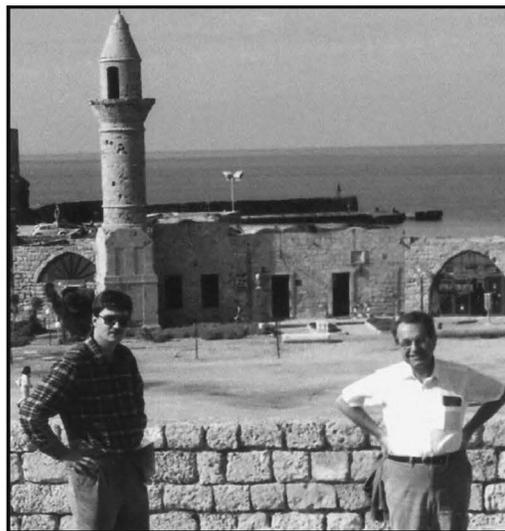
## HISTORY

Rob was born on March 26, 1957, in Paris, France, where his dad was stationed as a military advisor at the U.S. Embassy. Within three months of his birth, his family moved back to the United States, first to Garden City, New York, and then further west to Walnut Creek, California, when he was three years old.

Fortunately, Rob was exposed to great educators throughout his life; his mother taught college mathematics and his father taught elementary school and piano after retiring from the Navy. Rob attended Ygnacio Valley High School in Concord, California, where he was named the outstanding senior in both mathematics and science. When he entered the University of California at Davis, intending to major in either math or chemistry, the teaching assistant for his freshman chemistry class suggested that he could combine those subjects and major in chemical engineering instead. Like many entering freshmen in our field, prior to that time Rob ‘had not heard the words *chemical* and *engineering* used together in the same sentence!’

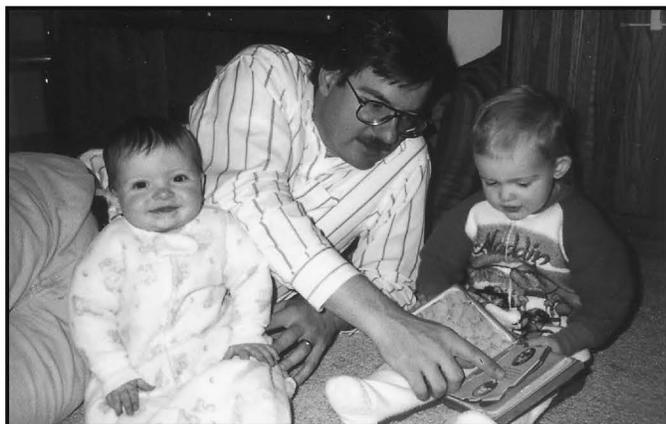
Rob displayed an early knack for leadership at Davis. During all four years he volunteered 15-20 hours a week to work with junior-high and high-school students through Young Life. In his senior year, he was President of the AIChE Student Chapter, which hosted the regional AIChE Student Chapter Conference. He also organized the First-Annual Kronecker Delta golf tournament, named in honor of a “favorite” tensor used by Professor Steve Whitaker in transport courses. Somehow, Rob also found time to study, and he received the University Medal in 1978 as the outstanding graduate from U.C. Davis in all disciplines.

For graduate school, Rob moved across the San Francisco Bay to Stanford, where he had the good fortune of working with Professor Andreas Acrivos. “I was the second in a line of several PhD students who studied the *Boycott Effect* with Andy,” Rob notes, “which refers to the phenomenon of an enhanced clarification rate in sedimentation vessels with inclined walls.” Rob’s dissertation work involved a combination of theory and experiment, a hallmark of his own research program ever since that time.



Before leaving Stanford for his postdoctoral position, Rob interviewed for a number of faculty positions and ultimately accepted an offer to come to the University of Colorado. Interestingly, this interview and selection process became the subject of an article written by Rich Felder regarding his observations while he was spending his sabbatical at Colorado.<sup>[1]</sup> At the time, it was clear that Rob would be an exceptional teacher, although his future research career and success was not as obvious. Rob notes, “I have always loved to teach, but I was less certain about research when I was interviewing for a faculty position. Fortunately, I quickly learned how much fun research can be, especially when working with students.”

More than twenty PhD students of Andy Acrivos have gone on to successful academic careers, including several (John Brady, Dave Leighton, Ashok Sangani, and Eric Shaqfeh) who overlapped with Rob. Many of these students did postdoctoral research in the Department of Applied Mathematics and Theoretical Physics (DAMTP) at the University of Cambridge, and Rob dutifully took up the call after completing his PhD in 1982. He was a NATO Postdoctoral Fellow at DAMTP for a year, working with



*Rob enjoys teaching students of all ages, even if only half of the class pays attention! With daughters Grace (right) and Allie (left) in 1993.*

Professor George Batchelor on particle aggregation and with Dr. John Hinch on elastohydrodynamic collisions and rebound.

Rob has always enjoyed working with young people, both inside and outside of the university setting. While in graduate school, he continued to spend 15-20 hours a week (and often more) leading a Young Life club. Young Life is a nondenominational Christian outreach to primarily non-church kids, and Rob led weekly club meetings, Bible studies, camping trips, and social events, in addition to co-leading and training a team of other volunteers.

Near the end of his time in graduate school, Rob became a student leader of the Menlo University Fellowship and met Shirley Giles, a member of the group. They married in December 1982, a few months after Rob finished his PhD and then part of his Postdoctoral year, while Shirley completed a BA in Communications from Stanford and then a mission experience in Bangalore, India. Rob and Shirley returned to the United States in late summer 1983 and moved to Colorado for Rob to begin the faculty position he had lined up the year before.

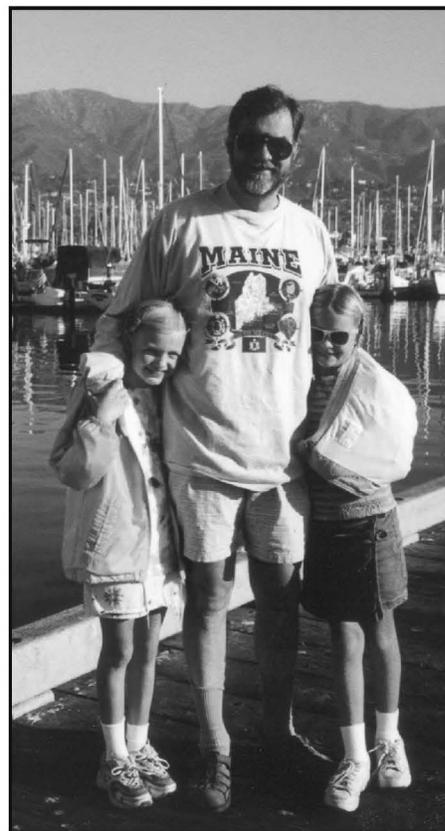
Shortly after moving from England to Colorado, Rob and Shirley began doing volunteer work with the high school program of the First Presbyterian Church in Boulder. After a year, they began working with the University Christian Fellowship, a program for CU-Boulder students sponsored by the same church. Rob was the volunteer director of this program for several years, and he and Shirley continue to be associates in the program. Their activities over the years have included teaching a Sunday class, leading Bible studies, housing interns, organizing retreats, and chairing the Messenger Committee to send teams of university students on summer projects in foreign countries.

Rob was promoted from Assistant to Associate Professor after only five years on the faculty and was promoted to full professor in 1992. In 1990-91, he received a Guggenheim Fellowship for his first sabbatical, which he took at the Massachusetts Institute of Technology. At MIT, he enjoyed interactions with Professors Bob Armstrong, Howard Brenner, Bob Brown, Clark Colton, and Greg Stephanopoulos, among others, as well as with Howard Stone at Harvard University. "I also enjoyed getting to know several bright PhD students and postdocs," Rob recalls, "including Nick Abbott, Stephanie Dungan, Gareth McKinley, and Ron Phillips, who have all gone on to

*Rob's first responsibility after becoming Dean in July 2002 was to buy a tuxedo for the black-tie functions that he and his wife, Shirley, would attend.*



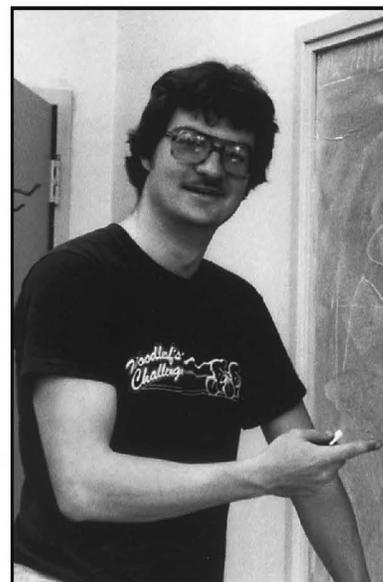
*Daughters Grace and Allie today, well on their way to being teenagers, on a trip to Santa Barbara.*



*“Punting” on the river Cam, a welcome break from postdoctoral studies at the University of Cambridge in 1982-83. ▼*



*Rob (on the left) leading songs for a Young Life retreat in 1980, with Robert Aguirre (now a Professor of English).*



*Rob in his Stanford office in 1982, explaining the concept of inclined settling. The T-shirt depicts his love of bicycling—he still rides a bike to work every day!*

successful academic careers.”

During this year at MIT, Rob and Shirley lived in the Back Bay area of Boston. While Rob walked across the Massachusetts Avenue bridge over the Charles River to MIT, Shirley walked upriver to Boston University, where she completed an MA degree in broadcast journalism.

After they returned to Colorado, their first daughter, Grace, was born in December of 1991, followed by their second daughter, Allison, born in June of 1993. “I never thought that I would enjoy young children as much as I enjoyed high-school and college students,” Rob says, “but I’ve changed my mind, now that I have my own children.” In the year between his daughters’ births, Rob became Department Chair (1992). Although his teaching load was slightly reduced to accommodate his new activities, throughout his ten years as department chair, Rob maintained his research program at its usual high level.

Rob took his second sabbatical in 1997-98, this time at the University of California at Santa Barbara, hosted

by Professor Gary Leal. Besides providing time for uninterrupted research, it was also a great opportunity for Rob to spend more time with Shirley and their young daughters. He notes that they had a picnic in their backyard or at the Goleta beach several evenings every week. The close-knit family now often travels with Rob for conference/vacation trips, especially to foreign countries. Closer to home, they love to camp, hike, bike, and ski, and Rob often brings the girls with him when he can’t stay away from the office on Saturdays!

More recently, Rob was appointed Dean of Engineering and Applied Science at the University of Colorado (July, 2002). While he took this position out of a sense of duty to the institution that has served him well for the past twenty years, he has found his new responsibilities “surprisingly fun.” In the current economic climate of limited resources for the traditional “dean-type” activities of adding new buildings, supporting new initiatives, and increasing the faculty, he remains excited about the challenges of nurturing faculty for excellence in both teaching and research, educating students in both traditional and active-learning environments, and allocating resources wisely to invest in excellence for the long term.

“I expect to be Dean for ten, plus or minus eight, years,” Rob jokes, “so making personal plans for the future is difficult.” He anticipates continuing a vibrant research program, although perhaps more modest in size. His current research group consists of nine PhD students and two research associates. Rob hopes to return to classroom teaching someday and plans to remain active in serving the profession. Most importantly, we expect Rob to continue to balance his priorities of family and faith along with his service to students, faculty, and the profession.

## The research that he has performed and the

### EDUCATION

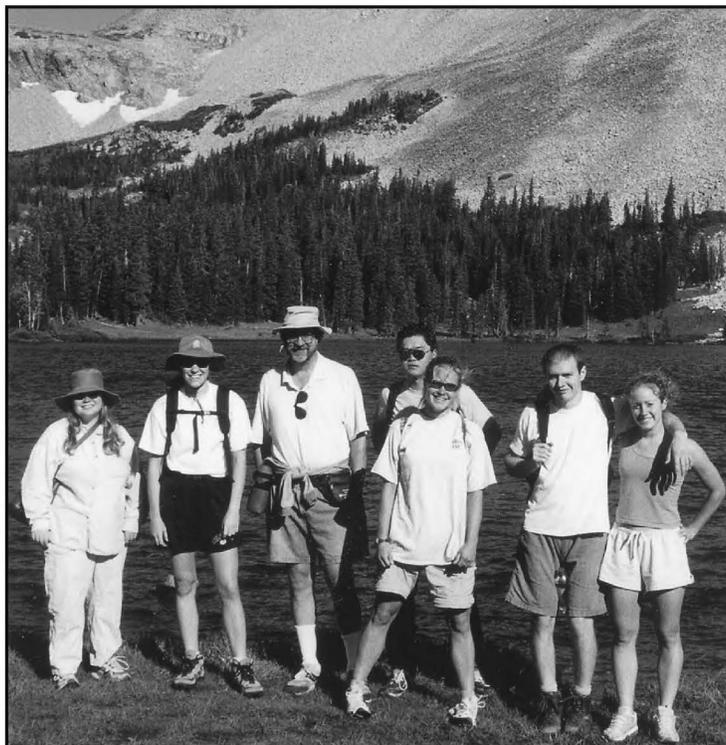
Rob is an outstanding classroom teacher and has won several departmental and college-wide teaching awards. He is respected by students for his high standards, superb organization, compelling lectures and demonstrations, as well as his compassion and fairness. In fact, Professor Bill Bentley (University of Maryland), a former PhD student who also had Rob as a professor, indicates that “Rob was singularly the best educator I’ve ever encountered, anywhere.”

The lasting influence of Rob’s educational work includes a half-dozen publications on teaching methods in peer-reviewed journals, the development of six new courses (five that are now taught by other faculty), organization of a special issue of *Chemical Engineering Education* on teaching fluid-particle technology, and development of the Interdisciplinary Biotechnology Program at the University of Colorado. Additionally, he directs or co-directs three Graduate Assistantships in Areas of National Need (GAANN) programs funded by the U.S. Department of Education, which support graduate-student training throughout the Department of Chemical Engineering. As part of these programs, Rob thoroughly enjoys taking the students on retreats and road trips. Despite his recent ascension (descension?) to the Deanship, Rob has continued to be active in these programs, including attending the retreats and other student interactions.

Rob is also an outstanding mentor and spends countless hours helping students and young faculty to think critically, to learn through discovery, and to communicate effectively. For the past three years, he has served as a faculty mentor to graduate students participating in an NSF-funded outreach program to local high schools and middle schools. He has also been research mentor to over 120 undergraduates, 50 graduate students, and 10 postdocs. As one significant measure of his success and lasting impact, ten of his former graduate students and postdocs are now full-time faculty members. As has been noted by several of these former students, the framework that Rob established, his mentoring style, and his concern for his students are all aspects that these former students hope to emulate.

### RESEARCH

Rob’s research philosophy is to perform fundamental research on problems selected from or motivated by practical engineering applications. He is a world



*Rob with some members of his research group on a hike in the Colorado Rocky Mountains in 2000.*

leader in the hydrodynamics of complex fluids, and his group has applied fundamental theory and principles in this area to an astonishing variety of problems.

In his twenty-plus-year academic career, Rob has published more than 160 papers and has received over \$18 million in grants to support his research program. Worth noting is the fact that, as evidenced by his references, publications, and funding, he has had a significant impact on three distinct research areas: fluid mechanics, biotechnology, and membrane separations. As one example of his creativity, Rob and a PhD student, Kim Ogden (now at the University of Arizona), showed that productive cells could be separated from unproductive cells and recycled in a continuous-flow bioreactor by coupling genetic markers for flocculation with the gene for the product of interest, so that the productive cells settled rapidly as flocs with fractal structures. Rob and his group later became the first to apply fundamental engineering principles to pioneer new bioreactor strategies for enzymatic production of ribonucleic acids, by immobilizing DNA templates on small beads and then recovering both DNA and enzyme (due to binding) along with the beads to achieve substantially improved yields of RNA product.

As another example, Rob applied fundamental transport principles, including the newly recognized phenomenon of shear-induced hydro-

## *impact he has had on other lives will last for many lifetimes.*

dynamic diffusion, to establish widely used models for crossflow membrane filtration. More recently, his group has developed and analyzed several novel strategies for membrane-fouling control: rapid backpulsing, dynamic secondary membranes, and surface modification by photografting.

In more basic research on multiphase flow, Rob developed the first elasto-hydrodynamic theory (with coupled solid and fluid mechanics) for particle collisions with other particles or surfaces in liquids or gases, to predict whether particle rebound or adhesion occurs, and then later elucidated the friction/lubrication nature of particle contacts in liquids. This pioneering work is now used in diverse fields such as granulation, wet granular flow, suspension flow, and air filtration. Moreover, his group has analyzed the related problems of drop and bubble interactions in near contact, showing how small deformations due to lubrication forces retard coalescence and how large deformations may promote alignment, breakup, and/or coalescence.

### **SERVICE AND LEADERSHIP**

When Rob became the Department Chair, it was one of the best possible things that could happen to our department. As Chair, Rob undertook a major program to improve the Department in all areas and at all levels, including undergraduate students and programs, graduate students and programs, and faculty. Since Rob took over, the number and quality of the undergraduate and graduate student populations have improved, funding and publications per faculty member have more than doubled, and the faculty has grown in size—half of the current faculty were hired while Rob was Chair. Faculty have also received numerous national and international awards from professional societies (Materials Research Society, AIChE, ACS, and ASEE) and foundations (Dreyfus, Packard, Sloan, Howard Hughes Medical Institute) that recognize its progress, with most of these awards based on nominations that Rob carefully prepared for his colleagues. In fact, in just the last three years, three different faculty have won singular national awards from ASEE (two Curtis W. McGraw Awards and Rob's selection as the 2002 Dow Lectureship winner). The State of Colorado has also twice designated the Department as a Program of Excellence.

Rob is a tireless advocate for chemical engineering education and research, as well as for the people involved in those activities. In addition to numerous responsibilities at the University of Colorado (including his service as Chair (1992-2002), with only one sabbatical break, and now as Dean), his professional activities have included organizing the IUTAM Symposium on Hydrodynamic Diffusion of Suspended Par-

ticles in 1995, the technical program of the AIChE Annual Meeting in 1999, and the technical program of the North American Membrane Society Annual Meeting in 2000. He co-organized a series of workshops on "Teaching Fluid-Particle Processes" for the 1997 ASEE Summer School for Chemical Engineering Faculty, and he served as Guest Editor of a special-feature section of *Chemical Engineering Education* in 1998, which contained seven articles related to the recommendations of this workshop. He also served as the Director of the Colorado RNA Center (1992-2001) and co-Director of the Colorado Institute for Research in Biotechnology (1987-2001), in statewide efforts to promote research, student training, and industry/university cooperation, including management of an annual symposium, seed grants program, graduate fellowships, and student internships. Rob was the co-Chair (along with Scott Fogler and Mike Cutlip) of the 2002 ASEE Summer School for Chemical Engineering Faculty, held last July at the University of Colorado.

In 1995, Rob was invited to make a presentation at the AIChE Young Faculty Forum, and he chose the subject "Getting Along With (and the most out of) Your Department Chair." Based on session evaluations, his presentation received the Outstanding Paper Award for the 1995 AIChE Annual Meeting. As the co-Chair for that session, it was readily apparent to me that Rob's advice to the younger faculty, as well as to those aspiring to be young faculty, was extremely well received. He was also not afraid to challenge the common assumptions about what young faculty should do—he challenged them to participate in service activities that had a high outcome-to-input ratio and not to simply neglect service until after being tenured. Excerpts of his advice to young faculty are soon to be submitted as an article in *Chemical Engineering Education*.

### **SUMMARY**

*If your vision is for one year, plant wheat.  
If your vision is for ten years, plant trees.  
If your vision is for a lifetime, plant people.*

Old Chinese Proverb

In fact, that is exactly what Robert Davis has spent the last twenty years doing! As a researcher, he has trained PhD and undergraduate research students who will lead the next generation; as a teacher, he makes sure that his students know the basic principles and fundamentals; and as a Department Chair and Dean, he has mentored faculty and provided a framework in which all are encouraged and enabled to be successful. The research that he has performed and the impact he has had on other lives will last for many lifetimes. □

# PRODUCTIVITY AND QUALITY INDICATORS

## For Highly Ranked ChE Graduate Programs

PHILLIP E. SAVAGE

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Comparative assessments of graduate programs have been made for at least eighty years. Such assessments are useful to prospective students and to those seeking an academic position. They are also used in the political arena to make or justify policy and appropriations decisions. Within engineering, the most visible rankings are those from *U.S. News*,<sup>[1]</sup> the NRC Report,<sup>[2]</sup> and the Gourman report.<sup>[3]</sup> The *U.S. News* ranking is arguably the best publicized and most widely used ranking today.

*U.S. News* ranks the graduate programs for individual engineering disciplines. These discipline-specific rankings are based exclusively on a department's reputation as determined from a peer-assessment survey. Engineering deans (or their designees) nominate up to ten departments in a particular discipline (e.g., chemical engineering), and the total number of respondents who nominate a department determines its rank. The most recent ranking<sup>[1]</sup> of graduate programs was compiled in January 2002, based on data from a survey distributed in the fall of 2001.

This article expands the reputation-based *U. S. News* rankings of chemical engineering departments by providing and comparing quantitative quality and productivity indicators for the top twenty chemical engineering departments in its 2002 ranking. One objective of this study was to determine how well the rankings, which are based exclusively on reputation, correlate with different publicly available productivity and quality indicators. A second objective was simply to assemble the database of quantitative indicators, an exercise that has not been completed for at least ten years.

The productivity indicators examined here are the number of published articles and reviews and the number of bachelor, master, and doctoral degrees granted annually. The quality indicators are the number of NAE members, the number of AIChE Institute awards received, the number of highly cited papers, the number of citations per paper, and the total

number of citations to the department's published articles and reviews. This last quantity is an indicator of both quality (citations) and productivity (number of publications).

The study also included data on the research expenditures for each department. Some would contend that total research expenditure is not an indicator of productivity or quality, but research funding is a necessary input for a high-quality graduate program. Moreover, one could argue that the ability to compete successfully for peer-reviewed federal funds is an indicator of quality. Therefore, the study included data for federally funded research expenditures for each department.

None of the indicators used in this study are perfect or complete measures of quality or productivity. They are simply quantities that most chemical engineering educators would likely agree are among the most relevant indicators. Similarly, the indicators used in this study do not constitute an exhaustive set of all relevant indicators. Other relevant indicators (e.g., non-AIChE awards, patents, faculty appointments for PhD recipients, etc.) exist but were excluded here to make the demands of data gathering consistent with the resources available for the task.

Many of the indicators considered here have been used previously to rank graduate programs. Diamond and Graham<sup>[4]</sup> argued that per capita citation density (citations per faculty member) is perhaps the best single indicator of a program's



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excellence. Their article also provides an interesting discussion of the history and limitations of subjective peer assessments (reputational rankings). Angus, et al.,<sup>[5]</sup> proposed a ranking system that uses data for publications, citations, research support, and awards. Their system included a greater variety of awards than NAE membership and AIChE Institute awards, which are the only awards considered here.

Both articles provided rankings of chemical engineering programs. These rankings were based on the publication and citation data that appeared in the 1995 NRC report. The data were gathered in 1993, so the rankings in these articles as well as in the NRC report itself reflect the landscape as it existed ten or more years ago. Additionally, there were inaccuracies in some of the citation data in the 1995 NRC report.<sup>[4]</sup>

It is worthy of note that the NRC is currently evaluating various methodologies for its next comparative study of graduate programs at U.S. universities, release of which is anticipated to be in 2005. Given that at least a decade has passed since a comprehensive set of indicators has been assembled for chemical engineering graduate programs, we set out to develop such a database for the top twenty programs in the *U.S. News* 2002 rankings. One purpose in doing so is to assess the degree of correspondence between the subjective rankings and the various publicly available quantitative indicators.

## METHODOLOGY

This study examines data for both productivity indicators and quality indicators for the twenty chemical engineering departments ranked by *U.S. News*. One of the quality indicators is the number of faculty members in a chemical engineering department who are also members of the National Academy of Engineering (NAE). This information was compiled by comparing the list of NAE members<sup>[6]</sup> at each institution with the list of faculty in each department.<sup>[7]</sup> A second quality indicator is the number of AIChE Institute awards that faculty members in a given chemical engineering department in 2002 had received between the years 1992 and 2001.<sup>[8]</sup>

Additional productivity and quality indicators involve publications and citations. The average annual number of publications from each chemical engineering department was determined for 2000 and 2001. These data were obtained from a search of ISI's Web of Science.<sup>[9]</sup> The search was conducted by department (or school) and not by each individual faculty member. It provided all publications in which at least one author self-identified with the specific department.

The search included only "articles" and "reviews." It pro-

vided no data specifically for the chemical engineering programs at Caltech and at Minnesota. Caltech authors in both chemistry and chemical engineering identified themselves with the Division of Chemistry and Chemical Engineering.

Thus, the search returned publications for both departments and no attempt was made to determine the subset that could be attributed to chemical engineering. Minnesota's chemical engineering program is part of the Department of Chemical Engineering and Materials Science, and the search returned papers published by the entire department. These departmental totals were included in this study because the chemical engineering portion of that department is easily the larger of the two.

The ISI database was also used to discover the total number of citations made to each "article" and "review" published by a given chemical engineering department in 1998 and 1999. This search also provided the total number of articles and reviews published by that department during that two-year span. The number of citations reported is the number as of the dates of the searches (May 23-24, 2002). Thus, the citation statistics reported herein are for papers that had been in print for two-and-one-half to four-and-one-half years. There may be a benefit to using a

longer time in print for the citation analysis (capture more completely the total impact of the articles), but there also exists a disadvantage (using older papers makes the citation data less reflective of the impact of a department's recent work).

The number of papers published by most departments in 1998/99 was within 10% of the number published in 2000/01. Since the departmental publication rates are similar for these four years, and since the citation statistics are for only a two-year sample, the citation statistics are not likely to suffer from a publication-rate-profile bias.<sup>[10]</sup> Moreover, the citation statistics presented herein are free of many of the "pitfalls" enumerated by Grossmann.<sup>[11]</sup> Other authors<sup>[4,5]</sup> have also discussed the strengths and weaknesses of using citations as an indicator of quality so these issues will not be rehashed here.

Note that ISI computes statistics for the citation impact in chemical engineering for different institutions. These statistics are determined from citations to all publications from a given university in a set of journals ISI classifies as "chemical engineering" journals. Thus, a portion of the data will be from articles contributed by other departments, and more importantly, work published by chemical engineering faculty will be excluded if it is published outside the traditional chemical engineering journals. It is for these reasons that this statistic was not used in the present study. Finally, note that one

***One objective of this study was to determine how well the rankings, which are based exclusively on reputation, correlate with different publicly available productivity and quality indicators.***

could devise a scheme to calibrate the citation statistics (perhaps using impact factors for journals or fields) to account for field-to-field differences in citation frequency. This calibrated citation frequency could be a useful complement to the total citation frequency reported here.

Another indicator of productivity is producing engineering graduates. The ASEE website<sup>[12]</sup> provided the number of bachelor, master, and doctorate degrees, respectively, granted in chemical engineering in 2000 and 2001. The data available for the University of Minnesota includes chemical engineering and materials science together. This site also provided the number of full-time, tenured, or tenure-track faculty in each department for these two years. Note that these data do not account for fractional academic appointments nor do they include non-tenure-track faculty. Accurate data for the number of faculty full-time equivalents in each department would have been useful, but such data do not appear to reside in a publicly available database.

Finally, the study included information regarding research expenditures made by each department. The ASEE website provided the total annual expenditure for 2000 and 2001. These total research expenditure figures include both sponsored and internally funded research. No research expenditure data were available on the ASEE website for Caltech,

Georgia Tech, or Northwestern. The National Science Foundation<sup>[13]</sup> also compiled and reported research expenditure data. The most current data are for fiscal year 2000, and both the total and the federally sponsored research expenditures are available for all of the departments of interest.

## RESULTS AND DISCUSSION

Table 1 provides the data for each department. The first column, "Rank," provides the *U.S. News* ranking. "NAE" is the number of faculty members in a chemical engineering department who are also members of the National Academy of Engineering. The next column shows the number of AIChE Institute awards that faculty members in a given chemical engineering department in 2002 received between 1992 and 2001. The column "Pubs" shows the average annual number of publications from each department. "B," "M," and "D" are the mean number of bachelor, master, and doctorate degrees, respectively, granted annually in chemical engineering for 2000 and 2001. "FTF" is the mean number of full-time (tenured or tenure-track) faculty.

The first "Total Research Expenditure" column is an annual average for 2000 and 2001, as compiled by ASEE, and the other two Research Expenditure columns contain data from NSF<sup>[13]</sup> for fiscal year 2000. The next column lists the

**TABLE 1**  
Extensive Indicators for Chemical Engineering Departments

Rank	AIChE			Research Expend. (\$K)							Cit. per Pub	>50 Cites	
	NAE	Awd	Pubs	B	M	D	FTF	Total <sup>1</sup>	Total <sup>2</sup>	Federal <sup>2</sup>			Cit.
1. MIT	9	10	134	79	39	34	33	17,958	16,106	10,131	3751	12.0	8
2. Minnesota <sup>3</sup>	7	2	143	156	10	43	32	7,551	9,057	5,682	2283	6.7	2
3. UC Berkeley	3	2	94	80	7	13	18	13,205	4,842	1,880	1577	8.6	1
4. Caltech	4	4	n.d.	11	6	6	10	n.d.	5,105	2,772	n.d.	n.d.	n.d.
5. Wisconsin	2	1	90	93	6	16	17	8,862	7,317	4,295	1210	7.0	1
6. Stanford	1	1	58	14	31	6	11	6,019	6,424	5,378	1068	10.8	2
7. Texas	3	1	91	126	20	18	20	5,405	7,469	3,823	1412	7.2	0
8. Delaware	2	2	86	45	10	19	21	3,380	5,890	2,940	1168	6.8	2
9. Illinois	1	0	54	79	18	9	13	2,825	5,160	3,001	675	5.8	0
10. Princeton	3	7	70	27	2	11	17	3,644	3,130	1,564	1412	9.8	1
11. Michigan	0	3	79	130	22	10	17	4,143	3,623	2,315	1267	8.6	5
12. UC Santa Barbara	6	2	73	17	3	10	19	4,610	4,995	3,907	2648	15.9	11
13. Georgia Tech	3	2	62	135	10	15	34	n.d.	5,938	2,460	793	6.0	1
13. Purdue	0	1	63	112	8	12	21	6,699	6,624	2,403	655	5.0	0
15. Carnegie Mellon	3	2	78	41	9	13	19	3,603	3,379	2,223	1029	7.3	0
16. Cornell	1	0	36	58	12	8	13	3,397	3,020	1,647	770	7.9	0
16. Pennsylvania	2	2	38	30	14	7	9	1,738	1,777	1,300	638	9.7	2
18. Northwestern	1	2	45	46	6	10	15	n.d.	4,086	2,084	643	7.1	0
19. Penn State	1	1	50	141	8	6	20	3,172	14,257	8,491	718	6.1	1
20. Texas A&M	0	1	49	116	14	15	18	11,826	9,364	1,963	381	4.9	0

<sup>1</sup> From ASEE data

<sup>2</sup> From NSF data

<sup>3</sup> For chemical engineering and materials science

total number of citations to all articles and reviews published by a given department in 1998 and 1999. The mean number of citations per research publication appears in the next column. This quantity was calculated as the total number of citations divided by the total number of articles published during those two calendar years. The final column lists the total number of articles in the sample that had been cited more

than fifty times as of the date of the citation search.

Different sources sometimes report different values for the same statistic. A manifestation of this discrepancy is apparent in the "Total Research Expenditure" data in Table 1. Substantial differences between the NSF and ASEE databases appear for four departments (Berkeley, Delaware, Illinois, and

Penn State). The NSF data are for fiscal year 2000 and the ASEE data are for the academic year, but it is difficult to envision such large differences being attributable to different ending dates for a fiscal and an academic year. The chemical engineering programs at Berkeley and at Illinois do not reside within the College of Engineering, so this administrative structure might play a role in the discrepancies. Data reported by different sources for degrees granted by a given department also exhibited variability (but not as much as the research expenditure data).

The data in Table 1 afford an opportunity to determine which departments had the highest values for the different extensive quality and productivity indicators. Table 2 lists the top ten departments (of the twenty considered) in several of the categories. For each of the five indicators in Table 2, at least half of the departments listed

are also among the top ten in the *U.S. News* ranking. In fact, the only top-ten schools absent in more than two of the columns in Table 2 are Stanford and Illinois. Carnegie Mellon (CMU), Michigan, and UC Santa Barbara (UCSB) are the only schools ranked in the second ten by *U.S. News* to appear in at least two of the columns. Each of these schools appears on three or four of the lists.

All of the data in Table 1 except for citations per paper are extensive indicators of the productivity or quality of each department. That is, they are total quantities and their values can depend on the size of the department. To analyze the data more thoroughly, intensive indicators were obtained by

**TABLE 2**

**Top Ten<sup>1</sup> Departments in Different Productivity or Quality Indicators**

	<i>Citations/Pub<sup>1</sup></i>	<i>Citations<sup>1</sup></i>	<i>Publications<sup>2</sup></i>	<i>NAE Members</i>	<i>Doctorate Degrees</i>
1	UCSB	MIT	Minnesota	MIT(9)	Minnesota
2	MIT	UCSB	MIT	Minnesota (7)	MIT
3	Stanford	Minnesota	Berkeley	UCSB (6)	Delaware
4	Princeton	Berkeley	Texas	Caltech (4)	Texas
5	Pennsylvania	Princeton	Wisconsin	Berkeley (3)	Wisconsin
6	Michigan	Texas	Delaware	Texas (3)	Georgia Tech
7	Berkeley	Michigan	Michigan	Princeton (3)	Texas A&M
8	Cornell	Wisconsin	CMU	CMU (3)	Berkeley
9	CMU	Delaware	UCSB	Georgia Tech (3)	CMU
10	Texas	Stanford	Princeton	3 depts w/2	Purdue

<sup>1</sup> Of the 20 ranked by *U.S. News*

<sup>2</sup> Excluding Caltech because of lack of data

**TABLE 3**

**Intensive Indicators for Chemical Engineering Departments**

<i>Rank</i>	<i>AICHE</i>						<i>Research Expend. (\$K)</i>			<i>Cit.</i>	<i>&gt;50 Cites</i>	
	<i>NAE</i>	<i>Awd</i>	<i>Pubs</i>	<i>B</i>	<i>M</i>	<i>D</i>	<i>Total<sup>1</sup></i>	<i>Total<sup>2</sup></i>	<i>Federal<sup>2</sup></i>			
1	MIT	0.28	0.31	4.14	2.42	1.18	1.03	553	496	312	115	0.25
2	Minnesota <sup>3</sup>	0.22	0.06	4.47	4.86	0.30	1.33	236	283	178	71	0.06
3	Berkeley	0.17	0.11	5.22	4.42	0.36	0.69	734	269	104	88	0.06
4	Caltech	0.40	0.40	n.d.	1.10	0.55	0.55	n.d.	511	277	n.d.	n.d.
5	Wisconsin	0.12	0.06	5.42	5.64	0.36	0.94	537	443	260	73	0.06
6	Stanford	0.09	0.09	5.27	1.23	2.82	0.55	547	584	489	97	0.18
7	Texas	0.15	0.05	4.55	6.28	1.00	0.88	270	373	191	71	0.00
8	Delaware	0.10	0.10	4.17	2.17	0.46	0.93	165	287	143	57	0.10
9	Illinois	0.08	0.00	4.28	6.28	1.44	0.68	226	413	240	54	0.00
10	Princeton	0.18	0.41	4.12	1.59	0.09	0.65	214	184	92	84	0.06
11	Michigan	0.00	0.18	4.62	7.62	1.29	0.59	244	213	136	75	0.29
12	UC Santa Barbara	0.32	0.11	3.84	0.89	0.16	0.50	243	263	206	139	0.58
13	Georgia Tech	0.09	0.06	1.85	4.01	0.30	0.43	n.d.	177	73	24	0.03
13	Purdue	0.00	0.05	2.98	5.31	0.38	0.55	319	315	114	31	0.00
15	Carnegie Mellon	0.16	0.11	4.22	2.22	0.49	0.68	195	183	120	56	0.00
16	Cornell	0.08	0.00	2.88	4.64	0.96	0.64	272	242	132	62	0.00
16	Pennsylvania	0.22	0.22	4.17	3.33	1.50	0.78	193	197	144	71	0.22
18	Northwestern	0.07	0.14	3.07	3.14	0.41	0.66	n.d.	282	144	44	0.00
19	Penn State	0.05	0.05	2.56	7.23	0.41	0.31	163	731	435	37	0.05
20	Texas A&M	0.00	0.06	2.69	6.44	0.78	0.81	657	520	109	21	0.00

<sup>1</sup> From ASEE data

<sup>2</sup> From NSF data

<sup>3</sup> For chemical engineering and materials science

dividing all of the statistics in Table 1 by the number of full-time, tenured/tenure-track faculty (FTF) listed for each department. Table 3 lists these intensive indicators for each department. The data in Table 3 afford an opportunity to determine which departments had the highest values for the different intensive quality and productivity indicators. Table 4 lists the top ten departments (of the twenty considered) in several of the categories.

For each of the five indicators above, at least seven of the ten schools listed are also among the top ten in the *U.S. News* ranking. Illinois is the only top-ten school absent in more than two of the lists above for productivity or quality indicators on a per-FTF basis. CMU, Pennsylvania, Michigan, and UCSB are the only schools ranked in the second ten by *U.S. News* to appear on at least two of the lists above. CMU, Michigan, and UCSB also surfaced as the second-ten departments that most frequently appeared on the top-ten lists in Table 2 for the different extensive productivity or quality indicators. It appears that the chemical engineering graduate programs at CMU, Michigan, Pennsylvania, and UCSB have higher values for their productivity and quality indicators than one might expect based on their *U.S. News* rankings.

The data in Tables 1 and 3 allow identification of the indicators that correlate best with the *U. S. News* ranking. Table 5 presents the results of the correlation analysis in terms of the correlation coefficient (R) for each indicator. This coefficient was calculated as the covariance of the two data sets (the indicator and the ranking) divided by the product of their standard deviations. A negative correlation in Table 5 simply indicates that an increase in that particular quantity was accompanied by an improvement in the ranking.

The quantities in Table 5 with the largest correlations (absolute value) are the annual number of publications, publications per FTF, the number of times cited, the number of NAE members, the number of citations per FTF, and the number of doctorate degrees. This strong correlation between the ranking of a chemical engineering program and its publication output and citation rate was also evident in the results of the 1995 NRC report on graduate program quality. Note that three of the four most strongly correlated quantities are extensive (system-size dependent) variables; that is, they are the absolute numbers of publications, citations, and NAE members. Note too that each of the top four indicators (number of publications, citations, NAE members, and doctorate degrees) correlates better with ranking when considered on an absolute rather than a relative (per FTF) basis.

Table 5 shows that the *U.S. News* rankings do not correlate as strongly with research expenditures as with the other indicators itemized above. The data from the ASEE show the strongest cor-

relation, but keep in mind that this data set is missing entries for three departments. The NSF database included expenditures for all twenty schools, and these data show a poorer correlation with ranking. That there is a modest correlation between total research expenditures and ranking is evident, however, in that eight of the departments in the top ten in expenditures in 2000 (NSF) were in the *U.S. News* top twenty. That the correlation is not strong is evident in that only two of the next ten in total research expenditures were in the *U.S. News* top twenty. The schools with large research expenditures (according to the NSF survey) that were not among the top 20 in the *U.S. News* ranking were NC State (2<sup>nd</sup> in total expenditures), Case Western (10<sup>th</sup>), Auburn (11<sup>th</sup>), Oklahoma (12<sup>th</sup>), Utah (13<sup>th</sup>), Johns Hopkins (14<sup>th</sup>), South Carolina (15<sup>th</sup>), Florida (18<sup>th</sup>), New Mexico Institute of Mining & Technology (19<sup>th</sup>), and New Mexico State (20<sup>th</sup>).

One must keep in mind that the correlation analysis simply shows where correlations exist. It provides no direct information about causative effects. One might be tempted to conclude, for example, that a department that wants to improve its ranking should work hard at getting more NAE members on its faculty. Such an action might succeed, but the logic leading to that conclusion is faulty in that it is not supported by the mere existence of a correlation. It is possible, for example, that the correlation between a department's ranking and the number of NAE members on its faculty exists because it is easier for faculty at a top-ranked department to become NAE members. That is, the high-ranking of the department (or variables causing that high ranking) could be a partial cause of the high number of NAE members, not the result of it.

Finally, it is worth noting that the correlations found herein to exist between ranking and some indicators of productivity and quality for the twenty departments ranked by *U.S. News*

**TABLE 4**  
Top Ten<sup>1</sup> Departments in Different  
Intensive Productivity or Quality Indicators

	<i>Publications</i> <sup>1</sup>	<i>Citations</i> <sup>1</sup>	<i>Pubs w/&gt;50 cites</i> <sup>2</sup>	<i>NAE Members</i>	<i>Doctorate Degrees</i>
1	Wisconsin	UCSB	UCSB	Caltech	Minnesota
2	Stanford	MIT	Michigan	UCSB	MIT
3	Berkeley	Stanford	MIT	MIT	Wisconsin
4	Michigan	Berkeley	Pennsylvania	Pennsylvania	Delaware
5	Texas	Princeton	Stanford	Minnesota	Texas
6	Minnesota	Michigan	Delaware	Princeton	Texas A&M
7	Illinois	Wisconsin	Minnesota	Berkeley	Pennsylvania
8	CMU	Minnesota	Wisconsin	CMU	Berkeley
9	Delaware	Pennsylvania	Princeton	Texas	Illinois
10	Pennsylvania	Texas	Berkeley	Wisconsin	CMU

<sup>1</sup> Of the 20 ranked by *U.S. News*

<sup>2</sup> Excluding Caltech because of lack of data

likely become weaker as one includes more departments in the analysis. Previous analysis<sup>51</sup> showed that the correlation between reputational rankings and objective indicators is much weaker for departments that are not highly ranked.

## CONCLUDING REMARKS

This article provides objective indicators of the productivity and quality for the twenty chemical engineering departments ranked most highly by *U.S. News*. The indicators that correlated most strongly with the rankings were the number of publications, citations, NAE members, and doctorate degrees. For each of these four indicators, the extensive quantity was more strongly correlated with the ranking than was the intensive quantity. This result suggests that departments with more faculty members tend to be more highly ranked than departments with fewer, but equally excellent, faculty members.

**TABLE 5**  
Correlation of *U.S. News* Ranking  
with Different Indicators

Indicator	Correlation Coefficient
Number of Publications <sup>2</sup>	-0.819
Publications per FTF <sup>2</sup>	-0.718
Number of Times Cited <sup>2</sup>	-0.675
NAE Members	-0.602
Citations per FTF <sup>2</sup>	-0.572
Doctorate Degrees	-0.525
Doctorate Degrees per FTF	-0.518
NAE Members per FTF	-0.511
Total Research Expenditures <sup>1</sup>	-0.489
AIChE Institute Awards	-0.402
Federal Research Expenditures <sup>3</sup>	-0.354
Total Research Expenditures per FTF <sup>1</sup>	-0.333
Master Degrees	-0.302
AIChE Institute Awards per FTF	-0.285
Papers with >50 citations <sup>2</sup>	-0.285
Citations per paper <sup>2</sup>	-0.278
Full-Time Tenured/Tenure Track Faculty (FTF)	-0.273
Federal Research Expenditures per FTF <sup>3</sup>	-0.242
Total Research Expenditures <sup>3</sup>	-0.207
Master Degrees per FTF	-0.109
Total Research Expenditures per FTF <sup>3</sup>	-0.077
Bachelor Degrees	0.034
BS Degrees per FTF	0.244

<sup>1</sup> Excluding schools for which no expenditure data were reported, ASEE

<sup>2</sup> Excluding Caltech

<sup>3</sup> NSF report

There have been calls<sup>4,51</sup> for departmental rankings to use objective criteria that indicate excellence rather than relying solely on reputation. Rankings based solely on peer assessment surveys are akin to preseason college football polls that are good at identifying teams that have a history of sustained excellence, but which typically undervalue teams that are on the rise and overvalue teams that are declining. At the end of the season, though, those polled can use statistical data and won/loss records to assess the excellence of the teams. These year-end rankings, whether exclusively from a poll or from a combination of poll results and objective data (*e.g.*, the Bowl-Championship Series, or BCS, formula) provide a reasonable sorting of the different teams by their likely ability to win football games. Likewise, rankings of engineering programs could be improved by including some quantitative measures of objective indicators of productivity or quality. Survey respondents could use these indicators, along with their subjective judgment, to assess different programs (as in a coaches' or writers' poll in college football). Alternatively, these indicators could be used in some formula, along with survey results, to determine rankings (as in the BCS formula). That the ranking systems in college football make better use of objective indicators of excellence than the ranking systems used for chemical engineering graduate programs is revealing.

## ACKNOWLEDGMENTS

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# BUILDING MULTIVARIABLE PROCESS CONTROL INTUITION USING CONTROL STATION®

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Multivariable loop interaction is a well-known control problem that is discussed in a host of popular texts.<sup>[1-4]</sup> Computer tools such as Matlab/Simulink enable instructors and students alike to explore the phenomena by providing a high-level programming environment useful for simulating process control systems. The topics to be covered in a process control course, however, are numerous relative to the time allotted to them in the typical curriculum. Instructors must decide for themselves whether or not time spent with programming issues is time well spent in a process dynamics and control class. Many feel it is an appropriate use of time, and valid arguments can be made to support that viewpoint.

An alternative chosen by more than 150 college and university instructors around the world is the Control Station® training simulator. Control Station lets students design, implement, and test control solutions using a computer interface much like one they will find in industrial practice. It provides hands-on and real-world experience that the students will be able to use on the job. One of the primary benefits according to instructors who use the program is that the software is easy to use, permitting them to focus on teaching process dynamics and control issues rather than on program usage. Many students have related that because Control Station is so visual in its presentation, they believe it enhances their learning and knowledge retention.

Control Station provides a platform where broad and rapid experimentation can help students build fundamental intuition about a broad spectrum of process dynamic and control phenomena. Some of the topics that can be explored using the software include

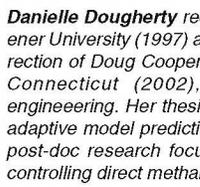
- Dynamic modeling of plant data
- Using process models parameters for controller tuning
- Tuning P-Only, PI, PID, and PID with Filter controllers

- Cascade controller design and implementation
- Feed forward control with feedback trim
- Smith predictor design for dead time compensation
- Parameter scheduling and adaptive control
- Dynamics and control of integrating processes
- Single and multiloop dynamic matrix control (DMC)

This paper will show how students can use Control Station to investigate the nature of multivariable loop interaction and how decouplers can minimize this undesirable behavior. The examples will demonstrate how students can use the software to quickly develop a host of multivariable process be-



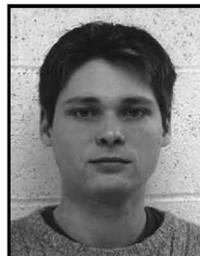
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**Danielle Dougherty** received a BS from Widener University (1997) and a PhD under the direction of Doug Cooper from the University of Connecticut (2002), both in chemical engineering. Her thesis was on multivariable adaptive model predictive control. Her current post-doc research focuses on modeling and controlling direct methanol fuel cell processes.



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haviors for exploration and study, and how they can then test the performance of control strategies using methods found in their text. Students performing this or similar study will certainly strengthen their understanding and intuition about this challenging subject.

## MULTIVARIABLE CASE STUDIES

Multivariable process control is increasingly important for students to understand at an intuitive level because in many industrial applications, when one controller output signal is changed, more than one measured process variable will be affected. Control loops sometimes interact and even fight each other, causing significant multivariable challenges for process control. Control Station provides a means for students to gain a hands-on understanding of multivariable process behavior and to practice how to design and tune controllers that address these behaviors.

One multivariable case study available to students is the multitank process. As shown in Figure 1, the process comprises two sets of freely draining tanks positioned side by side. The two measured process variables are the liquid levels in the lower tanks. To maintain liquid level, two level controllers manipulate the flow rate of liquid entering their respective top tanks. In this process, each of the upper tanks drain into *both* lower tanks. This creates a multivariable interaction because manipulations by one controller affect both measured process variables.

The distillation column case study is shown in Figure 2. This is a binary distillation column that separates benzene and toluene. The objective is to send a high percentage of the benzene out the top distillate stream and a high percentage of

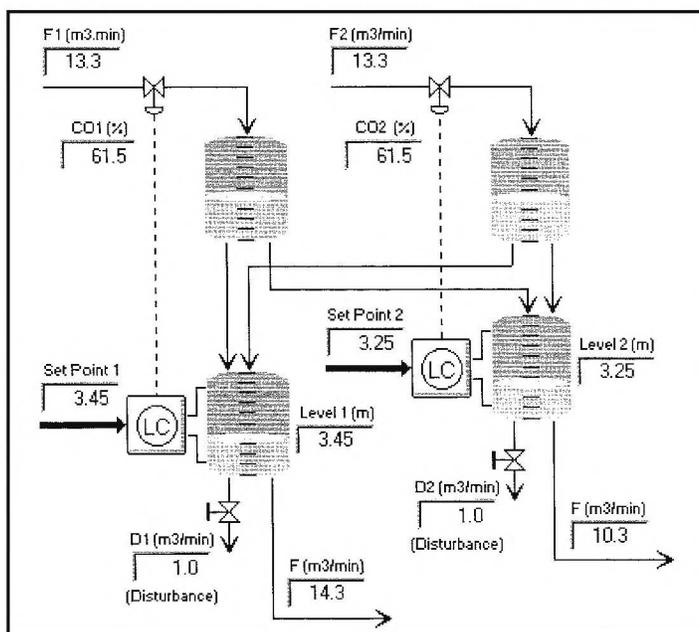


Figure 1. Control Station's multitank case study.

*We do not believe that the training simulator should replace real lab experiences since hands-on studies are fundamental to the learning process, but a training simulator can provide a broad range of meaningful experiences in a safe and efficient fashion.*

the toluene out the bottom stream. To separate benzene from toluene, the top controller manipulates the reflux rate to control the distillate composition. The bottom controller adjusts the rate of steam to the reboiler to control the bottoms composition. Any change in feed rate to the column acts as a disturbance to the process.

Multivariable loop interaction occurs in this process because when the benzene composition in the top distillate stream is below the set point, the top controller responds by increasing the cold reflux into the column. This cold liquid eventually spills to the bottom, cooling it and causing the bottom composition to move off the set point. The bottom controller "fights back" by increasing the flow of steam into the reboiler. The result is an increase of hot vapors traveling up the column that counteract the increased reflux by heating the top of the column.

## MULTIVARIABLE CUSTOM PROCESSES

Control Station's multiloop *Custom Process* graphic, used to simulate general multivariable systems created from dynamic models, is shown in Figure 3. Following the nomenclature established in popular texts,<sup>[1-4]</sup>  $G_{ij}$  represents the dy-

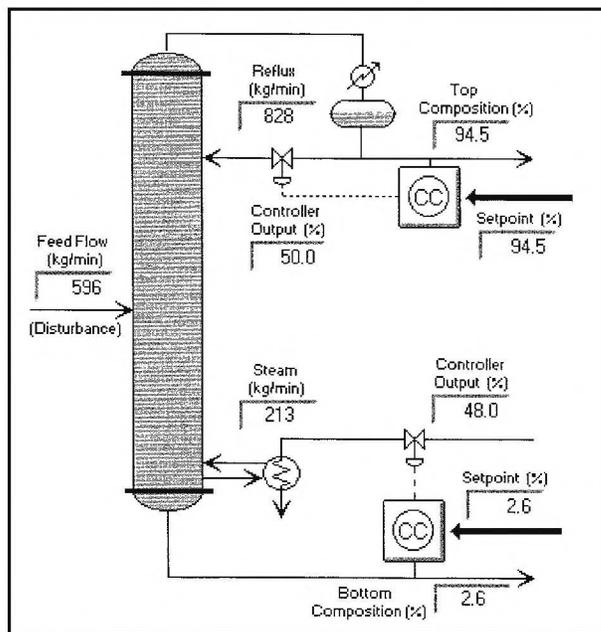


Figure 2. Control Station's distillation column case study.

dynamic behavior of the  $i^{\text{th}}$  measured process variable response to the  $j^{\text{th}}$  controller output signal. Hence, as can be seen in Figure 3, process  $G_{11}$  describes the direct dynamic response of measured process variable  $PV_1$  to changes in controller output  $CO_1$ , and interaction  $G_{21}$  describes the cross-loop dynamic response of  $PV_2$  to changes in  $CO_1$ .

## RELATIVE GAIN AS A MEASURE OF LOOP INTERACTION

Before exploring different multivariable process behaviors, we introduce the concept of *relative gain*.<sup>[5]</sup> Relative gain,  $\lambda$ , is popular because it

- Provides a convenient measure of loop interaction
- Is easy to compute
- Is dimensionless, so it is not affected by the units of the process data

Relative gain is computed from the steady-state process gains of the process models ( $K_{11}$  and  $K_{22}$ ) and the cross-loop interaction models ( $K_{12}$  and  $K_{21}$ ) that best describe observed process behavior (that results from model fits of process data). Following the nomenclature above, relative gain is computed as

$$\lambda = \frac{K_{11}K_{22}}{K_{11}K_{22} - K_{12}K_{21}} \quad (1)$$

In the remainder of this paper, we will show how Control Station helps students explore what the size and sign of  $\lambda$  implies for multivariable loop interaction and the ease with which a process can be controlled. Before starting that study, consider that our process has two controllers ( $CO_1$  and  $CO_2$ ) that regulate two process variables ( $PV_1$  and  $PV_2$ ). The controllers are connected to the process variables by wires and the connections can be wired one of two ways:

- 1)  $CO_1$  controls  $PV_1$  and  $CO_2$  controls  $PV_2$
- 2)  $CO_1$  controls  $PV_2$  and  $CO_2$  controls  $PV_1$

Each combination yields a different value of  $\lambda$ . An important lesson students learn is that *control loops should always be paired (wired) so the relative gain is positive and as close as possible to one*.

## EFFECT OF $K_p$ ON CONTROL LOOP INTERACTION

The students are taught the usefulness of relative gain as a measure of multivariable loop interaction by considering a variety of cases such as those listed in Table 1. These particular cases are simulated and studied here using Control Station's *Custom Process module*, as shown in Figure 3.

All of the direct process and interaction models used in the simulation studies are first order plus dead time (FOPDT). For each simulation case study, the direct process and cross-loop gains are listed in the table. All of the time constant and dead time parameters for the simulation case studies given in Table 1 are

Process time constant:  $\tau_p = 10$

Dead time:  $\theta_p = 1$

Also, all of the investigations use two PI (proportional-integral) controllers with no decoupling and with

Controller gain:  $K_c = 5$

Reset time:  $\tau_i = 10$

For all examples, when one PI controller is put in automatic while the other is in manual mode, that controller tracks set point changes with an appropriately small rise time and rapid damping. The issue the students study is process behavior when *both* PI controllers are put in automatic at

**TABLE 1**  
Exploring Relative Gain,  $\lambda$ , as a Measure of Loop Interaction

Case	direct $CO_1 \rightarrow PV_1$	cross-loop $CO_1 \rightarrow PV_2$	cross-loop $CO_2 \rightarrow PV_1$	direct $CO_2 \rightarrow PV_2$	$\lambda$
	$K_{11}$	$K_{21}$	$K_{12}$	$K_{22}$	
1	1	1.1	1.1	1	-4.8
2a	0	1.1	0.5	1	0.0
2b	-1	3.0	1.1	1	0.2
2c	1	-3.0	0.5	1	0.4
3	1	-1.1	0.5	1	0.6
4	1	0	0.5	1	1.0
5	1	1.1	0.5	1	2.2
6	1	1.1	.85	1	15.4

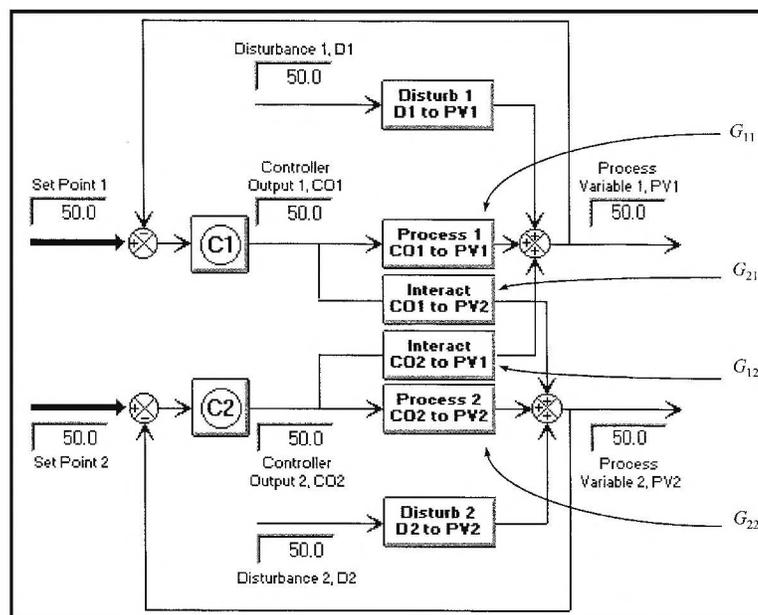


Figure 3. Control Station's multiloop custom process.

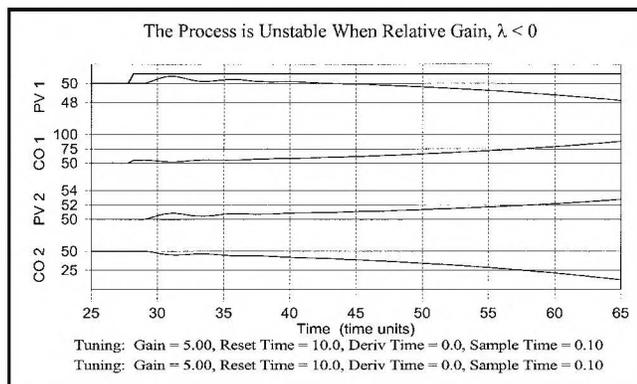
the same time.

► **Case 1:  $\lambda < 0$**  When the cross-loop interaction gains are larger than the direct process gain, as is true for Case 1 in Table 1, then each controller has more influence on its cross-loop measured process variable than it does on its own direct measured process variable. As listed in the table, the relative gain,  $\lambda$ , computed by Eq. (1) for this case is negative.

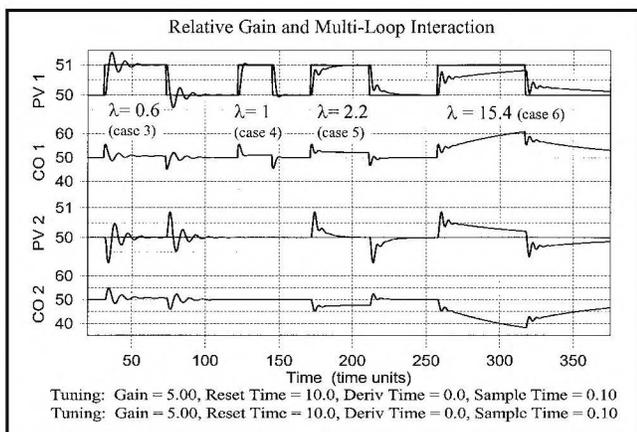
Figure 4 shows the set point tracking performance of the Case 1 process when both loops are under PI control with no decoupling (remember that for all simulations,  $\tau_p = 10$  and  $\theta_p = 1$ ; also,  $K_c = 5$  and  $\tau_I = 10$ ). As each controller works to keep its direct measured process variable on its set point, every control action causes an even larger disruption in the cross-loop process variable—and the harder each controller works, the worse the situation becomes. As can be seen in Figure 4, the result is an unstable, diverging system.

A negative relative gain implies that the loop pairing is incorrect. That is, each controller is wired to the wrong measured process variable. The best course of action is to switch the controller wiring. This switches the cross-loop gains in Table 1 to the direct process gains and vice versa.

Switching the loop pairing recasts Case 1 into a process



**Figure 4.** Incorrect loop pairing and an unstable process under PI control indicated by  $\lambda = 0$ .



**Figure 5.** Impact of  $\lambda$  on PI control loop interaction with no decoupling.

with a relative gain of  $\lambda = 5.8$ , which is a loop interaction behavior between Case 5 and Case 6. As we will learn, a process with this relative gain is challenging to control, but it is closed-loop stable and the loops can be decoupled using standard methods.

► **Case 2:  $0 < \lambda \leq 0.5$**  For the relative gain to be exactly zero ( $\lambda = 0$ ), one of the direct process gains must be zero. A direct process gain of zero means that a controller has no impact on the measured process variable it is wired to. Clearly, there can be no regulation if a controller has no influence.

Case 2a in Table 1 has  $K_{11} = 0$ , implying that  $CO_1$  has no influence on  $PV_1$ . Yet because the cross-loop gain  $K_{12}$  is not zero, changes in  $CO_2$  will disrupt  $PV_1$ . If a measured process variable can be disrupted but there is no means to control it, the result is an unstable process under PI control (no figure shown). Because both cross-loop gains are not zero in Case 2a, the loop pairing should be switched in this case to give each controller direct influence over a measured process variable. This would recast Case 2a into a process with a  $\lambda = 1.0$ , which is the interaction measure most desired. We study such a process in Case 4 below.

When the relative gain is near zero ( $0 < \lambda \leq 0.5$ ), then at least one of the cross-loop gains is large on an absolute basis (e.g., Case 2b and 2c). Under PI control with no decoupling and using the base tuning values of  $K_c = 5$  and  $\tau_I = 10$ , both of these processes are unstable and show considerable loop interaction (no figure shown). Detuning both controllers to  $K_c = 2$  and  $\tau_I = 10$  restores stability, but control-loop interaction is still significant.

Again, the best course of action is to switch the loop pairing. With the wiring switched, Case 2b yields  $\lambda = 0.8$  and Case 2c yields  $\lambda = 0.6$ , putting both relative gains closer to the desired value of one. While both processes still display loop interaction, the processes become stable under PI control with no decoupling, even with the base case PI controller tuning values.

► **Case 3:  $0.5 \leq \lambda < 1$**  When the relative gain is between 0.5 and one, the cross-loop interactions cause each control action to be reflected and amplified in both process variables. As shown in the left-most set point steps in Figure 5 for a case where  $\lambda = 0.6$ , this interaction leads to a measured process variable response that includes significant overshoot and slowly damping oscillations.

This amplifying interaction exists when stepping the set point of either loop. It grows more extreme and ultimately leads to an unstable process as  $\lambda$  approaches zero (see Case 2). Moreover, the interaction becomes less pronounced as  $\lambda$  approaches one (see Case 4).

► **Case 4:  $\lambda = 1$**  A relative gain of one occurs when either or both of the cross-loop gains are zero. In Case 4,  $K_{21}$  is zero, so controller output  $CO_1$  has no impact on the cross-loop measured process variable  $PV_2$ . Since  $K_{12}$  is not zero as

listed in Table 1, however, changes in  $\text{CO}_2$  will impact  $\text{PV}_1$ .

The second set point steps in Figure 5 show the control performance of the Case 4 process when the set point of  $\text{PV}_1$  is changed. As expected, the set point tracking actions of  $\text{CO}_1$  have no impact on  $\text{PV}_2$ . While not shown, a set point step in  $\text{PV}_2$  would cause some cross-loop disruption in  $\text{PV}_1$  because of loop interaction.

When both cross-loop gains are zero, the loops do not interact. Such a system is naturally and completely decoupled and the controllers should be designed and tuned as single-loop processes.

► **Case 5:**  $\lambda > 1$  Opposite to the observations of Case 3, when the relative gain is greater than one, the control loops fight each other. Specifically, the cross-loop interactions act to restrain movement in the measured process variables, prolonging the set-point response. The third set point steps in Figure 5 illustrate this behavior for a case where  $\lambda = 2.2$ .

As stated earlier, a process with a relative gain that is positive and close to one displays the smallest loop interactions (is better behaved). For Case 5, switching the loop pairing would yield a very undesirable negative  $\lambda$ . This means that the loops are correctly paired and the significant loop interaction is unavoidable.

► **Case 6:**  $\lambda \gg 1$  As the cross-loop gain product,  $K_{12}K_{21}$ , approaches the direct process gain product,  $K_{11}K_{22}$ , the relative gain grows and the restraining effect on movement in the measured process variables discussed in Case 5 become greater. This is illustrated in the right-most set point steps in Figure 5 for a case where  $\lambda = 15.4$ . Again, switching the loop pairing would yield a negative  $\lambda$ , so the loops are correctly paired and the significant loop interaction is unavoidable. Interestingly, as the cross-loop gains grow to the point that their product is larger than the direct process gain product (when  $K_{12}K_{21} > K_{11}K_{22}$ ), then  $\lambda$  becomes negative and we circle back to Case 1.

## DECOUPLING CROSS-LOOP $K_p$ INTERACTION

After gaining an appreciation for the range of open-loop dynamic behaviors, students then explore decoupling control strategies. A decoupler is a feed-forward element where the measured disturbance is the action of a cross-loop controller. Analogous to a feed-forward controller, a decoupler is comprised of a process model and a cross-loop disturbance model. The cross-loop disturbance model receives the cross-loop controller signal and predicts an “impact profile,” or when and by how much the process variable will be impacted. Given this predicted sequence of disruption, the process model then back calculates a series of control actions that will counteract the cross-loop disturbance as it arrives so the measured process variable, in theory, remains constant at set point.

Here we explore how *perfect decouplers* can reduce cross-loop interaction. A perfect decoupler employs the identical

models in the decoupler as is used for the process simulation. Using the terminology from Figure 3, these decouplers are defined in the Laplace domain as

$$D_{12}(s) = -\frac{G_{12}(s)}{G_{11}(s)} \quad \text{and} \quad D_{21}(s) = -\frac{G_{21}(s)}{G_{22}(s)} \quad (2)$$

Students are reminded to be aware that in real-world applications, no decoupler model exactly represents the true process behavior. Hence, the decoupling capabilities shown here must be considered as the best possible performance.

► **Case 1:**  $\lambda < 0$  A negative relative gain implies that the loop pairing is incorrect. Decoupling is not explored because the best course of action is to switch the controller wiring to produce a process with a relative gain of  $\lambda = 5.8$ . This loop interaction behavior is somewhere between Case 5 and Case 6 discussed below.

► **Case 2:**  $0 < \lambda \leq 0.5$  A relative gain of *exactly zero* ( $\lambda = 0$ ) implies that at least one controller has no impact on the measured process variable that it is wired to. There can be no regulation if a controller has no influence. Hence, decoupling becomes meaningless for this case and is not explored here.

When the relative gain is *near zero* ( $0 < \lambda \leq 0.5$ ), PI controllers with no decoupling must be detuned to stabilize the multivariable system. When the PI controllers are detuned and perfect decouplers (the identical models are used in the decouplers as are used for the process simulation) are included, the result is an unstable system (no figure shown). Detuning the decouplers (lowering the disturbance model gain) will restore stability, but interaction remains significant and general performance is poor. Again, the best course of action is to switch loop pairing.

► **Case 3:**  $0.5 \leq \lambda < 1$  When the relative gain is between

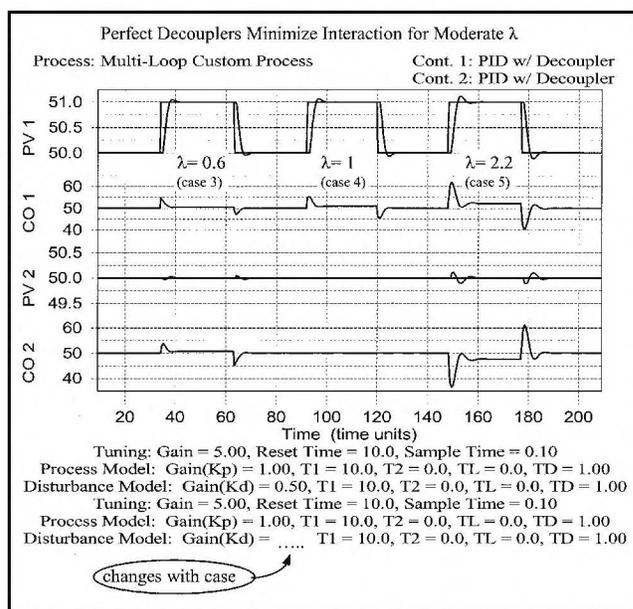


Figure 6. Decouplers work well when  $\lambda$  is near 1.

0.5 and one, the cross-loop interactions cause each control action to be reflected and amplified in both process variables. As shown in the left-most set-point steps in Figure 6 for the case of  $\lambda = 0.6$ , PI controllers with perfect decouplers virtually eliminate cross-loop interactions. This is not surprising since the relative gain is positive and close to one.

► **Case 4:**  $\lambda = 1$  A relative gain of one occurs when either or both of the cross-loop gains are zero. In Case 4 of Table 1,  $K_{21}$  is zero, so controller output  $CO_1$  has no impact on the cross-loop measured process variable  $PV_2$ . Consequently, a perfect decoupler will provide no benefit for this loop, and as shown in Figure 6 for the middle set-point steps, while a perfect decoupler causes no harm, a decoupler implemented on a real process will likely have imperfect models and would then create loop interaction.

Table 1 shows that  $K_{12}$  is not zero, so changes in  $CO_2$  will impact  $PV_1$ . A perfect decoupler will virtually eliminate cross-loop interaction for information flow in this direction (no figure shown). Thus, the Case 4 system can address the multi-variable loop interaction with a single decoupler on the  $CO_2$  to  $PV_1$  loop.

► **Case 5:**  $\lambda > 1$  When the relative gain is greater than one, the cross-loop interactions act to restrain movement in the measured process variables. The third set point steps in Figure 6 for the case where  $\lambda = 2.2$  illustrate that perfect decouplers substantially eliminate both this restraining effect and the level of loop interaction. Again, this is not surprising since the relative gain is positive and reasonably close to one.

► **Case 6:**  $\lambda \gg 1$  As the relative gain grows larger, the restraining effect on movement in the measured process vari-

ables due to loop interaction becomes greater. Case 6 in Table 1 is interesting because  $K_{21}$  is greater than  $K_{22}$ . This means that  $PV_2$  is influenced more by a change in controller output  $CO_1$  (its cross-loop disturbance) than it is by an equal change in its own controller output  $CO_2$ . Switching loop pairing offers no benefit as this makes the relative gain negative.

With perfect decouplers as shown in the *right* set-point steps in Figure 7 (the decoupler employs the identical models as are used for the process simulation), the system is unstable. This cannot be addressed by detuning the PI controller because even with lower values for controller gain,  $K_c$ , the system is unstable.

For a decoupler to be stable, the gain of the cross-loop disturbance model must be less than or equal to the gain of the process model, or in this case,  $K_{21} \leq K_{22}$ . That is, a decoupler must pass through at least as much influence of a controller output to its direct process variable as it does for any disturbance variable.

To address this, we detune the decoupler by lowering the cross-loop disturbance gain of the bottom loop so that in absolute value,  $K_{21} \leq K_{22}$  and  $K_{21} \leq K_{11}$ . Repeating the test in the *left* set-point steps of Figure 7 reveals a stable and reasonably decoupled system.

## CONCLUSION

We have presented examples of the lessons and challenges associated with multivariable process control and shown how Control Station can provide a better understanding of these complicated systems. Space prohibits the presentation of other multivariable studies available in Control Station, including the use of dynamic matrix control for multivariable model predictive control.

We do not believe that the training simulator should replace real lab experiences since hands-on studies are fundamental to the learning process, but a training simulator can provide a broad range of meaningful experiences in a safe and efficient fashion. The training simulator can be used to bridge the gap between process control theory and practice. If readers would like to learn more, they are encouraged to contact Doug Cooper at cooper@engr.uconn.edu, or visit <www.engr.uconn.edu/control>.

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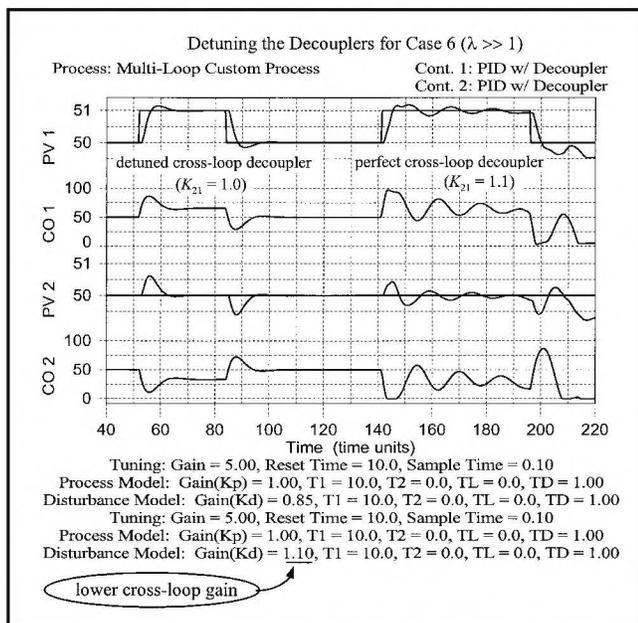


Figure 7. Decouplers can cause stability problems for large  $\lambda$ .

# Random Thoughts . . .

## FAQS. VI

### *Evaluating Teaching and Converting the Masses*

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**F**our years ago we raised ten questions that frequently come up in our teaching workshops,<sup>[1]</sup> and since then we have devoted five columns to answering eight of them.\* In this column we take up the last two:

1. My department head says that we can't count teaching in promotion and tenure decisions because there is no good way to evaluate it. *Is there a meaningful way to evaluate teaching?*
2. Most people who go to teaching workshops are already good teachers—the ones who most need them wouldn't go to one under any circumstances. *How can staunchly traditional professors be persuaded to use proven but nontraditional teaching methods?*

#### Evaluating Teaching

We have written several columns about evaluating teaching and so will simply provide a synopsis with references here.

The key to meaningful evaluation is *triangulation*—getting data from several different sources. Student ratings obviously should be included: students are the best judges of (among other things) whether instructors are effective lecturers, encourage active participation, are available and supportive outside class, and treat all of their students with respect. Extensive research attests to the validity of student ratings<sup>[2]</sup> and several things can be done to maximize their effectiveness at both evaluating and improving teaching.<sup>[3]</sup>

\* All of the FAQ columns can be viewed on-line at [http://www.ncsu.edu/effective\\_teaching/Columns.html](http://www.ncsu.edu/effective_teaching/Columns.html).

While necessary, however, student ratings are not sufficient. Most students are not equipped to judge certain aspects of teaching, such as the depth of an instructor's knowledge of the subject, the appropriateness of the course content and its compatibility with the department's curricular objectives, and the fairness of assignments and tests. Only other faculty members are in a position to make those judgments. *Peer review* is therefore another important component of teaching evaluation.

A proven approach to peer review (as opposed to the traditional unreliable one-shot classroom observation) calls for two raters to observe at least two class sessions, complete rating checklists for both sessions and other checklists for evaluating course materials, assignments, and tests, and reconcile their ratings.<sup>[4]</sup> Research-supported checklist items can be selected from lists provided by Weimer, *et al.*<sup>[5]</sup>

Additional evidence of teaching effectiveness can be obtained from retrospective senior evaluations and alumni evaluations, student performance on common examinations, and instructor self-evaluations. Student ratings taken over several quarters or semesters may be combined with peer ratings and outcomes of some of these other assessments into a

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teaching portfolio,<sup>[6]</sup> which provides the basis for an exceptionally meaningful evaluation of teaching.

### **Converting the Masses**

At almost every workshop we give, we are informed that we are preaching to the choir, and the faculty who most need to change wouldn't go to a teaching workshop at gunpoint. Some of our informants then ask how such individuals can ever be persuaded to change to more effective teaching methods.

We offer several notes of encouragement in response.

*In part due to programs such as the National Effective Teaching Institute<sup>[7]</sup> and local campus faculty development efforts, the number of faculty members using proven but (in engineering) nontraditional teaching methods has risen dramatically in the past decade, and the number is almost certain to keep rising.*

In a 1999 survey of engineering faculty members in the eight institutions that comprised the SUCCEED Coalition, 65% of the 511 respondents reported writing instructional objectives for their classes, 60% assigned small-group exercises, and 54% gave team assignments. Demographic data established that the respondents were truly representative of the entire 1621-person faculty and not disproportionately "true believers."<sup>[8]</sup> The survey results support our own observations. In the workshops we have given for over a decade, when we describe active learning (getting students to do things in class other than watch and listen to the instructor) we usually ask for a show of hands of the participants who regularly use this approach in their classes. Ten years ago, two or three hands would typically go up; now, one-third to one-half of them do.

ABET and the new accreditation criteria have been and will continue to be a driving force for the continuation of this trend. If we are to produce engineering graduates with mastery of such skills as communication and multidisciplinary teamwork, we must clearly do something in the preceding four years to equip them with those skills. Equally clearly, lecturing alone won't do it, but instructional methods such as active, cooperative, and problem-based learning when done correctly can promote development of all of the skills in ABET Outcomes 3a-3k.<sup>[9]</sup> Engineering instructors who are currently

the only ones in their departments using those methods are unlikely to be alone much longer.

*It is not necessary to convert the masses.*

It's certainly true that some instructors will never attend teaching workshops or use any of the methods promoted in them, but it's also not worth losing sleep over. Students can still learn in classes taught by skilled lecturers who do nothing else, and even if an instructor does not use cooperative learning, many or most students figure out the benefits of group work for themselves and form study groups on their own. As long as some instructors provide an optimal classroom environment—one that weans the students away from their dependence on professors and teaches them to rely on themselves and their peers as the primary sources of learning—the skills they acquire will carry over to their less expertly taught courses and later to their careers.<sup>[10,11]</sup>

In short, there is no need for all of your colleagues to see the light. If you simply do the best job of teaching you know how to do and share what you know with any colleagues inclined to hear it, you can relax—the students will be just fine.

***If you simply do the best job of teaching you know how to do and share what you know with any colleagues inclined to hear it, you can relax—the students will be just fine.***

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

# A SOLIDS PRODUCT ENGINEERING DESIGN PROJECT

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The design project forms an integral part of an undergraduate degree in chemical engineering accredited by the Institution of Chemical Engineers<sup>[1]</sup> and the Institute of Energy. It is a four-year program in which a major design project contributes one-quarter of the credits in the third year. Usually, different projects (supervised by an academic staff member) are assigned to groups of 3 to 6 students. The groups have a period of one year to work through a typical process industry problem. For assessment purposes, the students make a verbal and visual presentation to staff and peers in the first semester and prepare a joint poster and a detailed individual design dissertation in the second.

The project provides a necessary understanding of process design of unit operations such as separators, distillation columns, heat exchangers, and other process components as well as bringing together other elements of the degree course, such as thermodynamics, transport phenomena, and process safety. In addition to supplementing the technical skills learned in lectures, the project develops transferable skills such as communication, organization, and team-working.

Traditionally, the design project has been geared toward designing a theoretical process for manufacture of a commodity chemical that dominated the chemical industry during the twentieth century, such as cumene or ethanol. It is relatively unusual for projects to involve much solid processing, despite its importance in industry.<sup>[2-4]</sup> This is in part because of the intrinsic difficulty and in part because data and design procedures are less readily available. In addition, student projects normally use purity as the main or sole measure of the product's quality. For many solid products, however, the particle size distribution, flowability, and functionality in use may be equally or more important.

In the past, chemical engineers have designed processes

but have largely left product specification to others. In recent years, however, it has been suggested that they should be actively involved in product design, particularly for solids.<sup>[5,6]</sup> Courses and theoretical projects on product design now exist in some European and North American universities,<sup>[7]</sup> and there is now an undergraduate textbook.<sup>[8]</sup>

This project was restricted to MEng students. They are first-degree students who have achieved a higher minimum standard (55% instead of 40%) in earlier courses and who complete an additional year of study compared with BEng students. The project was offered to allow such capable and well-motivated students to actively engage in the design process for a real industrial product. Before starting the project, they had completed two years of laboratories and a mini-project. In the current scheme, students study particle science in the second year and particle processes in the third year.

A number of universities include experimental work as part of the MEng degree scheme, but they are generally research

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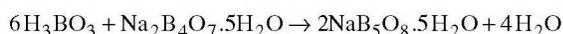
projects (albeit of an applied and often interesting nature). The project described here is unusual in that it uses laboratory measurements as part of a design exercise and uses real industrial materials.

## BACKGROUND

Boron is one of seven essential micronutrients required for normal growth and fruiting of most agricultural crops. Soil testing and plant tissue analyses have detected that of the essential micronutrients, boron is usually the most deficient in crops. Therefore, annual applications of boron are required for high yields and improved quality and to offset losses from crop removal and leaching. Plants, depending on soil type, management level, and method of application, require only small quantities of boron—around 0.2 to 4 kg per hectare per year.<sup>[9]</sup> Also, since borates are toxic to wood-boring insects but beneficial for plant growth, they are used as a wood preservative.

Boron is conventionally supplied in the form of granular borate compositions. In applications that require spraying, such as in agriculture, aqueous borate suspensions are prepared by heating, dissolving, and rapid cooling of the granules, incurring practical difficulties and additional costs. These suspensions are not self-structured and thus require the addition of a thickening agent to maintain the stability of the suspension.

Borax, a global supplier of borates, now has a patented self-structured aqueous borate suspension<sup>[10]</sup> that does not require a thickening agent to suspend the particles. Sodium pentaborate pentahydrate ( $\text{NaB}_5\text{O}_8 \cdot 5\text{H}_2\text{O}$ ) is formed by reacting boric acid ( $\text{H}_3\text{BO}_3$ ) with borax pentahydrate ( $\text{Na}_2\text{B}_4\text{O}_7 \cdot 5\text{H}_2\text{O}$ ) in the presence of water.



The product conveniently referred to as “borate cream” is sodium pentaborate pentahydrate and is, as yet, the only stable aqueous borate suspension found. As a consequence there is limited knowledge of the intermediate steps involved in its production. The suspension has a high solid content of 46 wt% and a 10% boron content. The reason the suspension is self-structured is believed to be caused by the weak attraction of the particles by van der Waals forces.

The self-structured suspension has many advantages over the previously prepared borate suspensions. Not only is the suspension physically stable, but it is also pourable (unlike the stiff compositions previously produced). The suspension can then be readily diluted in water for application, providing greater convenience for the consumers.

The demand for the “borate cream” in plant nutrition and wood preservation is expected to increase in the future. Other applications for the cream could also be discovered due to the diverse properties it exhibits.

To date, the cream has been entirely produced in a batch

process. Thus, Borax is collaborating with the University of Sheffield to establish the feasibility of increasing production by implementing a continuous process.

## PROJECT WORK

A group of four third-year chemical engineering students were given the task of meeting the project objective. The group first arranged a meeting with a Borax representative to discuss the requirements of the plant design and to obtain a more complete description of the current process. The company recommended features of the plant layout, sizing of equipment, and a production of 50,000 tonnes per year of 10% boron content cream. Product stability was critical, so it was necessary to investigate additives to prevent syneresis (separation) of the cream.

From this data, a preliminary overview of the process was devised. The process could be divided into four sections: silos, premixing and storage, solid conveying, and reactors.

In order to design and select the appropriate equipment for the handling and storage of these components, essential data on the nature of the bulk solids and water would have to be determined. The physical and chemical properties of water could be readily obtained from published data, but due to the originality of the process, relevant design data for the solid additives (such as specific densities and particle sizes) were less readily available. Therefore, these parameters were measured experimentally by the students to give the properties directly for the conditions that would be encountered in the design. In addition, the cream was produced by using the current batch procedure to give the students further insight into the process. This data could then be used to design the individual components of the continuous production plant.

Finally, a collective consideration of the design, economics, and safety and environmental aspects of the final proposed design was performed. The following paragraphs describe the work of the students in terms of both experimental and design work.

## EXPERIMENTAL WORK

The experimental work consisted of three major constituents: measuring the physical properties of the reactants and products, determining the formation characteristics, and measuring the viscosity of the final cream.

***Properties of the Reactants*** • The physical properties of the components that are vital in the design of the mixers, storage silos, and transportation system are the angle of repose, the bulk density, and the particle size, shape, density, and porosity.

The repose angle is required in the design of the storage silos and belt conveyors. It is the angle the particles make with a flat surface when a quantity of solid is allowed to form a heap. A standardized test procedure was used to give the

“poured” angle of repose for a given bulk solid.

In powder-handling systems, particle size is a key parameter in design calculations. There are a variety of particle-size-measurement techniques available in the department, but due to the smaller particles present in the powder distributions, the preferred measurement techniques were the laser-diffraction technique (LDT) and sieving. The general operating principle of LDT is that the angle of diffraction of a beam of light passing through the particles depends on the wavelength of the light and the size of the particles. We used the apparatus located in the department to give the particle size for powders within the measurement range of 4.5 to 875  $\mu\text{m}$ , with sieving used for all other circumstances. The frequency distribution obtained for additive “A” is shown in Figure 1.

The shape of particles can have a significant bearing on the packing and flow behavior of the bulk solid. Samples of boric acid and borax pentahydrate were analyzed underneath a low-powered microscope with suitable photographic attachments to determine the particle shapes. Micrographs of boric acid and borax pentahydrate are given in Figure 2.

It was evident from the micrographs that the particles were non-spherical and that some were even agglomerates. Hence, since nonspherical particles can affect the flow behavior and equipment wear, the particle’s shape was taken into account in the silo and conveying design.

Also, the particle density, bulk density, and porosity of the powders were measured using standard tests. All the measurements performed on the four bulk solids are summarized in Table 1.

**Formation of the ‘cream’** • The quality of the cream generated is highly dependent on three conditions of formation: agitation rate, concentration of solid com-

ponents, and temperature of operation.

The cream was produced under batch conditions in the laboratory to determine the optimum conditions to produce it in a continuous process, taking into account production, economic, and safety factors.

Initially, the cream was produced without any anti-settling agents,

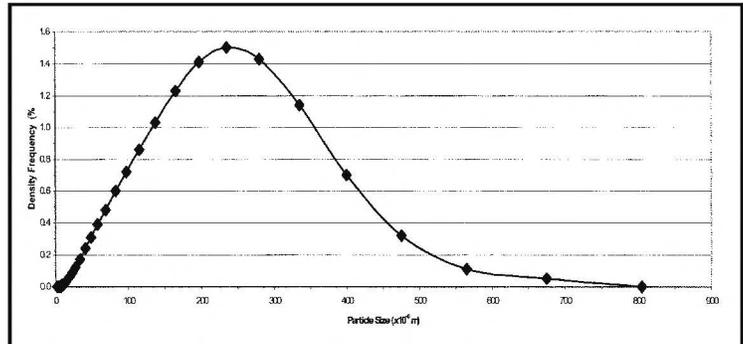


Figure 1. Frequency particle size distribution for additive ‘A’.

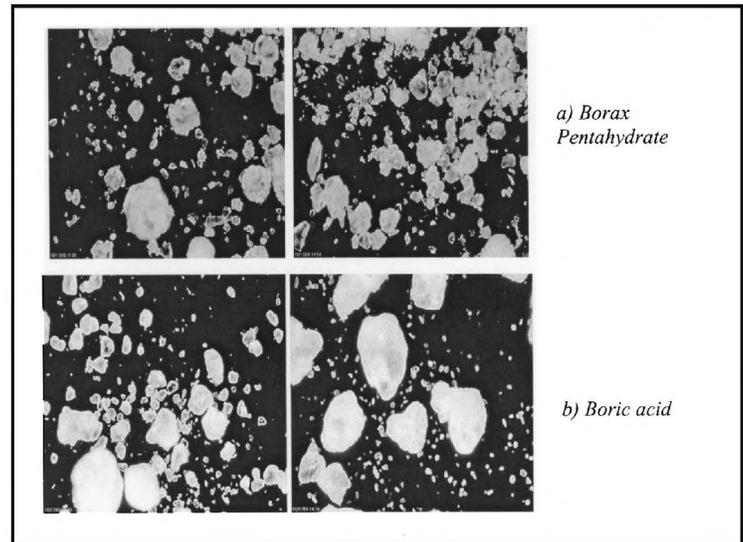


Figure 2. Micrographs of reagents: a) borax pentahydrate b) boric acid.

Property		Boric acid	Borax pentahydrate	Additive ‘B’	Additive ‘A’
Angle of Repose		34.5°	36.5°	32.0°	51.0°
Particle Size Parameters ( $\mu\text{m}$ )	$x_{16}$	142.80	190	2.70	77.2
	$x_{50}$	255.75	450	8.65	182.5
	$x_{84}$	444.70	860	32.50	316.8
	$\sigma$	1.76	2.13	3.49	2.03
Elongation		1.25	1.20	-	-
Bulk Density ( $\text{kg}/\text{m}^3$ )		950	1060	-	-
Particle Density ( $\text{kg}/\text{m}^3$ )		1520	2420	720	1760
Porosity		0.375	0.562	-	-

Table 1. Summary of physical measurements of the bulk solids.

but syneresis occurred when the suspension was allowed to stand for long periods, resulting in two distinct layers: an aqueous and a solid phase. Although mixing could readily restore homogeneity, this would greatly affect large-scale production. We found that adding two anti-settling agents to the water prior to adding the reagents minimized separation. Hence, later cream productions involved an additional premixing stage to hydrate the anti-settling agents prior to adding the reagents.

Understanding the mechanism of the cream formation is essential since it can allow possible improvements to the manufacturing process and could lead to the production of other borate suspensions. Therefore, samples taken at various intervals during the production of the cream were analyzed (in relation to temperature and pH readings) to determine the stages of production. It is known that mechanism of the formation of crystals involves two major phases: dissolution and nucleation.

A general temperature trend during the reaction phase was a U-shaped curve, as shown in Figure 3. Upon addition of the reactants, the temperature dropped sharply, resulting in a minimum temperature after approximately 20 minutes. We found that this period corresponded to the dissolution of the solid reagents in water via an endothermic process.

The temperature increased steadily between 20 and 60 minutes of reacting, but remained below the temperature before the addition of the reactants. This

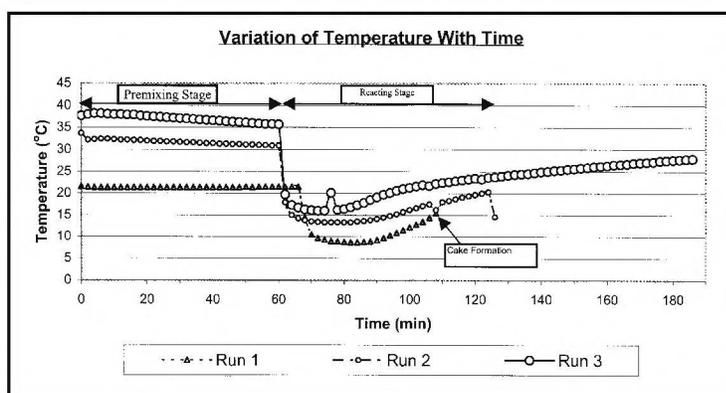


Figure 3. Temperature profile during cream production at varying initial temperatures.

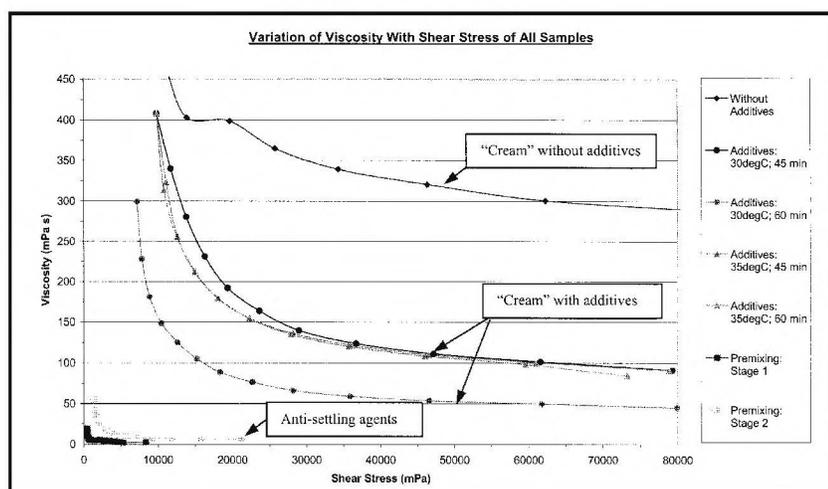


Figure 4. Variation of viscosity with shear stress for the cream produced with and without additives and the anti-settling agents.

temperature rise was found to be due to the commencement of nucleation, which is an exothermic process.

The experimental data allowed us to determine the effect of conditions on dissolution and nucleation (and hence the product quality) and were used to design the reactor stage under the optimum conditions for the desired product quality.

**Viscosity Measurements** • The viscosity is a fundamental fluid property that is necessary to predict the manner in which a fluid will react to applied forces such as pumping. Since the cream is non-Newtonian and exhibits complex flow behavior such as separation, the viscosity had to be determined experimentally for the conditions that would be encountered.

We measured the viscosities of the samples in a Rheomat 115 rotational viscometer located in the department. Its coaxial measuring system operates according to the Searle principle. The control instrument enables the rotational speed to be varied and the torque readout to be recorded. The shear rate and shear stress are determined from the rotational speed of the bob and the braking torque indication, respectively, allowing the rheogram to be plotted.

The viscosity of the cream should be as low as possible to allow ease of handling and to allow the cream to be dispersed in water during application. The variation of viscosity with shear stress for the cream produced with and without the additives and the anti-settling agents is shown in Figure 4. The experimental data suggest that for the cream produced with the anti-settling agents, high mixing time during the reaction stage and high temperature tend to give lower viscosity. The conclusions from this investigation were again incorporated into the process design.

## DESIGN WORK

Design of the proposed process was divided into two main sections: design of the individual components of the process and overall process design.

**Component Design** • The proposed process was divided into four distinct phases: containment of solids, solid conveying, premixing, and reaction. A flow diagram of the proposed continuous plant is given in Figure 5 (next page). The process features a storage silo for each of

the solid components. The two solid reagents have storage and feed silos to contain the large quantities of materials required. The silo design included material properties determined from shear testing using a Jenike shear cell.<sup>[11]</sup>

Pneumatic conveyors transport the material from storage to the feed silos, with cyclones positioned adjacent to the feed silos to separate the particles from the air stream. The solid conveying design included evaluation of the required air flow rate to give steady operation, design of a cyclone separator, and specification of a suitable air mover and rotary valve to discharge the cyclone and act as an air lock. As there are many system specifications that could be used, evaluation of the best design was performed. All the solid components are gravity fed from the feed silos to the first CSTR.

Since the two anti-settling agents comprise only a small part of the final cream, they are only stored in feed silos that are refilled manually. The anti-settling agents are hydrated in two batch premixers working alternately. The components need hydrating for a specific time of 1 hour, so the process has to be performed in batches. A continuous feed to the reactors is obtained by allowing the premixers to work alternately.

The reaction occurs in four reactors in a series arrangement. By increasing the number of reactors in operation, the process shifts from a continuous to a batch process, thus increasing the likelihood of complete reaction. Due to economic factors, however, four CSTRs in series were chosen. The reactors were designed by scaling up the laboratory data so that dissolution of the solid reagents in water occurs in the first CSTR and nucleation in the subsequent reactors.

The finished cream product is then stored in two large tanks prior to transportation to consumers.

#### Overall Process •

A collective consideration of the design, economics and safety and environmental aspects of the final proposed design was performed. A detailed cost analysis was carried out on the final plant design. The figures derived by the students were given and the capital

cost of the plant was estimated by using the factorial method. The purchase cost of equipment was obtained from quotations, when possible, to increase accuracy of the analysis.

The plant should be inherently safe since the process is enclosed and safe operation is inherent in the nature of the process. The solid reagents, the additives, and the 'borate cream' are not flammable, combustible, or explosive. Additive 'A' is combustible, but since it comprises only 0.1% of the cream, the danger is likely to be minor. Dust exposure can be controlled by a combining engineering and process control to prevent airborne dust concentrations. Basic safety and fire preventative measures were included in the design. Overall, the process should cause negligible damage under foreseeable circumstances.

A hazard and operability study (HAZOP)<sup>[12]</sup>—a systematic, critical examination of the operability of a process—was performed to indicate potential hazards that could arise from deviations from the intended design. A partial HAZOP Result Sheet is shown in Table 2. Any additional safety features from the analysis were included in the final P&I diagram. The unit P&I diagram for the premixing stage is given in Figure 6.

## CONCLUSIONS

Borax expressed its delight on a vital piece of work that would otherwise have been performed by the company. The exercise showed that students are capable of taking an active

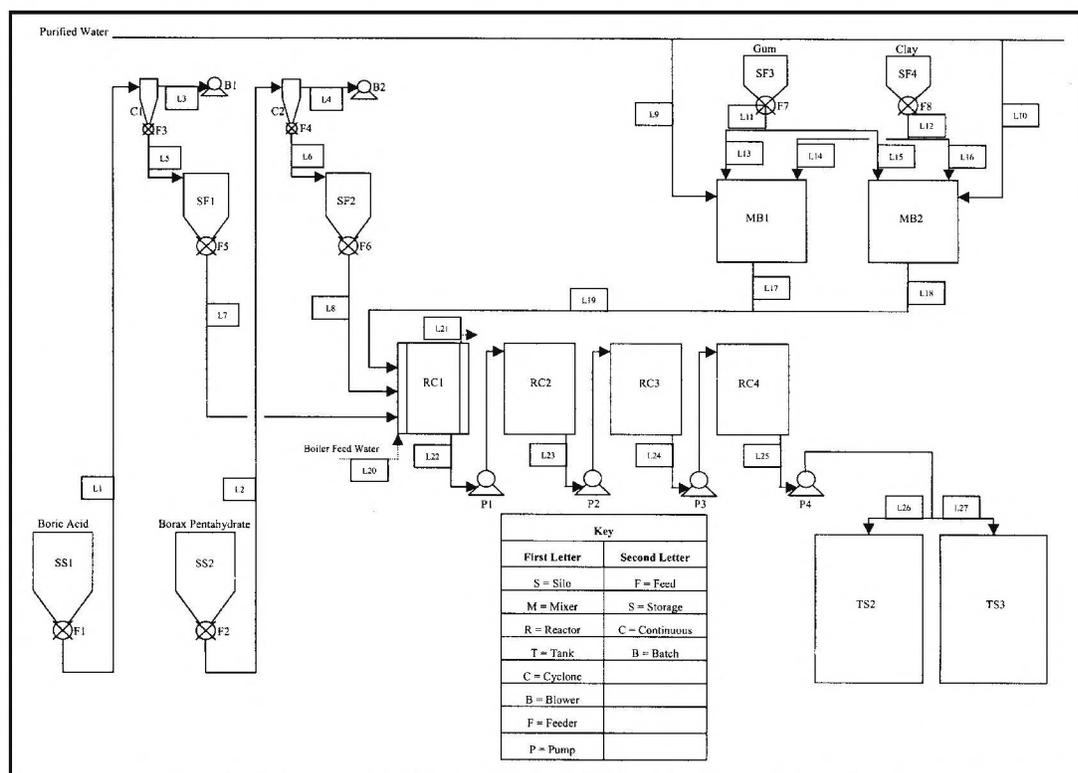


Figure 5. Flow diagram for continuous production of the cream.

role in an industrial design, not as part of an industrial year but as a major assessed project carried out at the university. The use of experimental measurements to define product performance rather than simply to collect property data was a valuable experience.

Student feedback indicates design projects tend to develop teamwork, presentation, and technical skills. In this particular case, the students also felt that obtaining experimental data on the product properties and producing the cream in the laboratory gave greater insight into the fundamental aspects of the process and provided a better means to meet the process objectives. Another beneficial aspect was dealing with company representatives and actual components rather than just theoretical data.

For traditional design projects, the problem with undergraduates getting experimental data is that materials in many traditional processes are toxic and the conditions involve high temperatures and pressures. In comparison, the materials involved in this process were relatively benign and the conditions were moderate. Many other industrial processes involving solids would also fall into this category. In the future, we hope to have more design projects that combine laboratory work with engineering design, preferably based on actual problems—collaboration that benefits students and industry alike.

## ACKNOWLEDGMENT

We would like to acknowledge the work of group members Jenny Richardson, Richard Heath, and Andrew Brown. Finally, we are grateful to Borax for allocating the project to the department and providing essential information and assistance.

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No flow	Blockage in line 9/10 Valve V3/V4 failure PLC faulty	Hydration does not occur	Put flow indicator in line 9/10
More flow	Valve V3/V4 failure	Insufficient hydration PLC faulty	Put weight control in premixers to detect quantity of material
Less flow	Valve V3/V4 failure	Insufficient hydration PLC faulty	Put weight control in premixers to detect quantity of material
Early flow	Timer faulty on PLC for V3/V4	Feed may enter in previous batch	Regular checks on timer on PLC
Late flow	Timer faulty on PLC for V3/V4	Feed may enter in next batch	Regular checks on timer on PLC

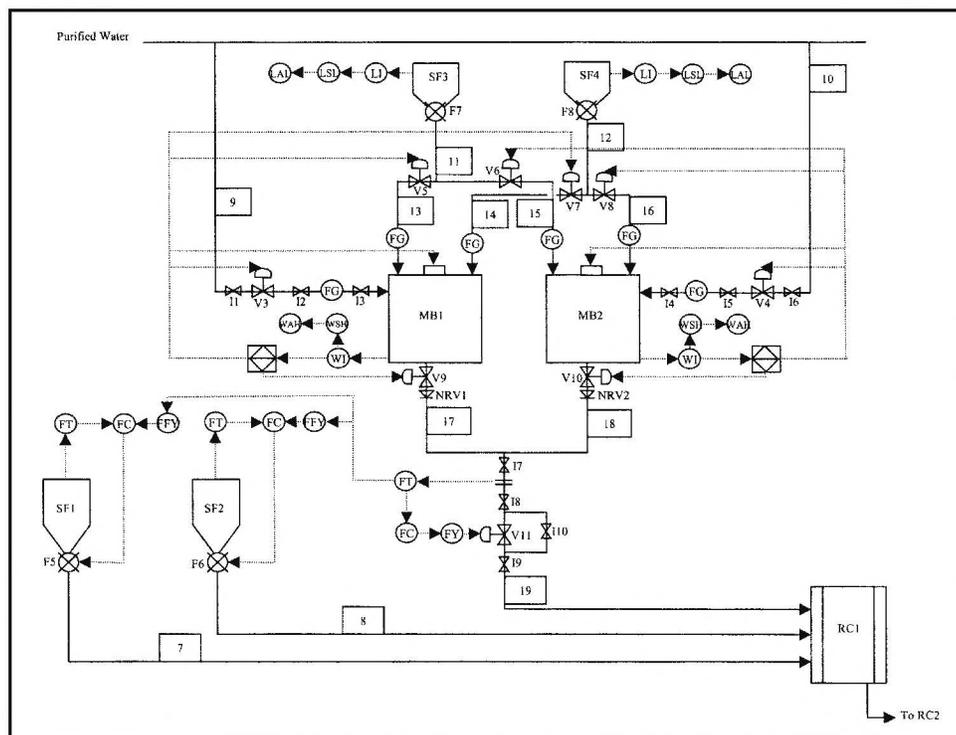


Figure 6. Unit piping and instrumentation diagram.

# COLLABORATIVE LEARNING AND CYBER-COOPERATION

## *In Multidisciplinary Projects*

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The National University of Singapore (NUS) and the Eindhoven University of Technology (TU/e) recently formed a strategic alliance with the aim of offering joint PhD programs. Existing scientific contacts between both universities and the preparation of this strategic alliance initiated the additional concept of joint collaborative learning among several interested departments at both universities.

The Department of Chemical and Environmental Engineering (ChEE) at NUS consists of more than forty faculty members and a thousand-plus student body. The undergraduate programs train over six hundred students who go on to foster the growth of chemical and environmental engineering in Southeast Asia. The quality of teaching in the ChEE department has been greatly enhanced by its in-depth and integrated research, which requires multidisciplinary expertise and can be generally categorized into the areas of chemical engineering fundamentals, environmental science and technology, materials and devices, and process and systems engineering.

TU/e is one of fourteen Dutch universities dedicated to educating over five thousand students in technical scientific education and research. It comprises eight faculties offering twelve full engineering degree programs (for the Dutch “ir” title). The five-year degree programs lead to an academic title equivalent to a Master of Science degree in engineering. In addition, TU/e offers a 3-year BSc and a 4-year PhD program.

Research teams at both TU/e and NUS carried out certain tasks to meet the objectives given by a company, Global Cooling, under comparable, yet different, settings. The TU/e team designed a photovoltaic refrigerator with a Stirling cooler, while the NUS team incorporated a direct-current compressor with an identical refrigerator. The project was partially sponsored by Global Cooling, with additional support supplied by the multidisciplinary project (MDP) program at TU/e and the Undergraduate Research Opportunity Program

(UROP) at NUS. The company participated by supplying the Stirling cooler and feedback on the design. Various overseas communication methods were established to facilitate communication and to ensure that the parameters and experiments were conducted under comparable conditions.

### UROP PROGRAM AT NUS

The Undergraduate Research Opportunities Program (UROP) initiated by the faculty at NUS is a special program that helps undergraduate students strengthen their research experience and their life-long learning ability. The program encourages research that involves cross-departmental participation, allowing undergraduate students to enhance and apply their knowledge of the latest technology. Due to the significance of the program, the National Science and Technology Board in Singapore elevated it to the national level by holding an annual UROP congress where the participating students could present their research findings and receive commendable recognition.

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The students participating in the UROP projects were required to start their research during their second- or third-year of study to ensure its completion. A minimum of 65 hours over two consecutive semesters was scheduled to complete a satisfactory project. Each student had to submit a 4-page paper for final assessment, and a pass-or-fail grade was awarded. It should be noted that additional requirements for the project were given due to the special nature of its international connection with the MDP program at TU/e. Specification of the requirements and assessment are discussed in detail below.

The working team at NUS comprised eight undergraduate students who were in their second year of study. Supervision was provided mainly by two full-time academic staff members in the ChEE department, while other engineering departments (such as the mechanical engineering and electrical/computer engineering departments) were occasionally consulted for relevant technical questions.

### MDP PROGRAM AT TU/E

The inter-departmental Centre for Sustainable Technology at TU/e played a key role during the 1990s in initiating multidisciplinary project work as an optional activity for students of different departments to work together on a subject related to sustainability. Participating departments include chemical engineering and chemistry (400 MSc students), mechanical engineering (700 MSc students), and applied physics (100 MSc students). Multidisciplinary projects are now a compulsory part of the curriculum for most TU/e departments.

In the departments of chemical engineering/chemistry and applied physics, the MDP program is placed in the fourth year of study, at the beginning of Master-degree work, so the students will have sufficient background to apply their knowledge and integrate different expertise from other students. On the other hand, other departments at TU/e, such as mechanical engineering, place MDP projects during the third year of the curriculum in order to conclude the phase of fulfilling the Bachelor degree. As a result, the various research teams of MDP programs often consist of students with different backgrounds in educational experience (different years) and scientific/engineering training (different departments).

An MDP group at TU/e usually consists of 5 to 7 students, preferably with different backgrounds. A 6-credit unit is awarded, requiring approximately 240 working hours to complete the project within a single trimester (10-12 weeks). The students usually work on the design of a prototype based on literature study. For the current project, the team at TU/e consisted of six undergraduate students from three different departments (chemical engineering/chemistry, mechanical engineering, and applied physics), some of whom had previous experience in collaborative project work. In addition to the supervision facilitated by two full-time faculty members, the students were encouraged to search for additional expertise,

both inside and outside the university.

### EDUCATIONAL GOALS

The proposed international Multidisciplinary Project (MDP) was a design-oriented collaboration with a specific economic and societal context. The operating procedures in the project were conducted in parallel by two research teams at NUS and TU/e. The educational goals to be achieved included

- *Working on projects*
- *Dealing with practical problems*
- *Applying already-acquired integrated (technical) knowledge*
- *Localizing and acquiring new knowledge and information*
- *Working on a team with students from different backgrounds*
- *Developing and applying communicative skills, presentation skills, and discussion techniques*

The purpose of an MDP is to involve undergraduate students in ongoing collaborative design work. MDP should benefit students by

- *Enhancing their knowledge of the newest technology*
- *Providing an opportunity to acquire skills for the intellectual process of inquiry*
- *Encouraging students, faculty members, and client companies to interact and form closer ties*
- *Rewarding students with certificates of participation for successful completion of an MDP project*
- *Exchanging information and ideas with a parallel group abroad*

In addition, to focus on the goal of group dynamics, a number of team-building sessions were held to address some of the aspects that play an important role within a group, such as decision making, leadership, communication, conflict handling, group-style inventory, and pilot peer-review.

The NUS group found that the project involved acquisition of new knowledge because the group members were only equipped with two years of undergraduate education and were still under basic training in chemical engineering. Hence, the group spent a substantial amount of time on self-study to familiarize themselves with the project-related subjects.

### THE INTERDISCIPLINARY STRUCTURE

The students operated as two teams of engineers from the virtual company MDP International (the virtual contractor) within a (virtual) budget agreed to by Global Cooling. Estimation of various costs was included as part of the project. Students participating in the program were from the Department of Chemical and Environmental Engineering at NUS, and the Departments of Chemical Engineering and Chemistry, Applied Physics, and Mechanical Engineering at TU/e.

Global Cooling and MDP International agreed on a contract and the groups were responsible for documenting and periodically reporting on the virtual cost. Global Cooling supplied the Stirling cooler and knowledge, while the team at TU/e purchased the refrigerators and (initially) the solar

panels for both parties, to ensure that the parameters and experiments were conducted under comparable conditions. On the other hand, the National Undergraduate Research Opportunity Program and the Centre for Advanced Chemical Engineering at NUS jointly supported the NUS group by offering the necessary facilities and funding for the purchase of a DC compressor, along with the construction materials and required accessories.

## OBJECTIVE OF THE JOINT PROJECT

The objective of the project was to design a photovoltaic refrigerator. The World Bank estimates that in today's world, about two billion people have no access to modern energy services. They live, for the most part, in developing countries in parts of Africa, Asia, and Latin America. For their energy supply, they are dependent on often-scarce biomass sources such as wood and dried dung. Photovoltaic (PV) energy technologies now make it possible to offer sustainable modern energy services to those who live relatively far from a central electric grid.<sup>[1,2]</sup> In most countries, there are three major areas in which PV will be preferably applied: lighting, communication, and cooking and cooling. This project focused on building a solar-powered cooling system.

The objective of the project was to design and manufacture two PV refrigerator prototypes to function as efficiently as possible, using either the Stirling cooler or the DC compressor. A test protocol had to be created that would enable comparison of the results for the two systems (PV-refrigerator connected to PV-panels). Finally, a testing report comparing both systems had to be presented. Efficiency was considered in terms of the conversion of sunlight energy to maintain the cooling chamber at desired temperatures. The teams used identical refrigerators and solar panels as their base material.

The requirements regarding the functioning of the refrigerator were

- *At environmental temperatures between 32°C and 43°C, the inner temperature of the cabinet should remain between 0°C and 8°C*
- *With respect to cooling rate, a minimum of 2 liters of water should be cooled down to 5°C within 24 hours*
- *The system was limited to using a thermal storage buffer (such as water), while the use of a chemical battery was not allowed*
- *Without sunlight, the thermal storage should be able to maintain the refrigerator at temperatures between 0°C and 8°C for at least 24 hours*

The refrigerator using the Stirling cooler was required to meet two additional conditions of

- *It should have a thermal siphon at the cold and the hot end of the system*
- *It should preferably have a maximum temperature difference over the heat exchanger of 5°C per side*

The variable factors in this project were the selection of

the cooling system and the interaction between the cooling system and the solar panel. The NUS team used a DC compressor as a cooling engine, while the TU/e team used a Stirling cooler. Initially, both groups focused on the theoretical research of the subject matter and individual components. Next, some experiments were conducted to assess individual components regarding the working properties, which included

- *Heat leakage in the Samsung refrigerator*
- *Variation of the output voltage of the solar panels with the intensity of light*
- *COP and capacities of the DC compressor at various conditions*

Apart from the actual design, attention was also given to areas such as safety, environmental concerns, and marketability. One of the major problems in producing equipment for markets in developing countries is the initially limited volumes to be marketed. The chances of a PV refrigerator being produced in substantial numbers would significantly depend on the richer parts of the world also presenting a market for such a device. One of the niches for this device could be the outdoor (sporting and camping) market.

An appreciable amount of attention was directed toward the question of sustainability. The subject of the MDP shows close relevance with the use of sustainable technology, and therefore sustainable technology had to be a key feature of the research question. That is, in addition to the technical aspects of the subject, students had to research environmental and social aspects of the subject and had to consider sustainability aspects. In this way, students were required to integrate their specific technical skill with knowledge of sustainability in their design and final report.

The students on both teams had assistance from technicians in building the prototype, to ensure sufficient progress. The main areas in which assistance was required were the construction of the buffer container and the disassembly of the original refrigerator.

A market analysis was conducted simultaneously with the construction of the photovoltaic refrigerators. Factors that were considered included pricing the photovoltaic refrigerators so that it would be attractive to targeted customers, namely the medical sectors in developing countries or sport and camping companies in developed countries. Other aspects included in this economic analysis were production volume, shipping, and assembly.

## TIME TABLE

Schedules of the academic year at TU/e and NUS vary greatly (trimester vs. semester), a severe drawback when scheduling such inter-university projects. The initial schedule was planned through a consensus between the staff members from both universities, with preliminary input from students being solicited. During the first videoconference, the schedule was modified subsequent to a discussion between

two student teams. To achieve comparable progress for evaluation, a 17-week timetable was eventually compiled (from September 2000 to June 2001) that accommodated the holidays and examination periods at the respective universities. Based on the expected 240 hours per student at TU/e, this corresponded to roughly 14 hours per week.

## PHASING OF THE PROJECT

The various phases of the project spanned 17 weeks and included the components of research, coupling, testing, marketing, and ending the project. It should be noted that some of the phases had to be done simultaneously to achieve proper progress. The following paragraphs contain more details about the activities planned for the various phases of the project.

**1st Phase (week 1 through week 4)** • This phase, which took about one-quarter of the total project time, was divided into two parts: orientation and purchase. Orientation was focused on gathering and processing information on the various elements of the photovoltaic refrigerator. The aim was to gain as much insight as possible regarding its operation and the efficiencies of the individual elements, which were an important consideration in the calculation of the required power of the solar panels.

A lot of self-reading and sales research was carried out in parallel to find a suitable DC compressor (the Stirling cooler was provided by Global Cooling). During this phase, a project plan was devised that required deliverable goals and realistic planning in detail. A financial budget that met the target range of the project served to conclude the first phase. The budget proposed by both teams actually showed virtual expenses. The “virtual” budget consisted of four primary costs: wages, equipment and material, working facilities, and stationery costs. The total virtual budget was around US \$14,000. In contrast, the real project budget, excluding the cost for wages and working facilities, came to about US \$2,500. The overall expenditures were about 92% of the proposed project budget (NUS team), which is a valuable outcome for executing the project.

**2nd Phase (week 5 through week 8)** • During the second phase, which spanned the same length of time as the first phase, students started their research relevant to the project. Attention was paid primarily to the design of couplings between the various elements. Couplings between the refrigerator and the DC compressor or Stirling cooler, between the solar panels and the refrigerator, and between the buffer and the refrigerator were investigated. The theoretical design was accomplished in the last two weeks of this phase,

while the prototype design was consolidated in the 6th week. At the end of the second phase, students had to produce an interim report with details about the relevant choices and assumptions that they had made, along with a report of their progress and possible adjustments for the remaining project. In addition, students had to present their up-to-date results.

**3rd Phase (week 9 through week 17)** • The third phase comprised the major milestones of the project over 9 weeks (half of the project time). During this phase, development of a test protocol was initiated. Both student teams used the initial period of this phase to clarify and streamline the measurement standards and criteria for reasonable comparisons between the prototypes. The first round of testing was carried out during weeks 13 and 14, and both teams conducted a second round of testing as well as some extra tests (which differed for each team) during the 15th week. In preparing the final report, each of the team members worked on a different chapter, with the results being compiled by a team editor. At the end of the third phase, students were expected to finalize their project and submit the final report. A final presentation during a videoconference concluded this MDP project.

## GRADING

Table 1 shows the assessment scale of the various grading criteria of the project. The grading criteria included (with corresponding weighing factor in parentheses) the final report (3), the final presentation (2), the project plan (2), in-between oral and written presentations (2), and group participation (1). The (sub) grades are on a 1-to-10 scale, rounded off to multiples of 0.5. Evaluation of teamwork effectiveness assessed delegation among group members and organization of the research work. The MDP students also had to give a formal interim presentation on their preliminary results to their respective project tutors at TU/e and NUS. They were asked to focus on the project progress as compared to the original project plan. In addition to the interim and final report, feedback from the client, Global Cooling, also played an important role in evaluating the final deliverables of the individual groups.

A pilot peer review that included individual and mutual assessment was part of the MDP educational goal at TU/e. It was first exercised on a trial basis halfway through the project. Students were asked to evaluate each other on two aspects: 1) specific (positive) ways a member contributed to teamwork and 2) additional improvement the student should strive for. In addition to discussion, the students compiled a brief confidential report for the supervising staff. This peer review

**TABLE 1**  
Grading Approach

<i>Assessment</i>	<i>Scale</i>	<i>Supervisor of</i>	
		<i>EUT OR NUS</i>	<i>Global Cooling</i>
Effectiveness of Team Work	1	•	
Project Plan	2	•	•
Interim Report	1	•	•
Interim Presentation	1	•	
Final Report	3	•	•
Final Presentation	2	•	
<b>Total</b>	<b>10</b>		

was also exercised at the end of the project to evaluate the progress of individual students in light of the previous suggestions from team members.

A final report (in electronic format) to the client and the tutors at both TU/e and NUS had to be submitted for grading a week before the final videoconference. A final evaluation was then completed by the client and staff members toward the end of the final videoconference. Within one week after grading, students were expected to submit a corrected report that addressed the remarks provided by the staff members at the respective universities and Global Cooling, so that the printed edition could be processed in time.

## ROLES OF CLIENT/COACH/ORGANIZER

There are a number of roles played by different people during the project. One role is the “contractor”—the person who has a research question and who is highly interested in the project’s outcome. This person is often an expert on the subject. The contractor can co-decide on the quality of the project plan and on the quality of the interim and final reports and presentations.

Another role is the “coach,” who follows the progress and process of the project and is the person to whom students can turn with daily questions. He/she can also act (if necessary) as an intermediary between the group and the people from the “outside world.” As a coach, this person can stimulate and motivate the group and guide and promote their progress.

A third role is the “organizer.” This person works mainly in the background, making sure that facilities such as special training, overall finance, and a place to work, are available.

Interaction between the three participants above and the students was made possible via regular e-mails and ICQ sessions. In addition, there were four videoconferences held during the program that facilitated idea exchange via direct “face-to-face” discussion. The MDP students were also required to give a formal interim presentation on their preliminary results to their respective project tutors at both universities. They were asked to focus on the project progress rather than the original project plan.

The feedback and comments from the client (Global Cooling) were considerations in grading the interim report, the presentation, and the final report. The MDP students used multimedia facilities to record the relevant project materials in electronic form (*e.g.*, CD-ROMS). These materials were mailed or e-mailed to the respective client, coaches, organizers, and partner-group members for their comments. The feedback was subsequently incorporated into the latter part of the MDP project work and report.

## COMMUNICATION FORMATS

Since the groups came from different cultures, mutual understanding between them was very important for stimulat-

ing constructive working dynamics and for enhancing comparable interpretation of the project. The leaders of both projects communicated at least once a week to monitor the groups’ progress and to ensure achievement of the short-term goals. In addition, frequent communication between the several subgroups at both universities took place via e-mail and ICQ sessions (real-time “chat” communication over the internet). Four videoconferences were scheduled to obtain mutual understanding and to enhance cohesive execution of the research project. Furthermore, there was communication between the academic staff members at both universities to resolve questions that arose and on administrative matters such as scheduling and the agenda of the videoconference.

Meeting minutes included actions taken, results obtained, and decisions made and were mailed to the other teams and coaches in order to achieve the desired synchronization. Each TU/e student had a notebook computer, and the group as a whole had its own MDP room with network connections. In addition, they had a group e-mail account and a separate website for communication purposes. Additionally, the students frequently used ICQ accounts for exchanging ideas and making decisions with the counter group abroad. The MDP groups at TU/e had a weekly meeting in which the academic staff members were present.

The NUS group members were given laboratory space in the engineering workshop that was equipped with networked personal computers and the necessary facilities for regular meetings. Individual group members took turns organizing the meetings to discuss the project’s progress.

## EXPERIMENTAL RESULTS

Individual prototypes built with a Stirling cooler and a DC compressor were accomplished at the end of the project. Both teams performed comprehensive and identical tests, comparing the efficiency of the systems. Daylight cycles were characterized and calibrated in both countries to ensure that the testing environments were comparable. Due to different voltage requirements by the Stirling cooler and the DC compressor, the exact daylight cycle and various parameters of the DC compressor, such as suction pressure, input voltage, and current, were investigated before the final tests. Initial experiments were conducted with varying buffer amounts and container types to obtain an estimate of the heat leakage rate from the refrigerator.

Water was chosen as the buffer material, due mainly to its availability and well-known properties. Using energy conservation laws, an estimate of the buffer amount was obtained after considering the heat transfer (enhanced by fins) between the buffer surroundings inside the refrigerator and the buffer itself. Due to the different power-supply levels, designing the buffer container and the fins was different for both groups. While certain additional adjustments were made by both teams before the final performance tests of the refrigerators coupled

with solar energy, a mutually agreed test protocol was established to assess the efficiency of the individual designs.

To examine the efficiency of the refrigerators, three major stages were evaluated as a function of time needed: the start-up stage, the temperature-maintenance stage, and the cool-down stage. The test results successfully met the requirements posed by Global Cooling. Table 2 shows one of the tests for both refrigerators. In general, the Stirling-cooler system showed a higher efficiency and demonstrated more steady temperature profiles, shorter start-up time, and longer “keep-cool” time. In contrast, the DC-compressor system gave faster cool-down, with favorable temperature profiles.

## EVALUATION

Part of the project evaluation was devoted to illustrating how the project objectives were achieved.

**Team Work** • Overall, the multidisciplinary project exposed students to a research project in a practical way. Although the initial period of team formation was fraught with difficulties in work allocation and coordination, the members learned to work with one another and coordinate advanced planning, establishing infrastructure, decision making, critical thinking, self-evaluation, corresponding improvement, dealing with conflicts, and overcoming differences.

**Applying Technical Knowledge** • The various tasks enabled students to apply learned knowledge and to acquire new knowledge. For example, foundation training may suffice to test the solar panels, but in-depth studies were required to resolve more complex problems such as the proposed power conditioning unit. Students also found that theories given in class don’t always agree with real life, so they developed creative approaches and independent thinking to properly interpret data for situations beyond their academic expertise.

**Resolving Practical Problems** • Students experienced several practical problems, such as how to best design the buffer container for the refrigerator powered by a compressor. Such first-hand experience in problem solving is not offered by current academic courses.

**Developing and Applying Communication Skills** • The students learned to refine their communication skills to efficiently pin-point useful resources, clearly convey problems, and effectively communicate with others. The videoconferencing presentations reinforced students’ technical communication skills, and they found it a challenging way to interact with overseas counterparts.

## CONCLUSIONS

This project contained the uniqueness of multidisciplinary, international, and industrial collaboration. Students were particularly challenged to apply fundamental knowledge, use their creativity, and interpret results. Furthermore, they ex-

**TABLE 2**  
**Test Results of**  
**Refrigerator Performance**  
(Courtesy contribution  
by both MDP groups)

	Stirling Cooler	DC Compressor
Start-up Time (hrs)	152	177
Cool-down Time (hrs)	12	5.8
Keep-cool Time (hrs)	47	31.6
Start-up COP (-)	1.32	0.97
Cool-down COP (-)	0.88	0.56
Heat Leak (W)	16.6	11.8

perienced the importance of communication skills and learned the importance of a constructive attitude.

Coordination of such a project is complicated and requires a lot of effort. It provides, however, a unique learning opportunity in working with peers, with different knowledge backgrounds and different cultural backgrounds.

The impact of different backgrounds was underestimated. It was late in the project that these differences were identified, because they resulted in misunderstandings. Solving these misunderstandings by intensive communication brought both groups much closer and greatly im-

proved cooperation.

The importance of video conferencing for decision making was overestimated, whereas the usefulness of chat sessions was underestimated. Chatting was preferred by the students in spite of local time differences. Direct communication proved essential for mutual understanding and agreement on important points.

Different academic calendars at the two universities made it difficult to plan the project, but spreading it over the entire academic year proved essential because of its practical and experimental aspects (*i.e.*, material delivery times, construction of and debugging the prototype, testing experiments).

The students were enthusiastic about the multicultural communication aspect and the opportunity for experimental design and consequently spent 70% more time on the project than originally intended.

## ACKNOWLEDGMENTS

The authors thank TU/e and NUS for the support of MDP (at TU/e) and CACHE and UROP (at NUS). Contributions from the MDP students are also appreciated: Arjan Buijsse, Paul Scholtes, Bastiaan Bergman, Ronny de Ridder, Maarten Blox, and Thijs Adriaans from TU/e, and Josephine Yeo Siew Khim, Ng Chwee Lin, Wuang Shy Chyi, Ashwin Balasubramanian, Kwong Bing Fai, Jason Chew Sin Yong, George Ng Ming Horng, and Ong Guan Tien from NUS. We also thank Dr. Suryadevara Madhusudana Rao for his technical support.

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## 2003 ASEE Annual Conference

# Chemical Engineering Division Program

June 22-25, 2003 ♦ Nashville, Tennessee

## Technical Sessions

### Sunday, June 22, 2003

#### Session 0413: Teaching Teaming, Writing, and Speaking

*Moderators: Steven W. Peretti, Lisa G. Bullard, Chris Anson, Deanna P. Dannels*

ABET requirements, as well as communication-across-the-curriculum initiatives, have focused faculty attention on how to effectively integrate teaming, writing, and speaking instruction within the engineering curriculum. Sponsored by an NSF-Action Agenda grant, a multidisciplinary faculty team at North Carolina State University has developed a set of teaming, writing, and speaking instructional materials for an engineering design course and an engineering laboratory course. Workshop participants will receive a CD and hard copy of instructional materials for both courses, evaluation rubrics for written and oral reports, and recommendations on effective implementation models based on the size of the department, the expertise of the instructor, and available campus resources.

### Monday, June 23, 2003

#### Session 1313: Novel Courses for ChEs

*Moderators: Jason Keith and Veronica Burrows*

1. "A New Chemical Engineering Senior Elective Course: Principles of Food Engineering," *Mariano Savelski*
2. "Integration of Microelectronics-Based Unit Operations into the ChE Curriculum" *Milo Koretsky, Chih-hung Chang, Shoichi Kimura, Skip Rochefort*
3. "Pediment Graduate Course in Transport Phenomena," *William Krantz*
4. "Sparkling Student Interest in Electrochemical Engineering," *Robert Hesketh, Stephanie Farrell, C. Stewart Slater*
5. "Teaching Packaging Engineering at Christian Brothers University," *Asit Ray*
6. "Fundamentals, Design, and Applications of Drug Delivery Systems," *Stephanie Farrell*

#### Session 1413: Design in the ChE Curriculum

*Moderators: David Silverstein and Priscilla Hill*

1. "Life-Long Learning Experiences and Simulating Multi-Disciplinary Teamwork Experiences Through Unusual Capstone Design Projects," *Joseph Shaeiwitz, Richard Turton*
2. "New Topics in Chemical Engineering Design," *Paul Blowers*
3. "An Economic Model for Capstone Design," *Rudy Rogers*
4. "A Web-Based Case Study for the Chemical Engineering Capstone Course," *Lisa Bullard*
5. "Challenging the Freshman: Freshman Design in ChE at Rose-Hulman Institute of Technology," *Atanas Serbezov, Carl Abegg, Jerry Caskey, Sharon Sauer*

### Tuesday, June 24, 2003

#### Session 2213: Recruitment and Outreach in ChE

*Moderators: Anne Marie Flynn and Mariano J. Savelski*

1. "Cookies and Diapers and Chemical Engineering," *Lisa Bullard*
2. "Integrating Chemical Engineering into High School Sciences Classrooms," *Deran Hanesian*
3. "OSU GK-12 Program for the Enhancement of Science Education in Oregon Schools," *Willie Rochefort, Dan Arp, Edith Gummer, Tricia Lytton, Haack Margie*
4. "Science, Technology, Engineering, and Mathematics Talent Expansion Program," *Taryn Bayles*
5. "Using an Enrichment Program to Introduce High School Students to ChE," *Paul Dunbar, Rhonda Lee, David Silverstein, Jim Smart*
6. "Chemically Powered Toy Cars: A Way to Interest High School Students in a Chemical Engineering Career," *Christi Luks, Laura Ford*

#### Session 2313: Innovations in the ChE Laboratory

*Moderators: S. Scott Moor and Jim Henry*

1. "The Fuel Cell—An Ideal Chemical Engineering Undergraduate Experiment," *Suzanne Fenton, James Fenton, H. Russel Kunz*
2. "A Novel Unit Operations Project to Reinforce the Concepts of Reactor Design and Transport Phenomena," *Sundararajan Madihally, Benjamin Lawrence, R.*

Russel Rhinehart

3. "Simple, Low-Cost Demonstrations for UO II (Mass Transfer Operations)," *Polly Piergiovanni*
4. "Use of Lab Experiments to Build Transport Concepts," *Nam Kim*
5. "A Novel Fluid Flow Demonstration/Unit Operations Experiment," *Ronald Willey, Alfred Bina, Ralph Buonopane, Guido Lopez, Deniz Turan*
6. "Institutionalizing the Multidisciplinary Lab Experience," *R. Worden*

Session 2613: **The Biology Interface**

*Moderators: Polly Piergiovanni and Stephanie Farrell*

1. "Teaching of Engineering Biotechnology," *Raj Mutharasan*
2. "Seamless Integration of Chemical and Biological Engineering in the Undergraduate Curriculum," *Howard Saltsburg, Gregory Botsaris, Maria Flytzani-Stephanopoulos, David Kaplin, Kyongbum Lee*
3. "Integrating Biology and Chemical Engineering at the Freshman and Sophomore Levels," *Kathryn Hollar, Stephanie Farrell, Gregory Hecht, Patricia Mosto*
4. "Microbiologically Speaking: Preparing Chemical Engineers for Careers in Life Sciences," *William French*
5. "ChE Power! A Hands-On Introduction to Energy Balances on the Human Body," *Stephanie Farrell, Robert Hesketh, Mariano Savelski*

**Wednesday, June 25, 2003**

Session 3213: **Learning Enhancements for ChE Courses**

*Moderators: Jim Smart and John Gossage*

1. "Improving Critical Thinking and Creative Problem Solving Skills by Interactive Troubleshooting," *Nihat Gurmen, H. Scott Fogler, John J. Lucas*
2. "Incorporating Computational Fluid Dynamics in the Chemical Reactor Design Course," *Randy Lewis, Sundararajan Madhally*
3. "Web-Based Instructional Tools for Heat and Mass Transfer," *Jason Keith, Haishan Zheng*
4. "Experiments in the Classroom: Examples of Inductive Learning with Classroom-Friendly Laboratory Kits," *S. Scott Moor, Polly Piergiovanni*
5. "Thermo-CD: An Electronic Text for the Introduction to Thermodynamics Course," *William Baratuci, Angela Linse*
6. "Development of an Intelligent Tutor for Teaching Material Balances to First-Year Students," *John Harb, Paul Miller, Kenneth Solen, Richard Swan*

Session 3413: **Advisory Boards and Program Assessment**

*Moderators: James Newell and Randy Lewis*

1. "Using Standardized Examinations to Assess Chemical Engineering Programs," *Keith Schimmel, Shamsuddin Ilias, Franklin King*
2. "Structuring Program Assessment to Yield Useful Information for ChE Faculty," *Helen Qammar, Teresa Cutright*
3. "Program Improvements Resulting from Completion of One ABET 2000 Assessment Cycle," *Sindee Simon, Lloyd Heinze, Theodore Wiesner*
4. "Departmental Advisory Boards—Their Creation, Operation, and Optimization," *Michael Cutlip*
5. "Involvement of the Departmental Advisory Board with Curriculum and Student Recruitment Issues," *Dana Knox, Basil Baltzis*
6. "Effective Use of External Advisory Boards," *Kirk Schulz*

Session 3513: **Statistics in the ChE Curriculum**

*Moderators: Valerie Young and Donald Visco*

1. "Variation, variation, very-action, everywhere, but . . .," *Milo Koretsky*
2. "The Use of Active Learning in the Design of Engineering Experiments," *Gerardine Botte*
3. "Use of an Applied Statistical Method to Optimize Efficiency of an Air Pollution Scrubber Within an Undergraduate Laboratory," *Jim Smart*
4. "Designing a Statistics Course for Chemical Engineers," *Valerie Young*
5. "Teaching Statistical Experimental Design Using a Gas Chromatography Experiment," *Douglas Ludlow, Robert Mollenkamp*
6. "Integration of Statistics Throughout the Undergraduate Curriculum: Use of the Senior Chemical Engineering Unit Operations Laboratory as an End-of-Program Statistics Assessment Course," *Michael Prudich, Darin Ridgway, Valerie Young*

Session 3613: **Teamwork and Assessment in the Classroom**

*Moderators: Joseph Shaeiwitz and Andrew Kline*

1. "Imbedding Assessment and Achievement in Course Los with Periodic Reflection" *Franklin King, Shamsuddin Ilias*
2. "Assessment in High Performance Learning Environments," *Pedro Arce, Sharon Sauer*
3. "Developing Metacognitive Engineering Teams," *James Newell*
4. "Observations on Forming Teams and Assessing Teamwork," *Joseph Shaeiwitz*
5. "Rubric Development for Assessment of Multi-Disciplinary Team Projects," *Kevin Dahm, James Newell*

**ChE Executive Committee Meeting**

(Breakfast, Ticketed)  
Monday, June 23, 2003  
7:00 AM - 8:15 AM

**ChE Lectureship Award  
Presentation**

Monday, June 23, 2003  
4:30 PM - 6:00 PM

**ChE Division Banquet**

(Off-site; Ticketed)  
Monday, June 23, 2003  
6:30 PM - 9:00 PM

**Division Business Meeting/Luncheon**

(Ticketed)  
Tuesday, June 24, 2003  
12:30 PM - 2:00 PM

**ChE Chairpersons Breakfast**

(Ticketed)  
Wednesday, June 25, 2003  
7:00 AM - 8:15 AM

## The Value of Good RECOMMENDATION LETTERS

GARY L. FOUTCH

Oklahoma State University • Stillwater, OK 74078

Whether you currently have a job, are looking for one, are up for promotion or tenure, or are pursuing some other opportunity, sooner or later you will most likely need a supporting letter. Let's say that you've just decided to apply for a position, or perhaps a fellowship or an award. You've spent hours conscientiously filling out the paperwork and you've asked the best people you can think of to write letters on your behalf. It seems like you've done everything right so far, doesn't it?

Well, maybe not.

What did your references say when they agreed to write a letter for you? Did the conversation go something like, "Professor X, I'm applying for the xyz fellowship. Would you be willing to write a letter of recommendation for me?" with the Professor replying, "Sure, I'd be happy to"? If that was the limit of your communication, you may have made a big mistake! You've just put your hopes into the hands of someone 1) who may be too busy to write a letter that truly reflects your talents, 2) who knows very little about you, even if you think otherwise, 3) who is unfamiliar with the criteria that will be used to evaluate your application, or 4) who may not think as positively about you as you think.

Do you think that someone's willingness to write a letter about you implies that the person supports you? If so, I suggest you rethink your strategy for getting appropriate letters of support.

I recently heard someone say, "I hear you write a good letter." It was clear this person wasn't looking for a letter that necessarily said something *good* about him personally, but carried the sense that "I hear that you can write letters that have a high probability of getting me what I want." Perhaps this doesn't sound like much of a difference, but I can assure you, it is quite different.

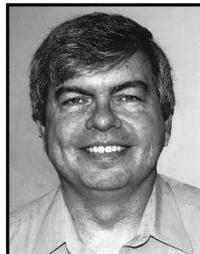
Let me begin by giving the reviewer's perspective of your application, based on my own experience. I have served four

years as a panelist for the NSF graduate fellowship program and four years for the Fulbright Foundation. The NSF fellowship program application pool consists primarily of college seniors, while the Fulbright program that I served on was for faculty sabbaticals in England, Ireland, and Canada. All applicants in these national and international competitions are bright, have strong backgrounds, and present good supporting documentation. Frequently, the deciding factor will come down to the *quality* of the reference letters supporting the application. Quality in this context not only means that the letter says good things about you, but also that it is believable and that it addresses the criteria for the award or position. As a reviewer, I have to believe the supporting letters—and in a tie-breaker, the most believable letter can make the difference.

The following examples paraphrase letters I've read. How would you feel if one of your references said something like

*I can't believe Joe Bob asked me to give him a recommendation. He was a horrible student in my class—when he bothered to show up. There must be someone more deserving of this award.*

What do you think of Joe Bob's chances for a highly competitive award if his application contained such a recommendation? Or, how would you like to be mentioned in a letter that said



**Gary L. Foutch** is Kerr-McGee Chair and Regents Professor at Oklahoma State University, having joined the School of Chemical Engineering in 1980. He received all his degrees in chemical engineering from the University of Missouri-Rolla, with part of his PhD work at the Technical University of Munich-Weihenstephan. His research is in the area of transport-limited kinetics and separations, with current projects on ultrapure water processing and high-temperature reactor design.

*I am Distinguished Professor X. I have a Nobel Prize in Chemistry. I know Joe Bob. Award him a fellowship.*

What has the committee learned about Joe Bob from this masterful piece of writing? All I learned was that he knows an egotistical chemistry professor. I learned nothing about Joe Bob himself.

Perhaps you think I'm making these letters up, but I assure you that within a word or two, I have seen them—the excerpts are as factual as my memory allows (we can't keep copies of applications). The good news for most of you (but not, unfortunately, for Joe Bob) is that of the approximately 1200 letters I've read, I estimate that only about 10 were that bad.

An example of a reference writer not understanding the criteria for an award is demonstrated by an excerpt from a supporting letter for a Fulbright that stated

*I can think of no better reward for Professor X's accomplishments at Distinguished U than allowing him and his lovely wife to enjoy a relaxing year at Cambridge.*

At the time, the criteria for the award for which Professor X was being considered focused on research and/or teaching collaboration between U.S. and foreign scientists and long-term benefits to both the visitor's and the host's institutions were important. A reward for past accomplishments, or a vacation in the English countryside, was most certainly not a goal of the program!

There is another type of letter that hurts an application. Some letter writers make up things, or cut and paste from other letters, or simply have no idea what to say about the applicant. These letters quite often contain errors in fact or actually contradict the body of the application. An example follows.

The NSF panels have twenty to thirty reviewers sitting in the same room who are, for the most part, reading. Occasionally, however, a comment will be made about a statement in an application. During one of these panels, a colleague noted that according to the department chairman's supporting letter, two students from the same class of about twenty had ranked in the "top 5% of the class." (Engineers appreciate these little mathematical oddities—it's just part of our nature!) This doesn't sound like a big deal so far, but then someone else remembered they had also seen that statement. Within a matter of minutes, seven applications that were submitted from this same department were checked, and each contained a letter from the department chairman indicating that each applicant had been in the top 5% of the class.

Those letters no longer contained any credibility.

Another possibility is that your references simply do not remember that much about you, or that they don't remember what you remember. A few years ago I had a wonderful student who I enjoyed teaching and who has kept me updated once or twice a year through e-mails. Several months ago he relocated and sent me a note with his new address, adding a personal note of a memory from his school days. He related that one day when he was walking down the hall after class, he met me and two visiting chemical engineers, and that I had invited him to go to lunch with us. He said that at the time he had been considering leaving chemical engineering, but that listening to the industry guys talk about their jobs and other general topics had revitalized him, and he ended up staying in the program and getting his degree. He wanted me to know and to thank me for that lunch invitation. I'm afraid that I have no recollection about that lunch whatsoever! I'm glad I did something to help him stay committed to engineering, but if he hadn't mentioned it I would never have known. While this is exactly the type of personal story that could be used in a letter of recommendation to show commitment and dedication, it can't be related if it isn't remembered.

How can you help yourself? There are several things I recommend in order to get supporting letters worthy of the time and effort you devote to your application:

- ▶ Determine if the letter-writers actually support your application. This is easily determined—just ask! Don't start with, "Will you write a letter of recommendation for me?" Instead, tell them that you are interested in applying for a particular program or award and ask them what they think your chances are. Do they feel you would be competitive? Ask if they have any advice on how to compete for the job or award. What do they know about your strengths and weaknesses that would allow you to be successful if you applied? Ask if they would be supportive of your application. DO NOT ask them to write a letter of support until you have heard their responses to the above and are convinced that they have your best interests in mind. If you're not sure, say thanks and walk away. After some thought, you may conclude that they should be one of your references after all, and in that case approach them again with "...remember the conversation we had the other day...."
- ▶ Educate your reviewers. Most potential reviewers will not know the criteria of the specific award or program.

***All applicants in these national and international competitions are bright, have strong backgrounds, and present good supporting documentation. Frequently, the deciding factor will come down to the quality of the reference letters supporting the application.***

Even if your letter-writers were familiar with the program several years ago, don't assume the criteria are the same today and that your references are up to date on them. You need to be sure they understand the criteria upon which you will be evaluated. Feel free to communicate which criteria you believe best match your skills and which you think need the most support.

- ▶ Tell your reviewers something about yourself. Tell them why this award or position is the perfect match for you. Allow them to make the letter as personal as possible. They won't have the perspective you have; you have more knowledge about yourself and why you should be the recipient than they do. If you can sell them on your dreams, they will be able to focus that energy into a letter that can truly support you.
- ▶ Meet their timetable! Don't ask for a letter that's due tomorrow. To ensure all deadlines can be met, I suggest planning ahead by at least two weeks. A rushed letter will most likely have omissions that could hurt your application.
- ▶ Consider having an extra letter sent. One too many is better than one too few. Read the application details or call the program administrator. Usually, an extra letter just goes into the file, but the bottom line is not to be a letter short of the required number. Feel free to get confirmation that letters were sent. Some application pro-

cesses have a return postcard so you can be sure.

- ▶ Try to guide the letter so it matches the narrative application and forms you have written. Don't write the letter for your reference, and if they suggest that you do so, I recommend you find someone else to do it. You want a sincere and honest opinion from a conscientious supporter. I suggest that you prepare a letter to your reference that contains the criteria and a bullet list of items you feel the letter should consider. A bullet list allows them to add their own prose as they address key points so that all letters won't sound alike. Also, just in case, if you have similar bulleted lists for different references, mix the order so they don't go down the line and hit the same points in the same sequence.

Let me add a note specifically to those of you applying for a Fulbright or other international award. For the high-demand locations such as England and Germany, you can assume that all applicants have invitation letters offering a desk and computer access. Look for *real* ties to your host institution. In today's world where it's easy to have collaborators from around the globe, you need to give the judges a reason for *physically* being there. Help your references explain why you *have* to be overseas. If possible, in addition to the host letter, have another colleague(s) within the same or a nearby country describe what your presence will mean to them.

Good luck! □

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## ChE *letter to the editor*

To the Editor;

Regarding the article "Making Phase Equilibrium More User-Friendly" by Michael J. Misovich,<sup>[1]</sup> we endorse some of the points made, but are also concerned by some general attitudes expressed about teaching this subject (and by extension, chemical engineering thermodynamics in general, since he makes passing reference to chemical reaction equilibrium).

On the positive side, we commend the considerable emphasis on the calculation of properties and presentation of the data graphically. We also agree with the importance of developing an intuitive understanding related to such things as order-of-magnitude values of thermodynamic quantities, and the likelihood of the occurrence of azeotropes.

On the other hand, some statements are made that seem to place the subject matter in a very limited position relative to other courses that he mentions. For example

- "Phase equilibrium . . . in which abstract concepts are

*presented to the near exclusion of practical examples."*

- ". . . most phase equilibrium courses (sic) do not connect these (calculations) to real processes or equipment."
- ". . . this class deals with techniques for generating data . . . to the total exclusion of applications."

It seems no wonder then that "students who perform calculations satisfactorily seem confused over the meaning of what they have learned." These statements also tend to run counter to Felder's TIP 1,<sup>[2]</sup> notwithstanding the subsequent emphasis on graphical presentation.

To the contrary, we believe that teaching this subject without overtly involving applications (processes and equipment) amounts to emasculation of it. One thing that should be emphasized is that thermodynamics (as the umbrella subject) provides limiting or boundary solutions to problems, but is silent on "efficiency," in various guises, that translates the limiting-case results into actual results. It is inevitable that

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this requires, however, the introduction of actual processes (and equipment), and in this way bridges can be built to these other courses.

The author is undoubtedly aware of many such applications, as he indicates, and we mention only a few (not necessarily directly related to phase equilibrium, but to equilibrium in general):

- Separation of a condensable from a noncondensable species (cooler-condenser); also related to humidification and dehumidification
- Eutectic behavior related to the use of ethylene glycol antifreeze coolant (automobile engine) and its vapor-liquid counterpart in "steam distillation"
- Vapor-compression refrigeration (compressor)
- Energy conversion (fuel cell or electrochemical cell in general)
- Equilibrium reaction yields, equilibrium species distribution in general (equilibrium-limited reactor, whether batch or flow system)

The author also expresses a strong preference for the use of computer spreadsheets, although he acknowledges the possible alternative use of metacomputing software (such as Maple<sup>[3]</sup>), which, in our opinion, is more efficient. In addition, this software does not require the trial-and-error or iteration approaches mentioned by the author for some of his assignments.

If the goal is to produce graphical visualization of behavior, then spreadsheets have the inherent limitation that the explicit generation of data must precede the generation of graphs. Spreadsheets can only easily generate such data if the equations are available in analytical form; otherwise, trial-and-error or iterative procedures must be used, as he notes. In contrast, metacomputing software provides graphing commands that do not require such explicit prior data generation.

Furthermore, any required data can be obtained separately, without trial-and-error or iterative procedures.

As an example, if plotting the graphs  $P(x_1)$  and  $P(y_1)$  for the ideal system in his Figure 1 is the objective of a student assignment, Maple requires only the following statements (only the first two lines are required for the plotting; the other lines relate to cosmetic aspects of the display):

```
> Psat1:=(value);Psat2:=(value);
> plot(Psat2+(Psat2-Psat1)*x,Psat1*Psat2/(Psat1+x*(Psat2-
Psat1)),x=0..1,
axes=BOXED,xtickmarks=10,labels=["x1,y1","P/mm Hg"],
labeldirections=[HORIZONTAL,VERTICAL],title=[P-x-y diagram])
```

Using the `implicitplot` command, we can readily construct Txy diagrams with Maple, for both ideal and nonideal systems, without trial-and-error or iterative procedures.

As a further example of the use of metacomputing software in phase equilibria, we note that Dickson, *et al.*,<sup>[4]</sup> have demonstrated the use of Mathcad<sup>[5]</sup> to obtain 3-dimensional vapor-liquid equilibrium envelopes.

In conclusion, although we agree with much of what the author says, we believe that there is more than he allows in "making phase equilibrium more user-friendly."

**R.W. Missen**

*University of Toronto*

**W.R. Smith**

*University of Ontario Institute of Technology*

### References

1. Misovich, M.J., "Making Phase Equilibrium More User-Friendly," *Chem. Eng. Ed.*, **36**(4), 284 (2002)
2. Felder, R.M., "How to Survive Engineering School," *Chem. Eng. Ed.*, **37**(1), 30 (2003)
3. MAPLE is a registered trademark of Waterloo Maple, Inc.
4. Dickson, J., J.A. Hart, IV, and Wei-Yin Chen, "Construction and Visualization of VLE Envelopes in Mathcad," *Chem. Eng. Ed.*, **37**(1), 20 (2003)
5. MathCAD is a registered trademark of MathSoft, Inc. □

# MATHEMATICAL MODELING AND PROCESS CONTROL OF DISTRIBUTED PARAMETER SYSTEMS

## Case Study: The One-Dimensional Heated Rod

LAURENT SIMON, NORMAN W. LONEY

New Jersey Institute of Technology • Newark, NJ 07102

**D**istributed parameter systems (DPS) such as chemical vapor deposition (CVD), nanostructured coatings processing, population balance, transdermal drug delivery, or film growth are normally represented by partial differential equations (PDEs). They have important industrial applications, but controlling them presents theoretical and practical challenges.<sup>[1]</sup> One of the methods employed to control first- and second-order systems uses an exact reduction of a distributed parameter system to a lumped one.<sup>[2]</sup> The theory of lumped parameter systems can then be used to design a controller that meets user specifications and desired quality objectives. Laplace transform is a common technique used to derive the lumped parameter system. Although the conversion is straightforward, the inversion of the resulting Laplace transform equation is usually not trivial.

This paper shows that certain materials covered in mathematical modeling and process control courses are good starting points for designing controllers for these systems. The work is divided into

- **Section 1**, dealing with the solution of a one-dimensional rod in the Laplace domain
- **Section 2**, using the residue theorem to invert the Laplace transform
- **Section 3**, dealing with the design of a PI controller for set-point tracking
- **Section 4**, includes experiences in teaching courses in mathematical methods and chemical process control

### SOLUTION OF THE ONE-DIMENSIONAL ROD PROBLEM

Consider a one-dimensional rod (see Figure 1). The boundary conditions are such that heat from a steam chest is added

to the system at  $z = 0$ , while the other end,  $z = 1$ , is perfectly insulated.<sup>[2]</sup> The variables are

$$x(z, t) = T - T_d \quad (1)$$

$$u(t) = T_w - T_{wd} \quad (2)$$

where  $T$  and  $T_w$  are the temperature of the rod and steam chest, respectively. Variables  $x$  and  $u$  represent deviations from the set-point values  $T_d$  and  $T_{wd}$ . The model equation is

$$\frac{\partial x(z, t)}{\partial t} = \frac{\partial^2 x(z, t)}{\partial z^2} \quad (3)$$

The boundary conditions are

$$\frac{\partial x}{\partial z} = \beta(x - u) \quad z = 0 \quad (4)$$

and

$$\frac{\partial x}{\partial z} = 0 \quad z = 1 \quad (5)$$

The initial condition is

$$x(z, 0) = 0 \quad (6)$$

To solve Eqs. (3) to (6), we first take Laplace transforms with respect to time:

$$sX(z, s) - x(z, 0) = \frac{d^2 X}{dz^2} \quad (7)$$

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$$\frac{dX}{dz} = \beta(X - U) \quad z=0 \quad (8)$$

$$\frac{dX}{dz} = 0 \quad z=1 \quad (9)$$

Using the initial condition, Eq. (7) becomes

$$sX(z, s) = \frac{d^2X}{dz^2} \quad (10)$$

In operator form

$$(s - D^2)X = 0 \quad (11)$$

The characteristic equation is

$$s - r^2 = 0 \quad (12)$$

with roots

$$r = \pm\sqrt{s} \quad (13)$$

The general solution is

$$X = a_1 e^{-(\sqrt{s})z} + a_2 e^{+(\sqrt{s})z} \quad (14)$$

in terms of exponential function, or

$$X = c_1 \sinh(z\sqrt{s}) + c_2 \cosh(z\sqrt{s}) \quad (15)$$

in terms of hyperbolic function.

Using the boundary condition, Eq. (8), one obtains

$$\left. \frac{dX}{dz} \right|_{z=0} = c_1 \sqrt{s} \cosh(0) + c_2 \sqrt{s} \sinh(0) = \beta [c_1 \sinh(0) + c_2 \cosh(0) - U(s)] \quad (16)$$

or

$$c_1 \sqrt{s} = \beta [c_2 - U(s)] \quad (17)$$

Furthermore, the boundary condition given by Eq. (9) yields

$$\left. \frac{dX}{dz} \right|_{z=1} = c_1 \cosh(\sqrt{s}) + c_2 \sinh(\sqrt{s}) = 0 \quad (18)$$

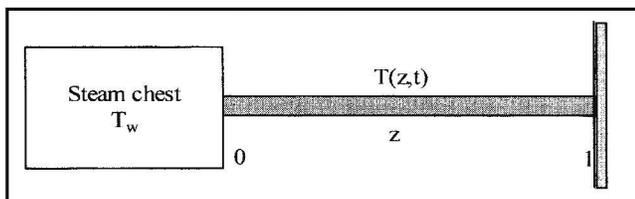
or

$$c_1 + c_2 \tanh(\sqrt{s}) = 0 \quad (19)$$

Solving Eqs. (17) and (19) results in

$$c_1 = \frac{-\beta U(s) \tanh(\sqrt{s})}{\beta + \sqrt{s} \tanh(\sqrt{s})} \quad \text{and} \quad c_2 = \frac{\beta U(s)}{\beta + \sqrt{s} \tanh(\sqrt{s})} \quad (20)$$

Therefore, Eq. (15) becomes



**Figure 1.** A one-dimensional rod heated by a steam chest of temperature  $T_w$ . The temperature of the rod at position  $z$  and time  $t$  is denoted by  $T(z, t)$ .

$$X(s, z) = \frac{-\beta U(s) \tanh(\sqrt{s})}{\beta + \sqrt{s} \tanh(\sqrt{s})} \sinh(z\sqrt{s}) + \frac{\beta U(s)}{\beta + \sqrt{s} \tanh(\sqrt{s})} \cosh(z\sqrt{s}) \quad (21)$$

or

$$\frac{X(s, z)}{U(s)} = \frac{\beta}{\beta + \sqrt{s} \tanh(\sqrt{s})} \left[ -\tanh(\sqrt{s}) \sinh(z\sqrt{s}) + \cosh(z\sqrt{s}) \right] \quad (22)$$

Since thermal energy is continually transferred from the upper end of the metal rod to the lower end, it is of particular interest to study the temperature profile at the lower end of the rod and the time it takes this temperature to settle down to equilibrium.

At  $z = 1$ , Eq. (22) becomes

$$\frac{X(s, 1)}{U(s)} = \frac{\beta}{\beta + \sqrt{s} \tanh(\sqrt{s})} \left[ -\tanh(\sqrt{s}) \sinh(\sqrt{s}) + \cosh(\sqrt{s}) \right] \quad (23)$$

Recall that

$$\cosh^2(z) - \sinh^2(z) = 1 \quad (24)$$

so Eq. (23) can also be written as

$$\frac{X(s, 1)}{U(s)} = \frac{\beta \operatorname{sech}(\sqrt{s})}{\beta + \sqrt{s} \tanh(\sqrt{s})} \quad (25)$$

## INVERSION OF THE LAPLACE TRANSFORM

In principle, control design for lumped parameter linear systems can be used to analyze Eq. (25), but the analysis is not trivial since the zeros and poles are not easily obtainable. We seek an expression of the form

$$G(s) = \frac{X(s, 1)}{U(s)} = \frac{P(s)}{Q(s)} \quad (26)$$

where  $P$  and  $Q$  are polynomials in  $s$  and  $Q(s)$  is of higher degree than  $P(s)$ .<sup>[3]</sup>

The inverse transform of  $G(s)$  is given by

$$L^{-1}\{G(s)\} = \sum_{k=1}^{\infty} \operatorname{Res}[F(s)e^{st}, s_k] \quad (27)$$

where the sum is taken over all the residues of the complex function  $F(s)e^{st}$ . The function

$$\rho_k(t) = \operatorname{Res}[F(s)e^{st}, s_k] \quad (28)$$

is the residue of  $F(s)$  at the singularities (poles)  $s_k$ . Its value is given by

$$\rho(t) = \frac{P(s_k)}{Q'(s_k)} e^{s_k t} \quad (29)$$

where  $Q'(s_k)$  is the value of  $dQ/ds$  evaluated at the singular points of interest.<sup>[3,4]</sup>

The quantity  $P(s_k)/Q'(s_k)$  can be written as

$$\frac{P(s_k)}{Q'(s_k)} = \lim_{s \rightarrow s_k} \frac{P(s)}{\frac{Q(s) - Q(s_k)}{s - s_k}} = \lim_{s \rightarrow s_k} (s - s_k) \frac{P(s)}{Q(s)} \quad (30)$$

When  $s_k$  is a multiple pole of order  $m$  of  $F(s)$ , then

$$\rho_k(t) = e^{s_k t} \left[ A_1 + tA_2 + \frac{t^2}{2!} A_3 + \dots + \frac{t^{m-1}}{(m-1)!} A_m \right] \quad (31)$$

or

$$\rho_k(t) = e^{s_k t} \sum_{i=1}^m A_i \frac{t^{i-1}}{(i-1)!} \quad (32)$$

where

$$A_i = \lim_{s \rightarrow s_k} \frac{1}{(m-i)!} \frac{d^{m-i}}{ds^{m-i}} \left[ (s - s_k)^m F(s) \right] \quad (33)$$

Recall that

$$\mathcal{L} \left\{ \frac{a}{n!} t^n e^{-bt} \right\} = \frac{a}{(s+b)^{n+1}} \quad (34)$$

$G(s)$  can now be written as a ratio of polynomials. In the discussion that follows, we will first show that for a step change in the amount of heat added to the steam chest, the temperature at  $z = 1$  follows a time trajectory before settling to a steady-state value. The amount of heat is usually determined from steady-state analysis, which is very common in chemical engineering. This is the case of most controlled membrane devices in which a specified drug concentration in the donor cell is used in order to reach a required steady-state concentration in the receiver cell.

This work shows that it is possible to change the heat from the steam chest in order for the temperature at  $z = 1$  to reach the desired value in a predetermined manner. In other words, both the system performance and the final value can be set a priori. A standard PI controller can be used for this purpose.

With  $\beta=1$ , Eq. (25) becomes

$$\frac{X(s,1)}{U(s)} = \frac{\operatorname{sech}(\sqrt{s})}{1 + \sqrt{s} \tanh(\sqrt{s})} \quad (35)$$

The identification of  $P(s)$  and  $Q(s)$  is not difficult in the case of polynomials. For expressions involving transcendental functions, one has to make certain that the numerator does not involve a singularity. Since the hyperbolic secant function does not have a singularity, the denominator is represented by

$$Q(s) = 1 + \sqrt{s} \tanh(\sqrt{s}) \quad (36)$$

The first four poles are  $s_1 = -0.7402$ ,  $s_2 = -11.7349$ ,  $s_3 = -41.4388$ , and  $s_4 = -90.80821$ . The function "FindRoot" in Mathematica® was used to compute these roots. Figure 2 shows a plot of  $Q$  as a function of  $s$ . Although an infinite number of poles are obtained, it is customary to use the first

two poles since they dominate the system response. Four poles are taken in this work for increased accuracy.

By taking the derivative of the denominator,  $Q'(s)$ , one obtains

$$Q'(s) = \frac{1}{2} \left[ \operatorname{sech}^2(\sqrt{s}) + \frac{\tanh(\sqrt{s})}{\sqrt{s}} \right] \quad (37)$$

From Eqs. (27) and (29), the inverse Laplace transform is

$$\mathcal{L}^{-1}\{G(s)\} = \frac{P(s_1)}{Q'(s_1)} e^{s_1 t} + \frac{P(s_2)}{Q'(s_2)} e^{s_2 t} + \frac{P(s_3)}{Q'(s_3)} e^{s_3 t} + \frac{P(s_4)}{Q'(s_4)} e^{s_4 t} \quad (38)$$

$$\mathcal{L}^{-1}\{G(s)\} = 0.8284e^{-0.7402t} - 1.7801e^{-11.7349t} + 1.9308e^{-41.4388t} - 1.9676e^{-90.8082t} \quad (39)$$

$G(s)$  is then

$$G(s) = \frac{0.8284}{s+0.7402} - \frac{1.7801}{s+11.7349} + \frac{1.9308}{s+41.4388} - \frac{1.9676}{s+90.8082} \quad (40)$$

or

$$\frac{X(s,1)}{U(s)} = \frac{-0.988583s^3 - 24.1254s^2 - 1300.31s + 32435.1}{s^4 + 144.722s^3 + 5421.46s^2 + 48092.0s + 32684.7} \quad (41)$$

## CONTROLLER DESIGN

In practice, the size  $A$  of the step change in  $U(s)$  (the steam chest temperature) necessary to get a desired value for  $X(s,1)$  (the temperature at the end of the rod) is usually known from steady-state analysis or experiments. Therefore,  $X(s,1)$  then becomes

$$X(s,1) = \frac{-0.988583s^3 - 24.1254s^2 - 1300.31s + 32435.1}{s^4 + 144.722s^3 + 5421.46s^2 + 48092.0s + 32684.7} \frac{A}{s} \quad (42)$$

An important concept in process analysis and control is the steady-state gain defined as the ratio of steady-state changes

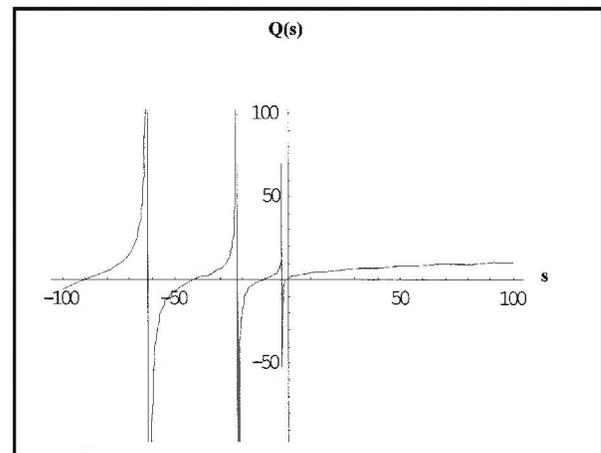


Figure 2. Characteristic equation  $Q$  as a function of poles  $s$ . The poles are in the range  $(-100, 100)$ .

in the process output to sustained changes in process input.<sup>[5]</sup>

Using the property

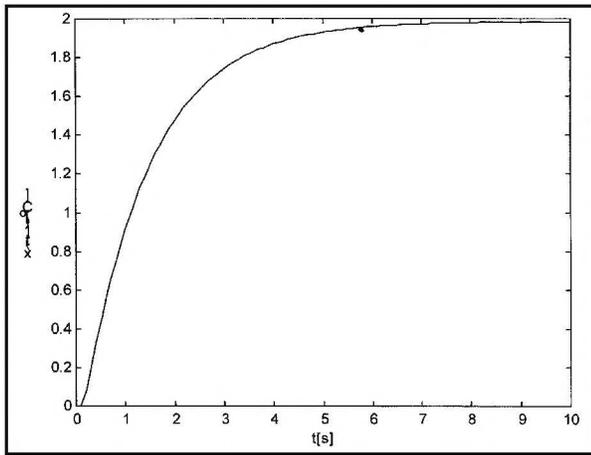
$$\lim_{t \rightarrow \infty} x(t,1) = \lim_{s \rightarrow 0} [sX(s,1)] \quad (43)$$

Eq. (42) becomes

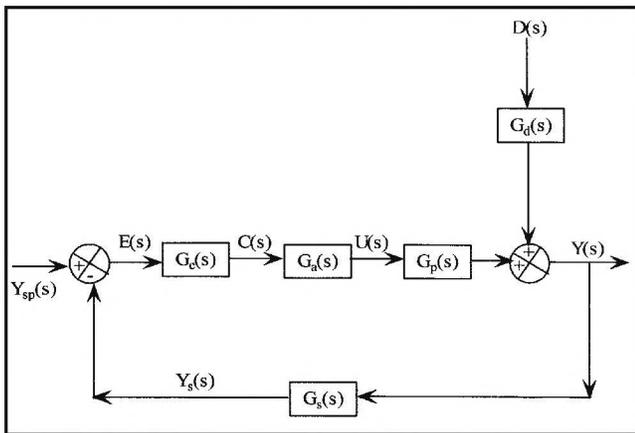
$$\lim_{s \rightarrow 0} [sX(s,1)] = \frac{32435.1 \text{ A}}{32684.7} = 0.9924 \text{ A} \quad (44)$$

The process steady-state gain is 0.9924, which means that each degree increase or decrease in  $u(t)$  will correspond to a change in  $x(t)$  of size 0.9924. To graph the response, one can invert Eq. (42) to get

$$x(t,1) = A[0.9924 + 0.02167 \exp(-90.8082t) - 0.04659 \exp(-41.4388t) + 0.1517 \exp(-11.7349t) - 1.1191 \exp(-0.7402t)] \quad (45)$$



**Figure 3.** Response  $x(t,1)$  as a result of an input step increase of size 2. This plot is generated using the “step” function in Matlab. The manipulated input variable is  $T_w$ .



**Figure 4.** Block diagram of a general feedback control loop. The transfer functions  $G_c(s)$ ,  $G_a(s)$ ,  $G_p(s)$ ,  $G_d(s)$ , and  $G_s(s)$  represent the dynamics of the controller, actuator, process, disturbance, and sensor, respectively. The inputs  $D(s)$ ,  $E(s)$ , and  $Y_{sp}(s)$  (in the Laplace domain) are the disturbance, error, and setpoint, respectively. The output of the system is denoted by  $Y(s)$ .

For example, if we use an A-value of 2 (step change size), the response  $x(t,1)$  is as shown in Figure 3. This plot is obtained by using the “step” function in Matlab. It is widely accepted that the response reaches its final value when it is within  $\pm 5\%$  of its final value and remains constant.<sup>[6]</sup> The final value is 1.9847. By setting  $x(t,1)$  to 95% of the final value (1.8855), Eq. (45) is solved to give a time  $t = 4.2097$  seconds, which is the time it takes the system to reach steady state.

The performance of the system can be improved by pole placement (also called direct synthesis). The main idea of pole placement is to design a controller such that the system has closed-loop poles at desired locations. In this work, only the methodology and the final results are outlined. Further details and derivations can be found in the literature.<sup>[5-7]</sup>

Consider the block diagram of a general feedback control loop (seen in Figure 4).<sup>[7]</sup> The transfer functions  $G_c(s)$ ,  $G_a(s)$ ,  $G_p(s)$ ,  $G_d(s)$ , and  $G_s(s)$  represent the dynamics of the controller, actuator, process, disturbance, and sensor, respectively.  $G_s$  represents how the sensor responds to a change in the temperature. In our example,  $Y(s)$  stands for the temperature at  $z = 1$ , which is measured by a thermocouple ( $G_s$ ). The measured variable is then compared with the desired value  $Y_{set}$ , yielding an error  $Y - Y_{set}$  (see Figure 4). This deviation is sent to a controller  $G_c(s)$ . The output of the controller (which is the temperature of the steam chest) goes to an actuator or final control element (*i.e.*, a steam valve) that regulates the temperature of the chest. Assuming no disturbance to the process ( $D(s) = 0$ ), it can be shown that the closed-loop transfer function for set-point tracking is given by<sup>[7]</sup>

$$G_{cl}(s) = \frac{Y(s)}{Y_{sp}(s)} = \frac{G_p(s)G_a(s)G_c(s)}{G_c(s)G_p(s)G_a(s)G_s(s)+1} \quad (46)$$

This equation relates the process output to the set point. The equation

$$G_c(s)G_p(s)G_a(s)G_s(s)+1=0 \quad (47)$$

is called the characteristic equation of the feedback loop. the roots of this equation are the poles of the feedback process. Consequently, they determine the response of the process. For our example, assuming  $G_a(s) = G_s(s) = 1$ , we obtain

$$G_{cl}(s) = \frac{G_p(s)G_c(s)}{G_c(s)G_p(s)+1} \quad (48)$$

Solving for  $G_c(s)$ ,

$$G_c(s) = \frac{G_{cl}(s)}{G_p[1-G_{cl}(s)]} \quad (49)$$

The pole-placement problem consists of placing the closed-loop poles at desired locations to meet performance specifications. A general controller can then be derived using this procedure. Based on issues related to pole-zero cancellations, however, and the fact that PID controllers are more available, we will derive a PI controller. The first step in the pro-

cedure is to approximate the plant as a first-order system with dead time

$$G_{pl}(s) = \frac{K_p e^{-\theta_p s}}{\tau_p s + 1} \quad (50)$$

where  $G_{pl}(s)$  is the transfer function of the first-order system. The gain  $K_p = (\Delta y / \Delta u)$  is the steady-state process gain. The quantity  $\theta_p$  is the time delay and  $\tau_p$  is the time constant. A reasonable choice for  $G_{cl}(s)$  is<sup>[5]</sup>

$$G_{cl}(s) = \frac{e^{-\theta_c s}}{\tau_c s + 1} \quad (51)$$

such that the closed-loop transfer function also contains a time delay. The time constant determines the dynamic path of the process as it approaches the new steady state. The parameters  $\theta_c$  and  $\tau_c$  are pre-specified design parameters. The condition  $\theta_p - \theta_c \geq 0$  must hold since the controller cannot respond to a set-point change in less than  $\theta_p$  time units.<sup>[5]</sup> From Eq. (49)

$$G_c(s) = \frac{\frac{e^{-\theta_c s}}{\tau_c s + 1}}{\frac{K_p e^{-\theta_p s}}{\tau_p s + 1} \left[ 1 - \frac{e^{-\theta_c s}}{\tau_c s + 1} \right]} \quad (52)$$

or

$$G_c(s) = \frac{\tau_p s + 1}{K_p (\tau_c s + 1 - e^{-\theta_c s})} \quad (53)$$

with  $\theta_c = \theta_p$ . Using a first-order Taylor series expansion,

$$e^{-\theta_c s} = 1 - \theta_c s \quad (54)$$

Equation (53) becomes

$$G_c(s) = \frac{\tau_p s + 1}{K_p (\tau_c s + \theta_p s)} = \frac{\tau_p s + 1}{K_p (\tau_c + \theta_p) s} = \frac{\tau_p}{K_p (\tau_c + \theta_p)} \left( 1 + \frac{1}{\tau_p s} \right) \quad (55)$$

which is the form of the PI controller with

$$K_c = \frac{\tau_p}{K_p (\tau_c + \theta_p)} \quad \tau_1 = \tau_p \quad (56)$$

where  $K_c$  is the controller gain and  $\tau_1$  is the reset time.

The original plant can now be approximated by

$$G_{pl}(s) = \frac{0.9924 e^{-0.1672s}}{1.379s + 1} \quad (57)$$

Figure 5 shows that Eq. (56) is a very good model of the plant dynamics.

Assuming that one wants to reduce the time constant by a half and one third (in this case  $\tau_c = 1.379/2 = 0.6895$  sec and  $\tau_c/3 = 0.4597$  sec, respectively), let us study how the system responds to a unit step change in the temperature

of the steam chest with these design parameters using a PI control. By using Eq. (56), one obtains  $\tau_1 = 1.3790$  sec in both cases. The controller gains ( $K_c$ ) are 1.6220 and 2.2166 for time constants of 0.6895 and 0.4597 sec respectively. Figure 6 shows the implementation of the controller using Simulink. Two loops are shown with the same plant transfer functions. The first loop is the closed-loop response with the PI controller, the second one is an open-loop. Both responses are recorded in block "scope." Figure 7 compares the open- and closed-loop responses. From the figure, the performance of the system is greatly improved. Figure 7 shows the system responses to an input step change of size two.

Using a discrete form for the transfer functions, one can easily implement the controller at desired sampling intervals. The Matlab function "c2d" converts the continuous system to a discrete-time system with specified sample time. The velocity form of the PI controller can then be used.<sup>[6]</sup> The end

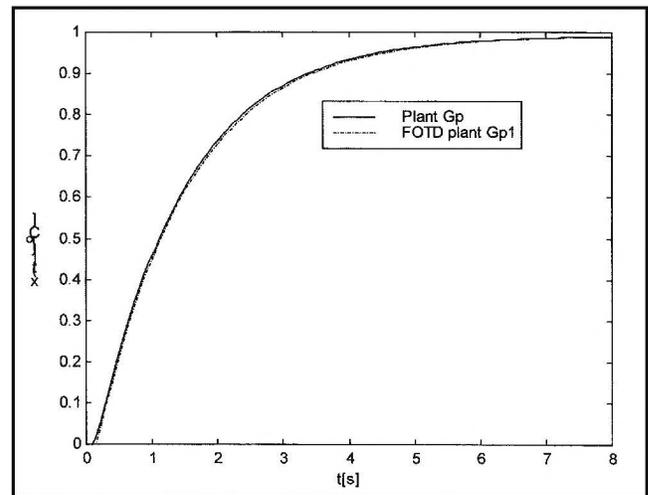


Figure 5. Comparison of the true (solid line) and approximated (dashed line) plant dynamics. The approximated plant is represented by a first-order plus delay (FOTD) model.

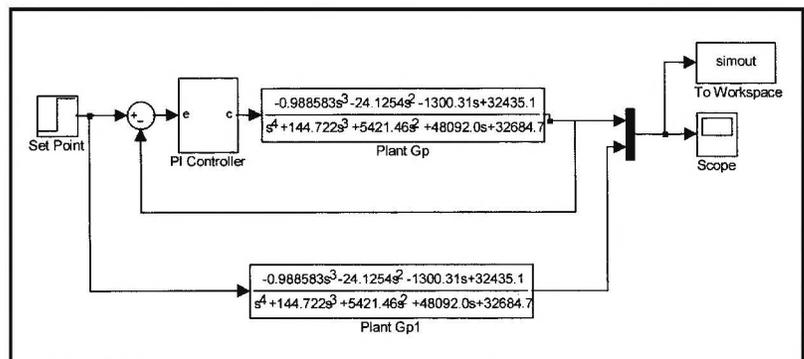
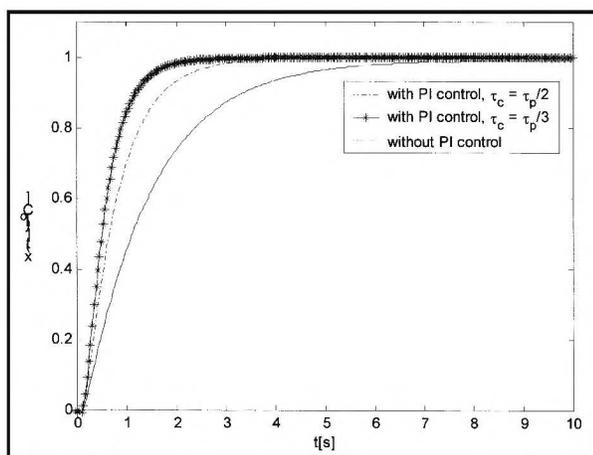


Figure 6. Diagram of the PI controller using Simulink. The step change is implemented by the block "Setpoint." The loop  $G_p$  is the closed-loop response with the PI controller,  $G_{pl}$  is part of the open-loop configuration. Both responses are monitored in block "scope." The block "simout" allows the closed and open-loop responses to be saved in the workspace.

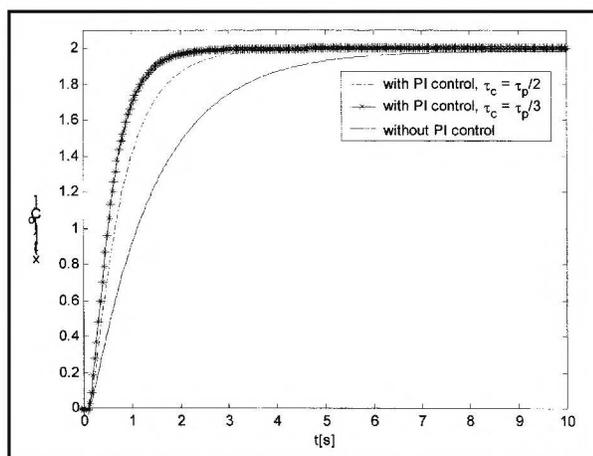
result is that at sampling time, a process operator can manually calculate the controller output using a hand calculator. Since a PI controller is relatively inexpensive, however, and in view of the increased performance of the system, it is advantageous to use one in line with the systems and in computing the best adjustable parameters computed off-line. It should be noted that a PI controller could be tuned with much less effort using classical tuning approaches such as field tuning, Cohen and Coon, and Ziegler-Nichols tuning methods.<sup>15-71</sup> Pole placement, however, can be used to develop a general controller (which may not have a PID or PI structure) designed to meet preset performance criteria.

## TEACHING MATHEMATICAL METHODS, DYNAMICS, AND CONTROL

First-year chemical engineering graduate students at NJIT



**Figure 7.** Closed-loop and open-loop response (—) for a simulation time of 10 seconds. The time constants were reduced by a half (---) and one third (-\*-). A unit step change was used.



**Figure 8.** Closed-loop and open-loop response (—) for a simulation time of 10 seconds. The time constants were reduced by a half (---) and one third (-\*-). A step change of size 2 was used.

take a 3-credit class in “Applied Mathematical Methods” in chemical engineering practice (see textbook<sup>31</sup>). They are also exposed to an undergraduate 4-credit course that deals with process dynamics and control. A course in the control of distributed parameter systems has not yet been offered in the department, but the potential is being explored through collaborative efforts among faculty members, mini-projects with industrial applications, and extensive research. Such problems are also ideal for independent studies.

Undergraduate chemical engineering students at NJIT react positively to the process dynamics and control of lumped parameter systems. With time, they understand Laplace transforms and have no difficulty analyzing dynamic behavior of feedback-controlled processes. The inversion of Laplace transforms is, usually, the most challenging part. Solving problems in class and completing homework assignments help considerably. These students are also encouraged to use mathematical software to plot, find roots, and take derivatives of special functions (*e.g.*, Mathematica, Matlab).

The students are given examples of industrial chemical processes in which they use their fundamental knowledge in mathematics to analyze the system open-loop and closed-loop dynamics. While using the techniques learned in class (transfer functions, closed-pole analysis, controller tuning) to solve practical chemical engineering problems, two things become apparent to them: first, the skills that they are learning are relevant and in demand; second, that they are imbued with knowledge and insight to solve these problems. The students respond very well to this approach, and some have even become interested in doing research in control of drug delivery systems.

## CONCLUSION

A one-dimensional perfectly insulated rod was solved in the Laplace domain with given boundary conditions. The solution in Laplace domain was inverted to the time domain using the residue theorem. The temperature profile (at the right end  $z = 1$ ) was approximated as a first-order system with a time delay of 0.167 sec and a time constant of 1.379 sec. A proportional-integral (PI) controller was then used to decrease the time constant of the process by 50 and 33%.

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# PROCESS SIMULATION AND MCCABE-THIELE MODELING

## *Specific Roles in the Learning Process*

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Standard texts on equilibrium staged separations<sup>[1,2]</sup> present the McCabe-Thiele, graphical approach as a primary tool for modeling and designing staged separation processes such as distillation, absorption, extraction, and stripping. The development of process simulation software, however, has impacted the way this material is taught. In a recent survey<sup>[3]</sup> of U.S. chemical engineering departments, 57% of the respondents indicated that they now use process simulators in teaching equilibrium-staged operations, and this number is presumably still growing. Recently, authors have discussed methods of integrating process simulators into lecture courses<sup>[4]</sup> and of using simulators to facilitate major project work.<sup>[5]</sup>

Simulators certainly have not, and should not, entirely replace “hand” solution techniques. The primary pedagogical concern regarding process simulators is that they function as black boxes. In many cases students can use them to solve specific problems without necessarily understanding the physical process they are modeling.<sup>[3]</sup> They are likely to accept the results of the simulation blindly, with no thought of the potential limitations of the modeling approach used.

One merit of traditional graphical approaches is that they provide some insight into what the simulator is actually doing. A further consideration is that graphical approaches provide a convenient framework for visualizing the process. Wankat<sup>[6]</sup> points out that even experienced engineers “commonly use McCabe-Thiele diagrams to understand or help debug simulation results.” But the merit of extending the hand calculations significantly beyond simple graphical models, such as using the Ponchon-Savarit method to include the energy balance, is less clear in the era of process simulation.<sup>[7]</sup>

It is such considerations that led Wankat to recommend “an eclectic approach that includes classical graphical and

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***The course organization is consistent with what is known about cognition and the progression of student understanding, and it appeals to students with varied learning styles.***

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analytical methods, computer simulations, and laboratory experience.”<sup>[6]</sup> This paper examines how an effective balance between these various components can be attained, using research into cognition and the learning process as a guide.

Over the past three years, the author has taught a 2-credit-hour, 14-week course (two 75-minute periods per week) on equilibrium staged separations (see Table 1 for a summary of its content). Enrollment varied between 14 and 22 first-semester juniors. In the fall of 1999, the course was taught using a lecture format almost exclusively. Material was presented in a purely deductive manner, closely following Wankat’s textbook<sup>[1]</sup> and making little use of process simulation.

In the fall 2000 and 2001 semesters, the course was organized as described in this paper (still using the Wankat text-



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book). Active learning exercises were employed throughout, with lab demonstrations, McCabe-Thiele modeling, and process simulation playing specific, complementary roles that are discussed in detail in this paper. Significantly, restructuring the course did not affect the class time requirements summarized in Table 1 and required no increase in preparation time on the part of the instructor aside from the one-time investment of learning to use HYSYS.

## COURSE ORGANIZATION

In a series of articles in *Chemical Engineering Education*, Haile<sup>[8-12]</sup> discussed the operation of the human brain and the learning process. This paper discusses how these insights on cognition were used to guide the course's organization and

the specific role McCabe-Thiele modeling and process simulation should play. This paper uses column distillation as an example, but the approach is readily applied to other physical processes and was integrated throughout the course.

Haile described<sup>[9]</sup> a "special hierarchy"—a progression of seven levels at which a student can understand concepts. These levels are summarized in Table 2 along with examples of capabilities of students who understand distillation at a particular level. The table assumes McCabe-Thiele is the primary modeling tool used.

Haile<sup>[11]</sup> also described a general hierarchy of modes of understanding that includes

*Somatic Understanding* • Tactile learning. Observing and handling something lays the groundwork for understanding it at higher, more abstract levels.<sup>[13]</sup>

*Mythic Understanding* • Oral traditions. Levels 1 and 2 of the special hierarchy fall within this realm.

*Romantic Understanding* • Characterized by abstractions such as writing and graphs. Level 3 of the special hierarchy is an example.

*Philosophic Understanding* • Logical reasoning. Levels 4 through 7 of the special hierarchy require a philosophic understanding.

The progression from Somatic to Philosophic understanding, in this case, suggests a course structure in which students are first exposed to a real distillation column, then they

are exposed to an abstract model of a column (such as a HYSYS model) that is already complete, and finally they learn to derive their own abstract model, namely the McCabe-Thiele model. The special hierarchy is also a useful guide. In Chapter 5 of Wankat's book, for example, the McCabe-Thiele model is derived and then used as a framework for illustrating such patterns as the trade-off between reflux ratio and the number of stages. The special hierarchy, however, suggests an alternative organization in which students are exposed to such concepts and patterns first (levels 1 through 3). This was accomplished by using HYSYS to generate simulated experimental data supporting an inductive presentation of the patterns. Derivation of a model came later in the context of solving problems (levels 4 and 5).

The following sections give a step-by-step discussion of strategy for advancing the students through the levels of understanding and the tools used to facili-

**TABLE 1**  
Topics in Equilibrium Staged Operations and Approximate Number of Class Periods Spent on Each

Topic (Number of 75-minute periods devoted to it)

- Introduction to Separations (1)
- Vapor-Liquid Equilibrium, Bubble/Dew Points (3)
- Flash Distillation, VLE Models (3)
- Binary Column Distillation (6)
- Multi-Component Distillation, Shortcut Methods (4)
- Absorption and Stripping (3)
- Liquid-Liquid Extraction (4)

**TABLE 2**  
Levels of Understanding in the Special Hierarchy as Described by Haile<sup>[9]</sup> and How They Might Manifest in Students Learning about Distillation

<u>Level of Understanding</u>	<u>Examples of Student Capability</u>
1. <i>Making Conversation</i>	• Describe in general how distillation works • Recognize a distillation column when seen
2. <i>Identifying Elements</i>	• Compare/contrast column distillation to flash distillation • Identify individual components of a column and explain their function
3. <i>Recognizing Patterns</i>	• Correctly predict relationships between column parameters, e.g., what happens to the heat duty in the reboiler when you raise the reflux ratio?
4. <i>Solving Problems</i>	• Use McCabe-Thiele model to determine the number of equilibrium stages required, given reflux ratio, top and bottom product compositions, and feed rate and composition
5. <i>Posing Problems</i>	• Use McCabe-Thiele model to solve a variety of distillation problems in which different sets of variables are used as "givens"
6. <i>Making Connections</i>	• Apply the McCabe-Thiele model to a column configuration (open steam heating, multiple feed, side stream product) that the student has never seen before
7. <i>Creating Extensions</i>	• Recognize that the McCabe-Thiele model is not valid for a given application and articulate how to modify the modeling technique to solve the problem at hand

tate each transition.

## ■ *Introduction to Column Distillation*

Haile<sup>[8]</sup> stated that because “learning creates new structures in the brain by modifying existing structures, learning can only begin from things the student already knows.” Flash, or single-stage, distillation is the logical lead-in for column distillation. The limitations of flash distillation were demonstrated by an example problem in which it took five flash stages to produce a desired product of >98% pure A from a feed of 50% A and 50% B. (This is similar to the presentation in Chapter 4 of Wankat’s text.) Students began to calculate flow rates and compositions for all streams, given equilibrium data, but they quickly recognized that, practically speaking, the process makes no sense. The “saleable” product stream had a tiny flow rate and there was a clear need to somehow recycle the intermediate fractions.

The class then moved to the Unit Operations Laboratory, where the ten-stage distillation column had been prepared and was operating at steady state. The instructor explained the counter-current functioning of the column and discussed the purposes of the various components of the column (condenser, reboiler, etc.). Next, the instructor posed the question, “How is this like flash distillation and how is it different?” This exercise followed the active learning strategy advocated by Felder, *et al.*<sup>[14]</sup> The class broke into groups of two to three students each, where they brainstormed lists of similarities and differences, and then the instructor led the full class in a discussion.

These activities were viewed as a vehicle to bring the students to Level 2 of the special hierarchy (Table 2). The next step, as outlined above, was to expose the students to an abstract model of the process and to help them recognize patterns.

## ■ *Use of HYSYS for Inductive Presentation of Concepts*

Induction consists of starting with observation and inferring the governing physical principles, as opposed to deduction, which consists of deriving the specifics of the case at hand from the general principles. Educators have begun to recognize that induction is a more natural learning mode,<sup>[15,16]</sup> but most traditional textbooks are written deductively. The chemical engineering department at Rowan University has previously implemented experiments to promote inductive learning of heat and mass transfer.<sup>[17]</sup> Here, the students gained a qualitative understanding of the physical process of distillation inductively, using the simulator as a rapid way to generate simulated “experimental data.”

After seeing the real column, students moved to the computer lab and loaded a HYSYS model of a distillation column, which had been prepared and converged ahead of time by the instructor. Students then went through a short (about five minutes) tutorial on the software, learning how to access significant column parameters ( $Q_c$ ,  $Q_r$ , reflux ratio, product compositions, temperature profile, internal liquid and vapor flow rates) and how to specify them. The class discussed why each of these parameters is of interest to the engineer—for example, the reboiler heat duty is significant because energy is expensive.

Next, the students were asked to collect simulated data in order to quantify certain patterns, such as

- *The effect of reflux ratio on product purity*
- *The effect of feed stage location on product purity*
- *The effect of reflux ratio on condenser and reboiler heat duty*
- *The effect of number of stages on product purity*

In response, the students took the column through a series of configurations and plotted graphs of the relevant data. After collecting the information, students broke into small groups to brainstorm physical explanations for the trends in preparation for full-class discussion.

During this stage of the process, students also observed that liquid and vapor flow rates throughout the column were nearly uniform. The physical reason for this, involving the energy balance on each individual stage, was another topic for discussion. Students were thus exposed to the physical justification for the constant molal overflow approximation before they knew of its significance in simplifying by-hand calculations.

HYSYS was specifically chosen for this process as part of a department-wide effort to introduce students to process simulation before the senior design sequence. Burns and Sung,<sup>[18]</sup> however, have created McCabe-Thiele models on spreadsheets and used them for comparable classroom demonstrations. The McCabe software package<sup>[19,20]</sup> developed at the University of Michigan is also ideally suited for inductive exploration of cause/effect relationships within a column.

The activities described in this section are viewed as a vehicle to instill a romantic understanding (Level 3 in the special hierarchy) of distillation in the students. The transition to a philosophic understanding (Level 4) was achieved by challenging students to devise their own model of the process.

## ■ *Hand Calculations*

After receiving this thorough introduction to the physical process, students were able to derive the model equations with relatively little guidance from the instructor beyond the

simple posing of questions. The sequence of questions is given here; for each, the students spent time working in teams before the full class discussed the results.

1. The instructor drew a control volume around the entire column and asked the students to list the process variables and brainstorm which of them would likely be given and which would likely be unknown.
2. The instructor then asked the students to write balance equations relating these variables to each other. The ensuing discussion led to a determination of the number of degrees of freedom in a column and the most likely ways of fulfilling them.
3. Next, the class wrote lists of variables and constraints (mass balance, energy balance, and equilibrium) for an individual stage and determined that no “new” degrees of freedom are introduced when one stage is added to the column.

At this point, the instructor pointed out that HYSYS models a column by solving these equations simultaneously with the constraint that all stages are at equilibrium. Thus, the function of the “black box” is elucidated.

Next, students were given an example problem involving a ten-stage distillation column and were able to demonstrate that the number of variables and constraints were equal—thus it was possible to attain a complete solution of all column parameters of interest. They also recognized the complexity of solving this many simultaneous equations “by hand.” The strategy of solving a system of equations that includes mass balances and equilibrium constraints by plotting both on the same y-x diagram was familiar to the students from the module on flash distillation. The instructor reminded the class of their observation that liquid and vapor flow rates throughout the column were essentially uniform and pointed out how the assumption of constant molal overflow led to mass balances in the form of straight operating lines. Students then learned the graphical technique of stepping off stages. This completed a deductive derivation of the McCabe-Thiele method, which was primarily carried out actively rather than in a lecture format.

While the McCabe-Thiele method was presented as a “pencil and paper” technique, the spreadsheet models<sup>[18]</sup> or McCabe<sup>[19,20]</sup> software package mentioned above could also be introduced at this stage. The crucial point is that the students have received a thorough exposure to the physical process, intended to provide the philosophic understanding required for true model building. They are therefore more likely

to appreciate the capabilities and limitations of the McCabe-Thiele model (in whatever form) and less likely to regard it as an arbitrary ritual.

## HIGHER LEVELS OF UNDERSTANDING

The activities outlined in the previous sections required, in total, approximately two weeks of class time. Progression through the higher levels (Levels 5 through 7) of the special hierarchy requires practice in problem solving through repetition and examination of variations.<sup>[10]</sup> In the fall of 2000 this was done exclusively using the McCabe-Thiele model for both in-class examples and homework problems, but in 2001 some homework problems were also completed on HYSYS so that students would have the experience of constructing models from scratch on the simulator. The final assignment in the 2001 module on distillation was one in which students designed the same two-column system both by hand and with HYSYS, comparing the results. This was intended to reinforce the students’ understanding of the assumptions and methodology behind both modeling approaches and the limitations of each, consistent with the highest levels of Haile’s special hierarchy of student understanding.

**... because “learning creates new structures in the brain by modifying existing structures, [and] learning can only begin from things the student already knows,” [flash], or single-stage, distillation is the logical lead-in for column distillation.**

## LEARNING STYLES

The course structure presented here used both process simulation and McCabe-Thiele modeling in a sequence that is logical according to the learning progression described by Haile. It was also consistent with the variety of learning styles<sup>[21]</sup> represented in any class

*Visual vs. Verbal Learning* • The students spent most of their class time discussing the system, either in small groups or with the full class. Throughout the process, however, visual learners were also stimulated. Introduction to distillation was carried out in the lab with a real, working column. Students transcribed the simulated data from HYSYS into graphical form and used the graphs as the basis for the discussion.

*Active vs. Reflective Learning*<sup>[22]</sup> • Small-group, active learning exercises were a feature of the entire course. The full-class discussions allowed the instructor to insure that the work from these activities was accurate and that no salient points were missed. But they were also intended to benefit the reflective learners in the class.

*Sensory vs. Intuitive Learning*<sup>[23]</sup> • Students were quickly immersed in studying and explaining physical phenomena, a

Continued on page 141.

# PERSONALIZED, INTERACTIVE, TAKE-HOME EXAMINATIONS

## *For Students Studying Experimental Design*

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In this day and age, many chemical engineers seek jobs traditionally filled by engineers from other disciplines, and the chemical engineering curriculum, particularly electives, can help enhance their prospects in that respect.<sup>[1]</sup> One crosscutting skill set that facilitates this trend is expertise in statistical methods.<sup>[2]</sup> Employers particularly value knowledge of the techniques of experimental design and quality control.<sup>[3,4]</sup>

The University of Missouri-Columbia's Department of Chemical Engineering offers a three-semester-hour course called "Experimental Design and Statistical Quality Control for Chemical Engineers." It is the most popular undergraduate elective, perhaps because it can be taken in lieu of a required course in probability and statistics offered in the College of Arts and Sciences. Graduate students, who must complete an additional semester project, also take the course.

The examinations described in this article are personalized and interactive in the sense that the students are allotted a prescribed number of experiments. Using a sequential approach in which some fraction of the experimental budget is expended in the first submission, each student submits a carefully formatted table of experimental conditions (factor-levels for each of the variables under consideration). The instructor uses a computer model that includes a random error term as a virtual laboratory to efficiently generate a unique data set for each submission. After interpreting the data from

the first set of experiments, the student submits additional experiments and receives additional sets of unique data until his or her experimental budget is expended. The appropriate set of experimental designs must be combined with accurate calculations and insightful analysis to arrive at "the truth,"

**TABLE 1**  
**List of Topics in "Experimental Design and Statistical Quality Control for Chemical Engineers"**

1. Normal distribution and the central limit theorem
2. Statistical quality control: creating, maintaining, and interpreting SQC charts
3. Statistical quality control: rational subgroups and interpretation
4. Significance testing
5. Z distribution
6. t distribution
7. Statistical dependence
8. Random sampling
9. Randomization
10. Blocking
11. Confidence intervals
12. Inferences about variances
13. Error propagation
14. Comparing more than two treatments
15. Empirical and theoretical models
16. Analysis of variance
17. Multiple comparisons
18. Randomized blocks with replication
19. Designs with more than one blocking variable
20. Balanced incomplete blocked designs
21. Full factorial designs
22. Interpreting the results of full factorial experiments
23. Determining significance of effects in factorial experiments
24. Applications of statistical quality control
25. Partial factorial designs
26. Design resolution
27. Confounding patterns
28. Sequential design of experiments; additional runs
29. Analysis of Residuals
30. Parsimony in empirical models
31. Linear regression
32. Nonlinear regression

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**TABLE 2**  
**Problem Statement**

You have accepted a job at Cavitron, a small start-up company. Cavitron is attempting to commercialize a turn-key, skid-mounted "pump-and-treat" system for use in oxidizing the organic and chlorinated organic compounds in aqueous mixtures.

Hydrodynamically induced cavitation is the operating principle for the treatment device, which is referred to as a "jet reactor." When polluted water is pumped at high pressure and high velocity through an appropriately designed nozzle and around an appropriately designed obstruction, microscopic bubbles form and implode in the fluid. Local temperatures reaching 800°C and local pressures in excess of 5,000 psi accompany the formation and implosion of the bubbles. Organic vapors predominate (relative to water vapor) in the bubbles. In the presence of dissolved oxygen and other oxidative species, as well as a miscible fluid catalyst (with appropriate vapor pressure), each bubble is a microreactor in which some fraction of the organic vapor is oxidized.

Your first project for Cavitron is to set up and operate a skid-mounted system for treating the leachate from a hazardous waste landfill. You will draw polluted water from the containment pond, treat it, and pump it back into the pond. Since each waste stream is different, the operating conditions for this application must be optimized. The response to be optimized is single-pass conversion (treatment efficiency). Table 3 lists seven standard process variables routinely evaluated at each installation. Factor level settings that experience has shown are in the proper experimental spaces are also provided. Your first task involves determining the effect of these seven "standard" process variables on treatment efficiency.

The Research and Development Department would also like you to evaluate four experimental modifications to the jet reactor. Field data is essential to verify laboratory results. At some point during your experimental campaign, you are to install the experimental modifications and proceed with testing. Table 3 also lists these experimental modifications (variables) and their factor level values. Your second task involves evaluating the effect of these experimental variables of treatment efficiency.

Your tasks are tabulated more specifically below.

**Task 1a:** Determine the sign and magnitude of the significant main effects and interactions of the standard process variables on the treatment efficiency of the unit.

**Task 1b:** Formulate an empirical model and evaluate its validity.

**Task 1c:** Recommend operating settings for these seven variables.

**Task 2a:** Determine the sign and magnitude of the significant main effects and interactions of the experimental modifications on the treatment efficiency of the unit.

**Task 2b:** Appropriately modify your empirical model from Task 1b and evaluate its validity.

**Task 2c:** Make recommendations about whether these four modifications should be adopted in future production units.

Time and budget constraints will allow you to perform 24 experiments. These may be submitted in whatever increments you choose over the next five days. Submit your sets of experimental conditions electronically and you will receive your data via return e-mail.

**TABLE 3**  
**Standard Variables and Experimental Variables/Modifications and Factor Levels**

*Standard Variables and Factor Levels*

Symbol	Description	- Level	+ Level
P	Pressure in the nozzle	2000 psi	3000 psi
L	Length of the pretreatment capillary	10 m	20 m
T	Temperature of the pretreatment capillary	25°C	70°C
C	Concentration of the catalyst	0.05 M	0.10 M
A	Angle of the obstruction	0°	5°
D	Diameter of the obstruction	5 cm	8 cm
X	Distance between nozzle and obstruction	0.5 mm	0.75 mm

*Experimental Variables and Factor Levels*

Symbol	Description	- Level	+ Level
S	Supersaturated oxygen	Off	On
K	Catalyst type	Standard	Experimental
O	Ozone generator	Off	On
N	Nozzle design	Standard	Experimental

an accurate estimate of the parameters of the model used to generate the data.

## COURSE STRUCTURE

The latest rendition of the course (spring semester, 2002) met for 50-minute sessions on Mondays, Wednesdays, and Fridays for fifteen weeks. Table 1 lists the topics discussed. They were selected to provide a practical statistical toolbox to chemical engineers in research, process engineering, and manufacturing.

The availability of computational tools, principally a personal computer and associated software, has allowed an increase in the complexity of calculations presented in chemical engineering classes, as well as in the homework assignments. In this class, most lectures (as well as all examples and homework solutions) were performed using the Excel™ spreadsheet program. These spreadsheets were made available, at the appropriate time, to the students via e-mail. This allowed the use of a relatively old but well-written and classic text that does not explicitly employ computer techniques or software.<sup>[5]</sup> Fortunately, on Mondays and Wednesdays the course met in a computer lab where each student had access to a computer. The use of a computer lab during class, however, is not required in the administration of this type of examination.

## DESCRIPTION OF THE EXAMINATION

It is difficult to give a comprehensive examination in a computationally intensive course when there are constrictions of class duration and/or access to computers in the classroom. Most chemical engineering examinations are completed during a single class period without the aid of computers. The availability of a computer lab does not circumvent the time constraint. The challenge for the instructor under these circumstances is to write an exam that promotes learning, discriminates among the students, and is consistent with the course content and homework.

Take-home examinations are an attractive option, but raise another problem: academic dishonesty. Although the percentage of students who collaborate improperly on take-home examinations is small, there is an opportunity for a minority to gain an unfair advantage. A take-home exam in which each student has a unique data set generated from a model including a random-error term eliminates the opportunity for one student to copy another's work. The use of several different models to generate the students' data sets provides a further obstacle to dishonest collaboration, but must be accounted for during record-keeping and grading.

Table 2 is the problem statement from a personalized, interactive, take-home examination based on this concept. Prior to the class in which it was presented, an electronic

version was e-mailed to each of the students as a worksheet in an Excel spreadsheet. This spreadsheet also included a worksheet containing Table 3, which includes the standard variables and the experimental variables/modifications as well as their factor-level settings. Also included was an abbreviated version of Table 4 (no factor levels, data, etc.), which was formatted for submission of experiments.

An individual student has a budget of 24 experiments. For a particular experiment, the model shown as Eq. (1) generates a data point:

$$y = I + \frac{P}{2}X_P + \frac{T}{2}X_T + \frac{D}{2}X_D + \frac{S}{2}X_S + \frac{O}{2}X_O + \frac{S \times O}{2}X_{S \times O} + \varepsilon \quad (1)$$

where  $y$  is the response, the single-pass conversion (%), and  $I$  is the overall average response ( $I = 15\%$ ). The  $X$ -variables ( $X_P, X_T, X_D, X_S, X_O$ ) have a value of -1 for the experiments in which the indexed variable is set at the minus level and +1 for the experiments in which the indexed variable is set at the plus level.  $X_{S \times O}$  is the factor level of the interaction between the  $S$  variable and the  $O$  variable, and its value is the sign of their product. The magnitudes of the main effects and interactions used in the model to generate the data are shown in Table 5. The student chooses the values of all 11 variables for each experiment. The variables that are not included in the model used to generate the data set ( $L, C, A, X, K, N$ ) are inert.

Equation 1 is an empirical model used to interpret data from factorial experiments. Theoretical models can also be appended with error terms to generate unique data sets for take-home examinations in core subjects such as thermodynamics and transport phenomena. More empirical curricula (*e.g.*, kinetics) are even more amenable to the technique.

The student submits a total of 24 experiments via e-mail over a period of five days. Most students submitted three sets of eight experiments each. It took about two minutes to open an e-mail, open the experimental design, insert the student's input into the model to generate a data set, save the data set, attach it to a return e-mail, and send. For example, if a class had 20 students, they would request 60 data sets, requiring the instructor to spend two hours generating data. The data generation process could be easily automated. The time required to write and grade this exam is similar to a conventional exam.

Based on the individualized data sets, the student must determine which of these variables has a significant effect on

**TABLE 5**  
Summary of Results

Main Effect/ Interaction	Model Parameter	Estimate from Data	Error	Recommended Setting
P	2.0	2.1	5%	+
L	—	—	—	-
C	—	—	—	-
T	-1.5	-1.8	-23%	-
A	—	—	—	-
D	-1.5	-1.7	-16%	-
X	—	—	—	-
S	3.0	2.9	4%	+
K	—	—	—	-
O	2.0	2.5	27%	+
SxO	3.0	3.0	0%	NA

**TABLE 4**  
Summary of Experimental Campaign

Exp. #	Standard Process Variables							Exp. Variables				Single Pass Conversion (%)	Empirical Model Prediction (%)	Residual (%)
	P	L	C	T = PxC	A = PxD	D = LxC	X = PxD	S	K	O	N			
1	-1	-1	-1	1	1	1	-1	-1	-1	-1	-1	11.8	11.1	0.7
2	1	-1	-1	-1	-1	1	1	-1	-1	-1	-1	14.8	15.0	-0.2
3	-1	1	-1	-1	1	-1	1	-1	-1	-1	-1	13.9	14.6	-0.7
4	1	1	-1	1	-1	-1	-1	-1	-1	-1	-1	15.5	14.9	0.6
5	-1	-1	1	1	-1	-1	1	-1	-1	-1	-1	13.2	12.8	0.4
6	1	-1	1	-1	1	-1	-1	-1	-1	-1	-1	16.4	16.7	-0.4
7	-1	1	1	-1	-1	1	-1	-1	-1	-1	-1	12.6	12.9	-0.4
8	1	1	1	1	1	1	1	-1	-1	-1	-1	13.4	13.2	0.2

Exp. #	P = SxK	L	C	T = SxO	A = KxO	D = X	S	K	O	N = SxO	Single Pass Conversion (%)	Empirical Model Prediction (%)	Residual (%)
10	-1	-1	-1	-1	1	-1	1	-1	-1	1	12.6	13.0	-0.4
11	-1	-1	-1	1	-1	-1	-1	1	-1	1	12.9	13.0	-0.1
12	1	-1	-1	-1	-1	-1	-1	1	1	-1	16.2	16.8	-0.6
13	1	-1	-1	1	-1	-1	-1	-1	-1	1	16.4	16.4	0.0
14	-1	-1	-1	1	-1	-1	-1	1	-1	1	18.7	18.4	0.3
15	-1	-1	-1	-1	1	-1	-1	-1	1	-1	12.2	12.6	-0.4
16	1	-1	-1	1	-1	1	-1	1	1	1	18.5	18.8	-0.3

Exp. #	P	L	C	T	A	D	X	S	K	O	N	Single Pass Conversion (%)	Empirical Model Prediction (%)	Residual (%)
18	1	-1	-1	-1	-1	1	-1	-1	-1	-1	-1	13.3	13.4	-0.2
19	1	-1	-1	-1	-1	1	-1	1	-1	-1	-1	15.3	15.1	0.2
20	1	-1	-1	-1	-1	1	-1	-1	-1	-1	-1	13.3	13.3	-0.1
21	1	-1	-1	-1	-1	1	-1	-1	-1	1	-1	14.5	14.7	-0.2
22	1	-1	-1	-1	-1	1	-1	-1	-1	1	-1	12.8	12.9	-0.1
23	1	-1	-1	-1	-1	1	-1	1	-1	1	-1	20.4	20.6	-0.2
24	1	-1	-1	-1	-1	1	-1	1	-1	1	-1	18.9	18.8	0.1

Variable	Main Effect (%)	Abbreviated Confounding Pattern
P	2.2	P + LxT + CxA + DxX
L	-0.2	L + PxT + CxD + AxX
C	-0.1	C + PxA + LxD + TxX
T	-1.0	T + PTL + AxD + LxX
A	-0.1	A + PxC + TxA + PxX
D	-1.6	D + LxC + TxA + PxX
X	-0.2	X + CxT + LxA + PxD
Average =	13.9	

Variable	Main Effect (%)	Abbreviated Confounding Pattern
P	2.0	P + SxK + TxD + OxD
T	1.5	T + PxT + SxO + KxN
D	-1.9	D + PxT + SxN + KxO
S	2.8	S + PxC + TxO + DxN
K	-0.3	K + PxC + TxN + DxO
O	2.7	O + PxC + TxS + DxK
N	-0.1	N + PxC + TxK + DxS
Average =	15.1	

Variable or Interaction	Main Effect (%)
T	-1.8
S	3.0
O	2.4
TxS	0.1
TxO	0.2
SxO	3.0
TxSxO	0.0
Average =	15.5

the single-pass conversion and which are inert. The sign and magnitude of the significant main effects must also be determined. Further, any significant interactions among the standard variables must be identified and their signs and magnitudes estimated. The student must also formulate an empirical model and evaluate its validity and recommend operating settings for these seven variables. Finally, each student must similarly assess the effects and interactions of four additional experimental variables of interest to the Research and Development Department.

Performing a full factorial experiment with eleven variables would require 2,048 experiments. As the experimental budget is about 1% of this amount, the use of highly fractionated partial factorial designs is required.

## SOLUTION TO THE EXAMINATION

The first step in one of many effective solution strategies is to design and perform a  $2^{7-4}_{III}$  partial factorial experiment focusing on the standard process variables. This is a resolution III “main effects” design because it estimates the main effects subject to a confounding pattern including two-way interactions. Aspects and advantages of this type of design are discussed in the course textbook.<sup>[5]</sup>

The first eight experiments shown in Table 4 prescribe this design. Pressure in the nozzle (P), length of the pretreatment capillary (L), and concentration of catalyst (C) are taken as the “live” variables. Their factor levels are assigned in standard order, as they would be for a  $2^3$  full factorial experiment.

The four remaining variables in the standard process variable set are temperature in the pretreatment capillary (T), angle of obstruction (A), diameter of obstruction (D), and distance between the nozzle and the obstruction (X). The levels of these variables are set according to the four combinations of interactions possible among the three live variables (*i.e.*,  $T=P \times L$ ,  $A=P \times C$ ,  $D=L \times C$ , and  $X=P \times L \times T$ ). Since all of the possible interactions among the three live variables were used as aliases for the additional variables, the design is referred to as fully saturated. The experimental variables/modifications are held at the minus (standard or unmodified) level for the first set of experiments.

Eight experiments were performed—therefore, eight parameters (the average and the seven main effects) can be estimated from the data. Each main effect is subject to confounding by fifteen other interactions. An abbreviated confounding pattern, including only the confounding two-way interactions, is also shown in Table 4. The data in the column headed “Single-Pass Conversion (%)” were generated using the model shown in Eq. (1).

Quantitative methods of determining significant effects are discussed in the course text<sup>[4]</sup> and will not be covered here. Examination of Table 4 reveals that the first eight experiments correctly indicate that P, T, and D may be important

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***Personalized, interactive, take-home examinations are not subject to the constraints of class duration and availability of computers . . . they can be more complex and thorough.***

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variables, while the remaining standard process variables (L, C, A, and X) may be relatively inert.

After evaluating the first set of experiments, the principle of sequential design of experiments must be practiced in the second design. This solution strategy involves another set of eight experiments, shown as experiments 9 through 16 in Table 4. In this design, the intent is to begin investigation of the experimental variables/modifications, while confirming and improving the estimates of the three standard variables judged to be significant. The experimental modifications/variables supersaturated oxygen (S), catalyst type (K), and ozone generator (O) are the live variables in a second  $2^{7-4}_{III}$  partial factorial experimental design. The alias for the final experimental variable/modification, nozzle design (N), is the three-way interaction among the live variables ( $N=S \times K \times O$ ). This design is also fully saturated in that the remaining three possible interactions among the live variables are used as aliases for the three variables judged to be significant during the first set of experiments ( $P=S \times K$ ,  $T=S \times O$ ,  $D=K \times O$ ). Table 4 also includes the data for these experiments, the abbreviated confounding pattern, and the parameter estimates based on the data.

The parameter estimates show that the experimental variables/modifications S and O may be significant, while K and N may be inert. Further, the estimates of the standard variable parameters P and D are confirmed. These estimates are subject to entirely different confounding patterns, lending credence to the assumption that it is these main effects and not their confounding two-way interactions that are significant.

The temperature variable, T, however, is a different matter. While both the first and second sets of experiments resulted in estimates of similar magnitude, the sign changed. This suggests the presence of a significant interaction. Careful examination of the abbreviated confounding patterns for both the first and second sets of experiments reveals that an interaction between S and O is the most likely candidate, as both are significant variables whose interaction has not been previously aliased to an inert variable. Therefore, the final eight experiments in the experimental budget are expended performing a  $2^3$  full factorial experiment using variable T, S, and O. This design has the advantage that all interactions are explicitly estimated. As shown in Table 4, this design provides an unambiguous estimate of the T effect, confirms and refines the estimate of the S and O effects, and reveals an important two-way interaction oxygen supersaturation and

ozone generation (SxO).

Table 5 summarizes the information gleaned from the experimental campaign and compares it to the actual parameters of the model used to generate the data. Three of the standard process variables were found to be significant, while the other four were determined to be inert. Two of the four experimental variables/modifications were determined to be significant, while the other two were inert. For all eleven variables, these determinations were correct (in agreement with the model used to generate the data). Further, the signs of all the effect and the interaction were also correct and the magnitudes were accurate between +/-30%. A column of recommended settings is also included in Table 5. For the inert variables, decisions about the settings are based on what might be expected to be easiest and cheapest.

Two empirical models can be developed from the data. The first

$$y = 13.9 + \frac{2.1}{2}X_P + \frac{-1.8}{2}X_T + \frac{-1.7}{2}X_D \quad (2)$$

predicts the single-pass efficiency of the jet reactor in its standard configuration (unmodified, all experimental variables/modifications at the minus level) as a function of the three significant standard variables. This model was used to generate the predicted values of the single-pass efficiency for the first eight experiments in Table 4.

The second model

$$y = 15.3 + \frac{2.1}{2}X_P + \frac{-1.8T}{2}X_T + \frac{-1.7}{2}X_D + \frac{2.9}{2}X_S + \frac{2.5}{2}X_O + \frac{3}{2}X_{S \times O} \quad (3)$$

predicts the performance of the jet reactor in its experimental configuration. It has a higher average and includes the S and O effects as well as their interaction. This model was used to generate the predicted values of the single-pass efficiency for the final sixteen experiments in Table 4.

Variables for both models are defined as in Eq. (1). Equation 3 is the experimental estimation of "the truth," as described by Eq. (1). Analysis of the residuals, tabulated in Table 4, was undertaken according to standard procedures and confirms the validity of the models.<sup>[5]</sup>

## STUDENT FEEDBACK

An interactive learning environment was established and persisted throughout the week of the exam. This excitement was felt by both the students and the instructor. Table 6 shows the results of a feedback survey administered to the class. There were 19 respondents. The results document that a personalized, interactive, take-home examination is not only a good learning tool, but is also popular with the students. Three estimates of the central tendency are included to aid in interpretation.

**TABLE 6**  
Summary of Anonymous Feedback Survey

(1 - Strongly Agree; 2 - Agree; 3 - Neutral; 4 - Disagree; 5 - Strongly Disagree)

	Avg.	Median	Mode
I understand the partial factorial experimental designs better as a result of this exam.	1.7	2	2
I understand the sequential nature of experimental design better as a result of this exam.	1.6	2	2
I like the individualized data concept.	2.0	2	2
I liked this exam.	2.2	2	2
I like take-home exams.	1.6	2	1
I learned a lot while working on this exam.	2.1	2	2
This exam was a superior learning experience relative to the other exams for this class.	2.4	2	2
This exam was a superior learning experience relative to exams in other engineering courses.	2.6	3	3
I spent more time on this exam relative to the other exams for this class.	2.1	2	2
I spent more time on this exam relative to exams in other engineering courses.	2.6	3	2
This exam really sucked.	4.0	4	4

## CONCLUSIONS

Personalized, interactive, take-home examinations are not subject to the constraints of class duration and availability of computers. Therefore, they can be more complex and thorough. Because a unique data set is generated for each student, the opportunities for dishonest collaborations are reduced. The use of several models to generate the students' data sets is a further barrier to cheating. Taking advantage of ubiquitous e-mail connectivity and the speed and storage capacity of modern personal computers, data generation and dispersal is expeditious.

The interactive aspects of the examination and the prescribed experimental budget allow a hands-on exploration of the concept of sequential design of experiments. Student feedback regarding the exam was favorable.

This type of examination can be adapted for use in other chemical engineering courses. In the future, elimination of the instructor interface during data generation will streamline the process.

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## Process Simulation

Continued from page 135.

process that should appeal to an intuitive learner. They did this, however, in a practical context that would also appeal to a sensory learner; they first saw a real column and did an example validating its importance, and then they used HYSYS, which is recognizable as a tool used by “real engineers.”

*Sequential vs. Global Learning*<sup>[16,24]</sup> • The structure was methodical and well-suited for sequential learners, but was also interspersed with “big picture” insights that were meant to benefit all students, particularly global learners. The first thing the class learned about column distillation was why it was useful. The class discussed the significance of each process parameter before attempting to calculate it or to even relate it to anything else.

### STUDENT RESPONSE

The course structure described in this paper was used in the fall 2000 and fall 2001 semesters at Rowan University. Table 3 summarizes the results of the course and teacher evaluations of it. Feedback was very positive, both toward the use of HYSYS for inductive teaching on concepts and toward the overall course. Specific student comments included, “Learning HYSYS and seeing what actually happens in a distillation column, etc., was very helpful,” and “The in-class HYSYS days were helpful for seeing how the whole process works.”

### SUMMARY

In assessing how modern process simulators should affect teaching of separations, chemical engineering educators have suggested a blend of simulation with traditional graphical modeling approaches. This paper describes an effective strategy for using these two modeling approaches that was successfully implemented in the fall 2000 and fall 2001 semesters at Rowan University. Students’ first introduction to distillation was exposure to a real column and discussion of the practical significance of distillation. Process simulation was used as a tool for inductive presentation of concepts to promote a thorough understanding of the physical process. This was followed by a deductive derivation of the McCabe-Thiele model. The course organization is consistent with what is known about cognition and the progression of student understanding, and it appeals to students with varied learning styles. It was an effective presentation, as evidenced by student feedback. This paper focused on column distillation as an example,

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but the approach is readily extended to other physical processes.

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# OPTIMUM COOKING OF FRENCH FRY-SHAPED POTATOES

## *A Classroom Study of Heat and Mass Transfer*

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**W**affles<sup>®</sup>. Ridges<sup>®</sup>. Pringles<sup>®</sup>. Tater Skins<sup>®</sup>. What do these trade names share? They are offered to the consumer as the perfect potato chip. And how might this so-called perfect potato chip be defined? Probably in terms of quality of taste and texture...balanced against a reasonable cost.

Along with pizza, students are seriously interested in potato chips—for the obvious reasons. At the University of Kentucky, we are always looking for new ways to stimulate learning in the classroom. Although chemical engineers do not traditionally study food engineering, we believe the exploration of various methods to cook the common potato helps motivate students to learn and apply the engineering principles of heat and mass transfer.

The preparation and manufacture of potato chips is a complex subject, spawning complete industries and intense research. Even doctoral dissertations have been devoted to the preparation of potato chips. Much of the recent research effort has been directed toward evaluation of cooking oils and seasonings, nutritional content, and product preservation. Other work has been done to optimize storage life with various protective barriers/packing materials and application of preservatives.

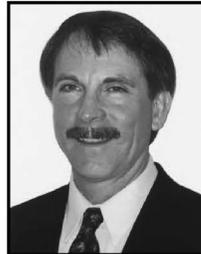
The following laboratory exercise deals with the optimization of french fry-shaped potatoes (rather than chip geometry) and is offered as an initial exploratory exercise for students. The complete exercise may be too lengthy for some laboratory allotments and portions may be modified or eliminated where appropriate. Faculty and students are invited to consult other excellent resources for further discussion of the technical aspects of food engineering.<sup>[1-4]</sup> Two other related articles recently featured in *Chemical Engineering Education* include a study of heat and mass transfer with microwave drying<sup>[5]</sup> and the use of a mathematical model for

cooking potatoes.<sup>[6]</sup> Finally, a recent popular article in *The New Yorker*<sup>[7]</sup> traced the origins of the development and optimization of the french fry in the U.S. by Ray Kroc of McDonald's fame.

### MOTIVATION

Students receive and learn information in accordance with three modalities: visual, auditory, and kinesthetic. Generally, academic environments appeal to these modalities by combining classroom theory and lab experimentation. In Kolb's four-stage learning model,<sup>[8]</sup> he calls this process reflective observation, abstract conceptualization, active experimentation, and finally, concrete experience (feeling). We believe most students (reported to be as high as 60%<sup>[9]</sup>) learn better when "hands-on" applications (active experimentation) are presented concurrently with classroom theory. Traditionally, students often wait between one to two years to apply a previously learned theory to an actual application in an experimental laboratory setting.

At the University of Kentucky, we offer an undergraduate course in the chemical/materials engineering curriculum called "Heat and Mass Transfer." Recently, our department has made concerted efforts to bring more experimental applications back into the classroom. One such experiment incorporated into the classroom environment is the study of



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heat and mass transfer and how it applies to a simple thing such as cooking a potato. Please note: these types of combined classroom/short experimental components are not intended to replace an existing separate laboratory experimental course. Instead, they are designed to complement and enhance traditional classroom theory.

## SCOPE AND OBJECTIVES

The purpose of this exercise is not to conduct an in-depth investigation into the best methods of producing potato chips, but rather to use fundamental principles of heat and mass transfer to demonstrate what effects these principles have upon possible food quality. Traditionally, the food industry has taken a “cook-and-look” approach to development of new foods. There is some evidence, however, that it is starting to take a more scientific approach because such an approach can reproduce successes and lead to more interesting differences in food textures.<sup>[10]</sup> The students in this exercise take advantage of the opportunity to explore some of the cooking variables involved in the preparation of products in the food industry.

Since the science and art associated with preparing the “perfect potato chip” is so complex, conditions in this exercise have been simplified to examine only fundamental components of the food preparation process. Potato chips are usually fried or prepared with various cooking oils, although there has been some interest lately in baking chips to reduce the fat levels. Using cooking oils, antioxidants, or seasonings (including salt) will not be considered in this exercise. Instead, various heat transfer equipment will be used to judge their effect on the drying (mass transfer) and cooking (heat transfer) of potato slices. Cooking equipment will include the conventional oven, a convection oven, a microwave oven, and a pressure cooker.

One might wonder—what is cooking and what is happening during the actual cooking process? The general cooking process is largely a matter of how heat is applied to a food product. In terms of unit operations, cooking is a combination of heat transfer and drying operations coupled with chemical reaction. Actually, cooking involves modifications of molecular structures and formation of new compounds, the killing of dangerous organisms, modification of textures, and the drying/browning of food materials. A typical potato is made up of water, starch, reducing sugars, pectin, and complex organic molecules.<sup>[11]</sup> During the cooking process, moisture levels and flavor components change. Also, bond strengths within the vegetable pectin are altered, which affects the mechanical properties of the potato.<sup>[12]</sup>

A word about the potato chip geometry: In our initial cooking experiments, the edges of the potato chips curled, which interfered with mechanical testing. Teflon holders were constructed to hold the chips in an upright position to promote heat transfer and to reduce edge curling. In the end, this chip

geometry was not the most desirable shape for heat-transfer modeling. Finally, a rectilinear geometry (french fry shape) was selected for ease of mechanical testing and approximation to cylindrical geometry for heat-transfer calculations.

Using a conventional oven to cook a potato stick, the student is prompted to define an “optimum potato” in terms of quantitative factors of mechanical hardness/deflection and qualitative factors of color, taste, feel, and smell. During the cooking process, there are two simultaneous phenomena occurring in the small potato stick. The inside of the potato is “cooked” during the process of unsteady-state heat transfer as heat progressively moves from the outside surface to the center of the potato. In a reverse gradient, mass is transferred as volatiles (water and organic molecules) move from the center of the potato to the outside surface during the drying process. Once the potato optimum is defined with a conventional oven, the student is challenged to reproduce the potato quality in other cooking equipment (convection oven, microwave, and pressure cooker).

## EQUIPMENT AND MATERIALS

Heat transfer (cooking) equipment includes a conventional oven, a convection oven, a microwave oven, and a pressure cooker. A gravimetric scale, capable of  $\pm 0.01$  g, is used to monitor loss of volatile materials during the cooking process. Surface firmness of cooked potatoes is monitored with a durometer.\* A compression force gage\*\* is used to test potato material strength by monitoring deflection. Dimensions of each potato test specimen are measured with a micrometer, and a thermocouple is used to monitor oven temperature. A french fry potato extruder\*\*\* is used to provide consistent-size test specimens.

## PREPARATORY STEPS

Before the actual cooking procedure is started, the available temperature ranges of the four ovens should be verified. To execute the heat transfer models, it is desirable to have the same temperature setting in each of the ovens. The conventional oven poses no problem because it can be varied from 38°C to 260°C (100°F to 500°F), but the temperature settings for the convection and pressure cookers will usually be pre-set by the equipment manufacturer. The temperature of the pressure cooker will be fixed by the pressure rating of the vessel. For example, our 6-quart pressure cooker is designed for 10 psig, or about 116°C (240°F).

All experimental equipment and plans should be carefully assembled before the potatoes are sliced. Raw potatoes readily turn brown upon exposure to air and this will affect the assessment of product color during the cooking test.

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\* McMaster-Carr Supply, Cleveland, OH; Shore OO range, model 1388T232m/#450)

\*\* McMaster-Carr Supply, Cleveland, OH; model 2115T11, \$65

\*\*\* HALCO french fry cutter, model K375, \$120

## GENERAL PROCEDURE

- 1 Select large, white baking potatoes (Russett variety) from one bag (same lot). Peel the potatoes and use a french-fry cutter to prepare consistently sized test specimens. Cut potato strips into 10.2 cm lengths (4.0 in) and pierce with short lengths of bamboo skewers so that the samples resemble a “carpenter’s saw-horse” (see Figure 1). Record the samples’ weight, including skewers, and place them in a conventional oven set at a moderately high temperature (204°C) to drive-off moisture and other volatile materials. Prepare a drying curve by plotting free moisture loss versus time.<sup>[13]</sup> This will entail removing the potato samples from the oven approximately every five minutes and recording weight changes. Weigh the samples and promptly replace them in the oven, as they will begin to cool and absorb humidity from the ambient air. See Figure 2 and 3 for typical examples of drying curves by students. Note the insertion of solid lines in Figure 3 to approximate the heat-up, constant-rate, and falling-rate regimes of drying. Much data scatter was the result of the potatoes removal from and reinsertion into the oven. If it is available, a laboratory drying oven with integral scale would allow more precise construction of classical drying curves.
- 2 Divide the drying curve into six segments: three points in the constant-drying-rate period and three points in the falling-rate period. Prepare seven new potato samples with skewers and place them in the conventional oven. Remove individual samples from the oven at those times corresponding to the points previously selected on the drying curve. Let the samples come to equilibrium in ambient air, and then conduct deflection tests, hardness tests, and panel evaluations tests on the samples as described below.
- 3 Repeat steps 1 and 2 for the conventional oven at a lower oven temperature setting (121°C).

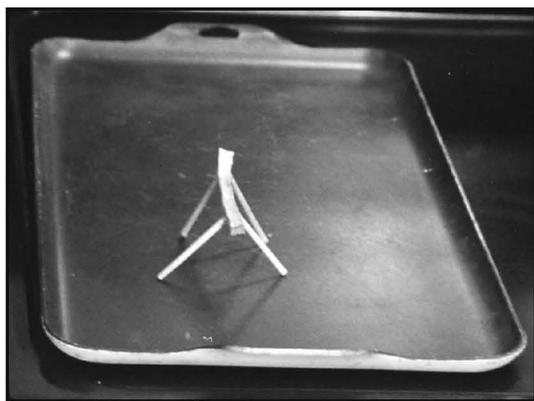


Figure 1. French-fry geometry on bamboo skewers.

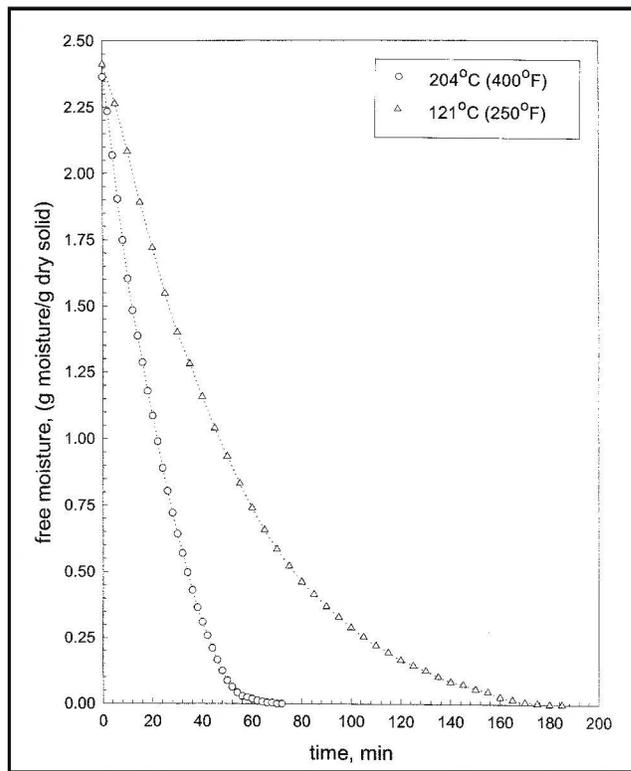


Figure 2. Free moisture versus time for constant drying conditions in a conventional oven.

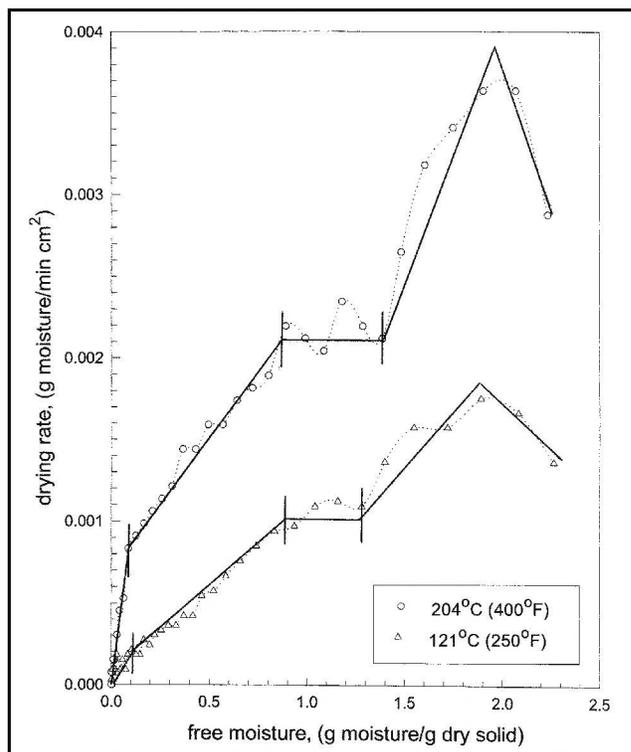


Figure 3. Drying curve for conventional oven.

- 4 Follow the same general procedure for sample testing in the convection oven, the microwave oven, and the pressure cooker.

## OPERATION OF HEATING EQUIPMENT

**Conventional Oven** • Locate a thermocouple near the potato samples to accurately measure the temperature, as deadbands on oven thermostats are known to vary widely.

**Convection Oven** • Forced circulation is used to improve heat transfer and reduce cooking time. In order to make heat-transfer calculations, the specific fan rating (standard cubic feet per minute, or scfm) for the oven must be determined. Depending on the oven design, the air flow can be measured in one of two ways: **1**) if the air is recirculated within the oven, a sheet metal shroud/duct apparatus can be constructed and pop-rieveted to the air suction or discharge. A pitot tube and micromanometer can then be used to measure air velocity through the known diameter duct (see Figure 4). **2**) If the oven design uses once-through air, this flow can be measured by a technique similar to one used by environmental engineers to measure breathing losses from atmospheric storage-



Figure 4. Student measurement of air velocity in a convection oven.

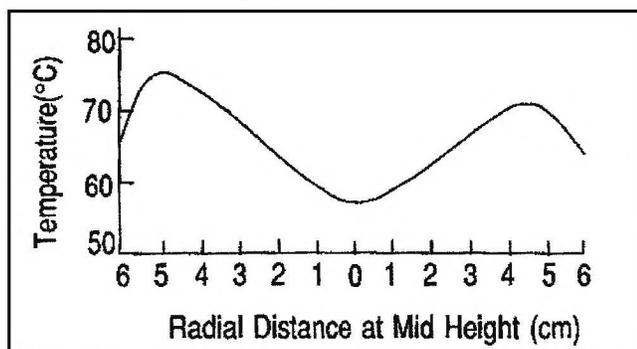


Figure 5. Experimental radial temperature profile in a cylindrical geometry of roast beef heated with microwaves.

tank discharge vents. With the oven at a very low heat setting, tape a plastic bag over the discharge vent of the oven to capture all air flow. Cut one hole along the outside edge of the plastic bag and insert a tube into it to measure static pressure with a micromanometer (resolution of  $\pm 0.001$  inches water). Cut another hole, with precisely measured diameter, approximately in the middle of one face of the bag. This hole will act as an orifice through which the air in the inflated bag will escape at a controlled rate. Use the following relationship to determine the cfm of the oven fan:

$$q = C_o A \sqrt{\frac{2 g_c \Delta p}{\rho}} \quad (1)$$

where

$q$	gas flow rate (=) $\text{ft}^3/\text{sec}$
$C_o$	correction coefficient for orifice $\sim 0.61$
$A$	orifice area (=) $\text{ft}^2$
$g_c$	gravitational conversion factor
$\Delta p$	pressure drop across orifice (=) $\text{lb}_f/\text{ft}^2$
$\rho$	gas density (=) $\text{lb}_m/\text{ft}^3$

As was done with a conventional oven, prepare a drying curve and conduct the testing protocol (deflection, hardness, panel-evaluation test) on the cooked potato sticks.

**Microwave Oven** • Using a microwave oven in cooking potatoes is advantageous because it results in faster and more uniform heating. Microwaves penetrate through various foods and their added energy causes dipoles of the water molecules to rotate in an alternating field. This alternating-rotation effect causes friction and provides a source of heat, which either thaws or cooks food. The governing energy equation for microwave heating is<sup>[14]</sup>

$$\frac{\delta T}{\delta t} = \alpha \nabla^2 T + \frac{Q}{\rho C_p} \quad (2)$$

where  $T$  is temperature,  $t$  is time,  $\alpha$  is thermal diffusivity,  $\rho$  is density, and  $C_p$  is the specific heat of the material. Note that the equation contains a heat-generation term,  $Q$ , that represents the conversion of electromagnetic energy to heat. For small-size food samples where spatial variations in temperature are negligible, such as our potato sticks, Eq. (2) can be simplified to

$$Q = \rho C_p \frac{\delta T}{\delta t} \quad (3)$$

For larger size food materials, the temperature distribution may vary significantly. Figure 5 shows the experimental radial temperature profile in a cylindrical geometry of roast beef heated with microwaves.<sup>[15]</sup> Note the higher temperatures just inside the edge of the cylindrical wall of the roast beef due to surface evaporation of moisture.

For our small geometries, thermal gradients within our potato samples are not expected to be significant. The generalized boundary condition for microwave heating is

$$-k \frac{\delta T}{\delta n} = h(T - T_{\infty}) + \varepsilon \sigma (T^4 - T_s^4) + m_w \lambda \quad (4)$$

where  $k$  is the thermal conductivity,  $n$  represents the normal direction to the boundary,  $h$  is the convective heat transfer coefficient, and  $T_{\infty}$  is the convective air temperature. The second term is for radiant heat transfer (to be ignored in our experiment), where  $\varepsilon$  is the surface emissivity and  $\sigma$  is the Stefan-Boltzmann constant. The third term describes evaporation at the surface, where  $m_w$  is the mass of water and  $\lambda$  is the latent heat of evaporation. This evaporation term is more important in the microwave cooking versus cooking in a conventional oven because moisture moves rapidly from the interior to the outside (due to uniform heating).

Although microwave heating provides a constant heat source, the highest temperature initially within foods that have large quantities of water (such as our potatoes) is the boiling point of water. After most of the moisture had been evaporated from the food, the temperature will rise to higher values and eventual surface charring will occur.

When cooking at different settings of a microwave oven, the power is not attenuated. Instead, different power settings cause the oven to cycle off and on. For example a 50% power setting means the oven is on at full power only 50% of the time.

One other unusual phenomenon that occurs with microwave heating of food that is not observed with conventional heating methods concerns the movement of internal moisture. A potato can be modeled as a capillary, porous body. With microwaves, thermal gradients within the potato can usually be ignored since essentially all parts of the potato are heated simultaneously. In conventional heating methods, moisture usually diffuses from inside the potato to the outside as a result of thermal and concentration gradients. With microwave heating, an additional driving force for moisture migration is due to generation of substantial pressure gradients within the potato. Positive pressures can build up within the potato that cause moisture to rapidly move to the surface, where it evaporates.

Prepare drying curves for potato sticks at maximum microwave setting.

**Pressure Cooker** • An added dimension of cooking is offered by using a pressure cooker. In addition to temperature and heat transfer effects, students can assess how elevated pressure affects cooking times and final product quality. With standard home-cooking pressure cookers designed for public consumers, low operating pressures are used for obvious safety reasons. By measuring the diameter of the opening in the top of a cooker and weighing the top floating element, students can determine the pressure rating (psi) of the cooker.

Boiling water within the cooker is used to generate a fixed pressure, and therefore only one temperature is available to

cook potatoes with this device. There are expensive pressure cookers that allow some control over the cooking pressure, but the pressure setting of the inexpensive models are pre-set by virtue of the weight of the top floating element. The pressure setting for our cooker was 10 psig, and our potatoes cooked at a temperature of 116°C (240°F). With the water boiling, place seven potato sticks with skewers in the bottom of the cooker (but out of the water), and tighten the lid. With a small-volume cooker, the pressure should build rapidly. Once operating pressure is attained, by evidence of escaping pressure, begin timing the cooking process. Every three minutes, quickly release pressure from the cooker and remove a potato stick. Retighten the cooker lid and resume pressure levels to cook the remaining potato sticks.

With a standard pressure cooker, there is no quick way to release pressure from the vessel. Pressure-cooker procedures instruct the operator to place the pan in cool water or wait until it cools to room temperature before removing the lid. This is for obvious safety reasons. For purposes of this exercise, our pressure cooker was modified by welding a half-inch ball valve (with Teflon seats) to the pan top. This provided a quick-relief method to depressurize the pan so that potato sticks could be removed and the pan expeditiously returned to steady-state operation. Note: in constructing and welding the ball valve to the lid, be careful to install the valve so that the integrity of the pan and the secondary relief device is not compromised. Once the valve is attached, test the final apparatus behind a safety hood to ensure a safe vessel prior to having students work with the unit.

## TESTING PROTOCOL

Initially, a “potato optimum” base case is established in a conventional oven. This optimum is defined by the student in terms of surface hardness (measured with a durometer), mechanical strength (determined with a compressive force gage), and qualitative factors (assessed by a product panel test). Once the optimum is defined, the student is challenged to predict this same optimum in other heat transfer equipment (convection and microwave ovens and a pressure cooker).

**Hardness** • Material hardness is a common material testing characteristic used to gauge surface hardness of rubbers, polymers, metals, textiles, printing, and forestry products. A raw, uncooked potato has a firm surface. As it is cooked, the surface will become softer as pectin bonds begin to loosen. As the potato is progressively heated, its surface become drier until finally it becomes quite firm if overcooked. Using the durometer hardness tester, stages of potato-surface hardness can be tracked over time during the cooking process.

**Deflection** • There are many ASTM (American Society for Testing and Materials) testing methods available ([www.astm.org](http://www.astm.org)) to measure compression, torsion, and tension of solid materials. Zhao<sup>[16]</sup> found that potatoes lose me-



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

# AN EXERCISE FOR PRACTICING PROGRAMMING IN THE ChE CURRICULUM

## *Calculation of Thermodynamic Properties Using the Redlich-Kwong Equation of State*

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Many students find it difficult to learn programming. One source of difficulty has to do with the complexity and relevance of the examples and exercises being used. Exercises that are simple enough for a student to write a working program in a reasonable length of time, without too much frustration, are often irrelevant to their chemical engineering studies. Consequently, they often do not see the benefit in learning programming and lose interest. More complex and realistic exercises, however, may require a long and frustrating debugging period, causing them to lose faith in their ability to make the program run and discouraging them from further programming attempts.

A good exercise to help students learn programming would be one of practical importance that can be constructed gradually in several steps. At each step, new types and more complex commands would be added to the program, but only after debugging of the previous step had been completed.

This paper presents such an exercise—one that involves analytical solution of the Redlich-Kwong equation for the compressibility factor and consequent calculation of molar volume, fugacity coefficient, isothermal enthalpy, and entropy departures. The solution is demonstrated using MATLAB,<sup>[1]</sup> but other programming languages (such as C or C++) can also be used.

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**Calculation of the Compressibility Factor and  
Derived Thermodynamic Properties  
Using the Redlich-Kwong Equation of State**

The two-parameter Redlich-Kwong (R-K) equation of state has an accuracy that compares well with more complicated equations that incorporate many more constants (when applied to non-polar compounds<sup>[2]</sup>). The R-K equation is a cubic equation in the volume (or in the compressibility factor) for which analytical solutions can be found.<sup>[3]</sup> After solving for the molar volume (or compressibility factor), several important thermodynamic functions (such as fugacity coefficient, isothermal enthalpy, and entropy departures) can be calculated.

In this exercise, the molar volume, the compressibility factor, the isothermal enthalpy departure, the isothermal entropy departure, and the fugacity coefficients are calculated and plotted for water vapor in the supercritical region. The values of reduced pressure and reduced temperature used are shown in Table 1.

**Equations and Numerical Data**

The R-K equation is usually written<sup>[4]</sup>

$$P = \frac{RT}{V-b} - \frac{a}{V(V+b)\sqrt{T}} \quad (1)$$

where

$$a = 0.42747 \left( \frac{R^2 T_c^{5/2}}{P_c} \right) \quad (2)$$

$$b = 0.08664 \left( \frac{RT_c}{P_c} \right) \quad (3)$$

and

P pressure (atm)

<b>TABLE 1</b>					
<b>Reduced Pressure and Reduced Temperature Values for Example 1</b>					
<i>P<sub>r</sub></i>	<i>P<sub>r</sub></i>	<i>P<sub>r</sub></i>	<i>P<sub>r</sub></i>	<i>P<sub>r</sub></i>	<i>T<sub>r</sub></i>
0.1	2	4	6	8	1
0.2	2.2	4.2	6.2	8.2	1.05
0.4	2.4	4.4	6.4	8.4	1.1
0.6	2.6	4.6	6.6	8.6	1.15
0.8	2.8	4.8	6.8	8.8	1.2
1	3	5	7	9	1.3
1.2	3.2	5.2	7.2	9.2	1.5
1.4	3.4	5.4	7.4	9.4	1.7
1.6	3.6	5.6	7.6	9.6	2
1.8	3.8	5.8	7.8	9.8	3
				10	

***The exercise presented here  
enables students to start a programming  
assignment at a fairly simple level and to  
build it up gradually to a more complex  
assignment of practical importance...***

- V molar volume (liters/g-mol)
- T temperature (K)
- R gas constant [R=0.08206 (atm liter/g-mol-K)]
- T<sub>c</sub> critical temperature (K)
- P<sub>c</sub> critical pressure (atm)

Eliminating V from Eq. (1) and writing it as a cubic equation of the compressibility factor, z, yields

$$f(z) = z^3 - z^2 - qz - r = 0 \quad (4)$$

where

$$r = A^2 B \quad (5)$$

$$q = B^2 + B - A^2 \quad (6)$$

$$A^2 = 0.42747 \left( \frac{P_R}{T_R^{5/2}} \right) \quad (7)$$

$$B = 0.08664 \left( \frac{P_R}{T_R} \right) \quad (8)$$

in which P<sub>R</sub> is the reduced pressure (P/P<sub>c</sub>) and T<sub>R</sub> is the reduced temperature (T/T<sub>c</sub>).

Equation (4) can be solved analytically for three roots, some of which may be complex. Considering only the real roots, the sequence of calculations involves the steps

$$C = \left( \frac{f}{3} \right)^3 + \left( \frac{g}{2} \right)^2 \quad (9)$$

where

$$f = \frac{-3q-1}{3} \quad (10)$$

$$g = \frac{-27r-9q-2}{27} \quad (11)$$

If C > 0, there is one real solution for z:

$$z = D + E + 1/3 \quad (12)$$

where

$$D = \left( -\frac{g}{2} + \sqrt{C} \right)^{1/3} \quad (13)$$

$$E = \left( -\frac{g}{2} - \sqrt{C} \right)^{1/3} \quad (14)$$

If C < 0, there are three real solutions for z:

$$z_k = 2\sqrt{\frac{-f}{3}} \cos \left[ \left( \frac{\phi}{3} \right) + \frac{2\pi(k-1)}{3} \right] + \frac{1}{3} \quad k = 1, 2, 3 \quad (15)$$

where

$$\phi = a \cos \sqrt{\frac{g^2/4}{-f^3/27}} \quad (16)$$

In the supercritical region, two of these solutions are negative, so the maximal  $z_k$  is selected as the true compressibility factor.

After calculating the compressibility factor, the molar volume ( $V$ ), the isothermal enthalpy departure ( $\Delta H^*$ ), the isothermal entropy departure ( $\Delta S^*$ ), and the fugacity coefficient ( $\psi$ ) are calculated from<sup>[4]</sup>

$$V = \frac{zRT}{P} \quad (17)$$

$$\frac{\Delta H^*}{RT} = \frac{3a}{2bRT^{3/2}} \ln\left(1 + \frac{b}{V}\right) - (z-1) \quad (18)$$

$$\frac{\Delta S^*}{R} = \frac{a}{2bRT^{3/2}} \ln\left(1 + \frac{b}{V}\right) - \ln\left(z - \frac{Pb}{RT}\right) \quad (19)$$

$$\psi = \exp\left\{z-1 - \ln\left[z\left(1 - \frac{b}{V}\right)\right] - \frac{a}{bRT^{3/2}} \ln\left(1 + \frac{b}{V}\right)\right\} \quad (20)$$

The numerical data needed for solving this problem include  $R = 0.08206$  liter atm/g-mol-K, critical temperature for water  $T_c = 647.4$  K, and critical pressure of water  $P_c = 218.3$  atm.

### Recommended Steps for Solution

1. Prepare a MATLAB m-file for solving the set of equations for  $Tr = 1.2$  and  $Pr = 5$  ( $C$ , in Eq. 9, is positive) and  $Tr = 10$  and  $Pr = 5$  ( $C$ , in Eq. 9, is negative). Compare the results obtained with values from generalized charts of thermodynamic properties.
2. Convert the program developed in part 1 to a function and write a main program to carry out the calculations for  $Pr = 5$  and the set of  $Tr$  values shown in Table 1.
3. Extend the main program to carry out the calculations for all  $Pr$  and  $Tr$  values shown in Table 1. Store all the results of  $z$ ,  $V$ , enthalpy and entropy departures, and fugacity coefficients in column vectors. Display the various variables versus  $Pr$  and  $Tr$  in tabular and graphic forms.

### Solution

The MATLAB program (m-file) for solving the set of equations for one value of  $Tr$  and  $Pr$  and displaying the values of selected variables is shown in Figure 1. Preparation of the program requires that students rewrite the equations using the MATLAB syntax. This stage includes changing some variable names to valid MATLAB names, changing some algebraic operators, and changing some

intrinsic function names (such as converting  $\ln$  to  $\log$ ). The use of the “max” intrinsic function to select the maximal compressibility factor from the values obtained in Eq. (15) requires storing these values in a vector.

The equations must also be reordered according to a proper computational order (thus a variable is not used before a value is assigned to it). This can be most easily achieved by first entering

```

R = 0.08206; % Gas constant (L-atm/g-mol-K)
Tc = 647.4; % Critical temperature (K)
Pc = 218.3; % Critical pressure (atm)
a = 0.42747*R^2*Tc^(5/2)/Pc; % Eq. (2), RK equation constant
b = 0.08664*R*Tc/Pc; % Eq. (3), RK equation constant
Pr = 6; % Reduced pressure (dimensionless)
Tr = 1.2; % Reduced temperature (dimensionless)
Asqr = 0.42747*Pr/(Tr^2.5); % Eq. (7)
B = 0.08664*Pr/Tr; % Eq. (8)
r = Asqr*B; % Eq. (5)
q = B^2 + B - Asqr; % Eq. (6)
f = (-3*q-1)/3; % Eq. (10)
g = (-27*r-9*q-2)/27; % Eq. (11)
C = (f/3)^3 + (g/2)^2; % Eq. (9)
if (C > 0)
    D = (-g/2 + sqrt(C))^(1/3); % Eq. (13)
    E1 = (-g/2 - sqrt(C)); % Eq. (14)
    E = ((sign(E1)*(abs(E1))^(1/3))); % Eq. (14)
    z = (D + E + 1/3) % Compressibility factor (dimensionless) Eq. (12)
else
    psii = (acos(sqrt((g^2/4)/(-f^3/27))))); % Eq. (16)
    zv(1) = (2*sqrt(-f/3)*cos((psii/3))+1/3); % Eq. (15)
    zv(2) = (2*sqrt(-f/3)*cos((psii/3)+2*3.1416*1/3)+1/3); % Eq. (15)
    zv(3) = (2*sqrt(-f/3)*cos((psii/3)+2*3.1416*2/3)+1/3); % Eq. (15)
    z = max(zv) % Compressibility factor (dimensionless)
end
P = Pr*Pc % Pressure (atm)
T = Tr*Tc % Temperature (K)
V = z*R*T/P % Eq. (17), Molar volume (L/g-mol)
Hdep = (3*a/(2*b*R*T^1.5))*log(1+b/V)-(z-1)
% Eq. (18), Enthalpy departure (dimensionless)
Sdep = (a/(2*b*R*T^1.5))*log((1+b/V))-log(z-P*b/(R*T))
% Eq. (19), Entropy departure (dimensionless)
f_coeff = exp(z-1-log(z*(1-b/V))-a/(b*R*T^1.5)*log(1+b/V))
% Eq. (20), Fugacity coefficient (dimensionless)

```

Figure 1. MATLAB program for calculating compressibility factor and thermodynamic properties for one value of  $Re$  and  $Pr$ .

TABLE 2  
Comparison of Calculated and Generalized  
Chart<sup>[5]</sup> Values for  $P_r = 5$

	$Tr = 1.2$		$Tr = 10$	
	Calc.	Chart	Calc.	Chart
Compressibility factor	0.7326	0.7	1.0373	1.0
Enthalpy departure $\Delta H^*/T_c$ (cal/g-mol K)	6.0167	6.5	-0.5515	-
Entropy departure $\Delta S^*$ (cal/g-mol K)	3.4616	4	0.0183	-
Fugacity coefficient $\psi$	0.4579	0.47	1.0376	1.05

```

% A script file for calculating compressibility factor and derived
% thermodynamic properties using the Redlich Kwong equation of state.
clear, clc, format compact, format short g
Tc = 647.4 ; % Critical temperature (K)
Pc = 218.3; % Critical pressure (atm)
Pr = 5; % Reduced pressure (dimensionless)
Tr_list=[1 1.05 1.1 1.15 1.2 1.3 1.5 1.7 2 3];
for j=1:10
    Tr = Tr_list(j); % Reduced temperature (dimensionless)
    [P,T,V,z,Hdep,Sdep,f_coeff]=RKfunc(Tc,Pc,Tr,Pr)
end

```

**Figure 2.** Main program for carrying out the calculations for one  $Pr$  and ten  $Tr$  values.

```

Tr_list=[1 1.05 1.1 1.15 1.2 1.3 1.5 1.7 2 3];
Pr_list=[0.1 0.2];
i=2;
while (Pr_list(i)<9.9)
    i=i+1;
    Pr_list(i)=Pr_list(i-1)+0.2;
end
n_Tr=10;
n_Pr=size(Pr_list,2);
for i=1:n_Pr
    for j=1:n_Tr
        [P(j,i),T(j,i),V(j,i),z(j,i),Hdep(j,i),Sdep(j,i),f_coeff(j,i)]=RKfunc(Tc,Pc,Tr_list(i),Pr_list(j));
    end
end
%
% Print tabular results
%
for i=1:n_Pr
    disp(' ');
    disp(['Tr = ' num2str(Tr_list(i)) ' T(K)= ' num2str(Tr_list(i)*Tc)]);
    disp(' ');
    disp(' Pr P(atm) V(L/g-mol) z Hdep Sdep f_coeff');
    Res=[Pr_list(:) P(:,i) V(:,i) z(:,i) Hdep(:,i) Sdep(:,i) f_coeff(:,i)];
    disp(Res);
    pause
end
%
% Plot results
%
plot(Pr_list,z(:,1),'-',Pr_list,z(:,2),'-',Pr_list,z(:,3),'-',Pr_list,z(:,4),'-',Pr_list,z(:,5),'-',...
Pr_list,z(:,6),'*',Pr_list,z(:,7),'o',Pr_list,z(:,8),'+',Pr_list,z(:,9),'v',Pr_list,z(:,10),'^');
legend('Tr=1','Tr=1.05','Tr=1.1','Tr=1.15','Tr=1.2','Tr=1.3','Tr=1.5','Tr=1.7','Tr=2','Tr=3');
title('Compressibility Factor Versus Tr and Pr')
xlabel('Reduced Pressure Pr');
ylabel('Compressibility Factor(z)');
pause
plot(Pr_list,f_coeff(:,1),'-',Pr_list,f_coeff(:,2),'-',Pr_list,f_coeff(:,3),'-',Pr_list,f_coeff(:,4),...
'-',Pr_list,f_coeff(:,5),'-',Pr_list,f_coeff(:,6),'*',Pr_list,f_coeff(:,7),'o',Pr_list,f_coeff(:,8),...
'+',Pr_list,f_coeff(:,9),'v',Pr_list,f_coeff(:,10),'^');
legend('Tr=1','Tr=1.05','Tr=1.1','Tr=1.15','Tr=1.2','Tr=1.3','Tr=1.5','Tr=1.7','Tr=2','Tr=3');
title('Fugacity Coefficient Versus Tr and Pr')
xlabel('Reduced Pressure Pr');
ylabel('Fugacity Coefficient(f/P)');
pause

```

**Figure 3.** Part of the main program in its final form.

the equations to a program that automatically reorders them (POLYMATH, for example). The ordered set of equations can then be pasted into the MATLAB editor. In addition to the “assignment” statements, this simple program requires only the “if” statement. No commands for printing the results are used, but selected variables are shown during the program execution by selective addition or removal of the semicolon from the ends of the commands. Good programming practice requires clear descriptions of the variables and the equations by adding comments.

The results obtained for compressibility factor, enthalpy and entropy departures, and fugacity coefficient by the MATLAB program are compared to values of generalized charts (Kyle<sup>[5]</sup>) in Table 2. The differences between the calculated values (presumed to be more accurate) and the generalized chart values are small enough to validate the correctness of the MATLAB program. For  $Tr = 10$ , no generalized chart values are available for enthalpy and entropy departure, but the calculated values match the trend observed in the generalized chart.

The principal change that has to be introduced in the program, when proceeding to the second step of the development, includes the addition of the function definition statement

```
function[P,T,V,z,Hdep,Sdep,f_coeff]=RKfunc(Tc,Pc,Tr,Pr)
```

and removal of the definition of the variables  $Tc$ ,  $Pc$ ,  $Tr$ , and  $Pr$ . The  $Tr$  and  $Pr$  are the parameters that are changed in the main program. Putting the definition of  $Tc$  and  $Pc$  in the main program enables easy modification of the program for different substances. All the variables that should be displayed in tabular or graphic form are included in the list of returned variables. The main program that calls this function in order to perform the calculations for  $Pr = 5$  and the ten  $Tr$  values (shown in Table 1) is displayed in Figure 2.

The program starts with commands that are not specific to the problem at hand and fall into the category of “good programming practice.” The workspace and the command window are cleared and the preferred format for printing is defined. The ten specified  $Tr$  values are stored in a row vector  $Tr\_list$  and a “for”

statement is used to call the function while changing the parameter values. The results are displayed in a very rudimentary form, just by omitting the semicolon after the call to the function.

After verifying that this function works properly, the assignment can be finished by adding to the main program the set of Pr values shown in Table 1, storing the results, and displaying them in tabular and graphic forms. Part of the main program in its final form is shown in Figure 3.

In this program, a “while” statement is used to input the required Pr values into the row vector Pr\_list. The intrinsic function “size” is used to determine the number of elements in Pr\_list. The values returned from the function are stored in two-dimensional matrices, one column for each Tr and one row for each Pr value. Tables of results are printed for a constant Tr value, where the respective columns of the results matrices are united into a single matrix, “Res” which is displayed.

Only the code for plotting the compressibility factor and the fugacity coefficient is shown, and the additional variables can be plotted similarly. The plots of the compressibility factor versus Tr and Pr and the fugacity coefficient versus Tr and Pr are shown in Figures 4 and 5, respectively. These plots are almost identical to the generalized charts that can be found in the thermodynamics textbooks.

## CONCLUSION

The exercise presented here enables students to start a programming assignment at a fairly simple level and to build it up gradually to a more complex assignment of practical importance in chemical engineering. It demonstrates several aspects of good programming practice:

- *The use of comments to clearly describe equations and variables*
- *Clearing the workspace and command window before starting execution*
- *Proper ordering of the equations*
- *Modular construction of the program, where each module is tested separately before its integration with the other components*

A variety of the variable types (*i.e.*, scalar and matrix), intrinsic functions, and simple and complex commands are used. Thus, the exercise can cover a considerable portion of a programming course.

Because of the gradual increase of difficulty in building this program, most students can successfully complete it and thus gain confidence in their ability

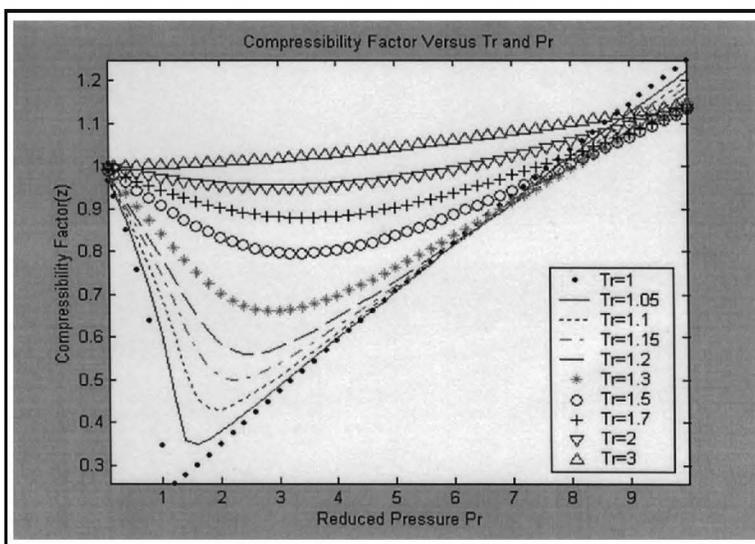


Figure 4. Plot of the compressibility factor versus reduced temperature and pressure.

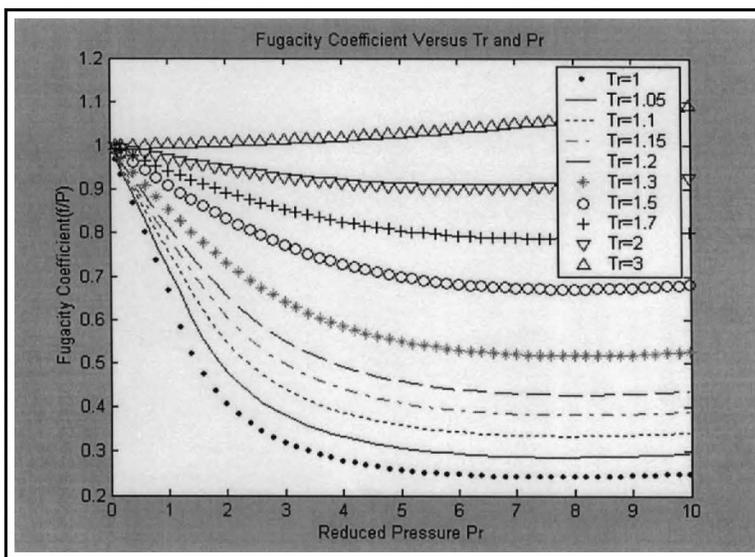


Figure 5. Plot of the fugacity coefficient versus reduced temperature and pressure.

to write a “real” program. The outcome of the exercise, the set of diagrams that for many decades has been a very important component in all thermodynamic textbooks, provides an excellent demonstration of the importance of programming in chemical engineering.

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# Optimum Cooking of Potatoes

Continued from page 147.

## STUDENT DELIVERABLES

1. Prepare single drying curves for potato samples cooked in a conventional oven, a convection oven, and a microwave oven. Construct two drying curves (low and high temperature settings) in a conventional oven. Compare and contrast all drying curves.
2. Determine the "potato optimum" cooking time (based on results from hardness, deflection, and panel tests) at a low temperature setting in a conventional oven. Using heat-transfer calculations, predict this optimum at a high temperature setting in the conventional oven and at low and high temperature settings in a convection oven.
3. Using a microwave oven, determine the potato optimum. Discuss how this optimum compares to other optimums obtained in other heat-transfer equipment. Discuss the advantages and disadvantages of potato cooking with a microwave oven. Place a damp paper towel over the potato stick and cook under previous "optimum" conditions. What happens to the potato quality and why?
4. Using a pressure cooker, determine the potato optimum. Discuss the nature of this optimum and how it compares to other optimums obtained in other heat-transfer equipment. Show calculations to determine the pressure and temperature conditions within the cooker.

## STUDENT FEEDBACK AND OUTCOMES

Students found this exercise to be both energizing and meaningful in engineering education. Applying principles of heat and mass transfer to foods they commonly consume generated considerable interest. Student feedback on the exercise during class evaluations was extremely positive. As an instructor, I like this exercise because students appear motivated, the experimental setup is relatively inexpensive, and the activity integrates multiple concepts of drying operations, conduction, and convective heat transfer.

The outcomes achieved from this classroom experience were:

- Enhanced total learning experience from combining classroom theory with an experimental component
- Reinforcement of ABET outcomes criteria, including (b) an ability to conduct experiments and to analyze/interpret data, and (d) an ability to function in multidisciplinary teams
- Letting students address the open-ended question of what the "optimum potato" is and how it might be produced
- Examination and appreciation of temperature and pressure effects on heat and mass transfer in a food-engineering application.

## CONCLUSIONS

Students found this simple exercise to be a welcome addition to traditional classroom theory of heat and mass transfer.

This experimental application seemed to be both motivational and an excellent learning vehicle. It provided application of fundamental engineering principles learned in the classroom to an everyday kitchen environment. Based on calculated rates of heat transfer, students could evaluate the effects of cooking and drying operations on something they frequently eat—the common potato.

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# USING A COMMERCIAL MOVIE FOR AN EDUCATIONAL EXPERIENCE

## *An Alternative Laboratory Exercise*

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I have used a commercial film, *Acceptable Risks*,<sup>[1]</sup> educationally for ten years. I give it to small groups of students in the timetable slot for a laboratory exercise and then have them write a report on it. It is not an educational film; it is a commercial cinema thriller—a “disaster” movie centered around a chemical plant. It is a drama involving human beings and is actually surprisingly sympathetic to those who work in the chemical industry. It is available on video for a modest price (vastly less than what is charged for some educational films). Although it did not get the media attention of *The China Syndrome*,<sup>[2]</sup> (which was about a nuclear power plant, released at about the same time as the Three-Mile Island incident), it is equally dramatic and watchable. In some respects, it resembles the Bhopal disaster, but it takes place on American soil and has characters that we get to know. Brian Dennehy plays the manager of a Citychem chemical plant in Oakbridge, under pressure from his bosses to maintain production and keep costs down. Eventually there is a toxic chemical release.

For chemical engineering students, however, there are many lessons to be learned. More than any other film I have seen (including specifically educational ones), it shows the technology and working practices of a plant, from the labeling of tanks to operating procedures; it shows what people actually do in a plant...management, operators, and technicians in particular.

There are technical issues. Understanding what goes wrong in this film and witnessing the consequences can give students insight into safety technology and techniques. Moreover, there is the human side. Perhaps one day some of these students will find themselves, like characters in the film, under pressure to speed up production and/or to save money. They see how there are conflicts and interactions between various groups, or how the company may go under if they cannot meet the price or order date, resulting in major job

losses and devastating effects on the local economy, or they see the conflict between politicians and environmentalists who fight for their own agendas.

As the students themselves recognize, this exercise demands some intellectual effort and provides a different learning experience from a traditional experiment and report. Analyzing what went wrong is more complex than just interpreting experimental data.

### USING THE VIDEO AS AN ASSESSED PRACTICAL EXERCISE

Typically, I give the film to second-year students in the time period allotted to a laboratory exercise. Three to six students in a room with a video player are told to watch the movie through to the end. The film takes an hour and a half, and the students have three hours for the practical. They then have to write a three-part report:

- 1) Write a news item for *The Chemical Engineer* (the main UK subject journal) reporting on the events as if they had just

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*Janet Robinson is a third-year student of chemical and process engineering at the University of Sheffield. When she wrote the report contained in this paper she was a second-year student.*

happened, remembering that the details will not yet be known and that the publication is subject to the libel laws. Their reading audience will expect to be told the company's name and the chemicals involved (so far as they are known) as accurately as possible.

- 2) Make a personal assessment of what went wrong and who was to blame.
- 3) Report on how valuable the experience of watching the film was. Did it give any insight into industrial practice in chemical plants? Did it affect your ideas about industrial safety? Was it a worthwhile alternative to a laboratory exercise?

## STUDENT RESPONSES

The student response has been overwhelmingly favorable. The small number of negative comments acknowledge that the student would have preferred to do an actual hands-on practical. Some of the responses to part three of the report were:

- The film allowed me to picture the kind of work I might be involved with in the future and the quick thinking that is necessary in a chemical plant in an emergency.
- Although the film is about things going wrong, it would have been pretty dull had it not. It did not put me off working in the chemical industry. Indeed, it may have confirmed that this is what I want to do.
- In particular, it reminds us that monetary gains should not be played off against human safety. In addition, the issue of plant location is raised, something that is currently very topical because of the recent disaster in Toulouse.
- I did consider the film worth watching. I think it was an insight into the chemical industry from a perspective that I might not otherwise have had. It highlighted many important safety, economic, and social issues.
- It was a challenging exercise, and I had to redevelop writing skills, very different from those I would use in writing laboratory reports, that I have not really used since I was studying GCSE English.
- Having watched this film, my awareness for the importance of safety in industry has definitely been increased.
- In the course of watching the film, I have learned how a chemical plant operates, about industrial practice, and about the safety procedures inside a plant.

### A Student's Appraisal (Janet Robinson)

*Personally, I think I gained quite a lot from watching the video and writing this report. Not just about the chemical plant and industrial practice, but also about writing in a new style compared to my normal work. I actually found the task a lot harder than writing a traditional lab report. I had to think in more depth about what I was going to write and make sure that, in the first place, I did not blame anyone, and in the second place, that I contributed my own opinions and not just what I had been told. That is considerably harder than it seems because there are quite a few people who could be blamed and it was hard to sort out the correct procedures from the incorrect ones since I have never been in a situation such as that.*

*The film showed me just how important safety issues within a chemical plant are—even simple but very serious things such as understaffing and an out-of-date evacuation plan. That sort of thing should be high on the agenda and should be sorted out before anything is produced. It has also shown me that you should not skimp on safety procedures just because a certain amount of chemical has to be produced. Safety should always come first, no matter how much pressure you are under. I think this is a very valuable thing to know when I go into industry.*

*I feel the film was worth watching and it taught me a lot. I think it is an acceptable alternative to the laboratory experiment and should be made compulsory for a number of reasons. It breaks up the traditional lab report. You gain valuable new skills such as writing in a different manner. I also think it teaches a lot about the day-to-day running of an industrial plant and shows that slight errors in procedures can have disastrous effects.*

## CONCLUSION

Watching a commercial film can be a valid educational experience if students are required to analyze and comment on it. Chemical engineering is not just about technical processes—it is also about people. It is clear that students have gained insights from watching this film that they did not get from visiting a plant. I also find this film a useful preparation for my course in Process Safety and Loss Prevention (where I show films about Bhopal and Feyzin).

A video can be a useful back-up if some laboratory experiments are temporarily unavailable. It can also be used as a timetabled class or borrowed for a project. Other films of relevance to chemical engineering are *The China Syndrome*<sup>[2]</sup> (about problems in the nuclear industry), *Erin Brockovich*<sup>[3]</sup> (about the effects of chemical pollution), and *Thirst*<sup>[4]</sup> (about purifying water, with a real chemical engineering finale). The film *Silkwood* is briefly concerned with the 1970s nuclear industry, but has, I think, little value in this context.

Since many chemical engineering departments now have teachers with degrees in other subjects and no industrial experience, *Acceptable Risks* might be a useful primer for them also.

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3. *Erin Brockovich* (2000) Universal Studios, NTSC, PAL, DVD (Supposedly based on a true story about people being poisoned by contamination of water supplies by hexavalent chromium. No real process information, but you could ask students to research Cr(VI) and water supplies; possibly also useful for discussion of ethical issues.)
4. *Thirst* (1997) New Line Studios, NTSC (TV movie. The hero is probably a civil engineer, but the story is about bugs in the water supply getting through filters. There are technical and environmental issues. The resolution is definitely chemical engineering.) □

# USING MOLECULAR-LEVEL SIMULATIONS TO DETERMINE DIFFUSIVITIES

## *In the Classroom*

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When engineers require a diffusivity for a chemical species in a fluid mixture for which experimental data is not available, there are several methods of obtaining a value. The most obvious method is to experimentally determine the value of the diffusivity, but frequently time and money constraints rule out this method. In that case, a theoretical approach to obtain the diffusivity can be used.

There are a variety of established methods for theoretical determination of diffusivities. For self-diffusivities and transport diffusivities of binary systems in gases, we can obtain values from kinetic theory and corresponding states arguments, a corresponding state chart, and the Chapman-Enskog theory,<sup>[1-3]</sup> and for self-diffusivities and transport diffusivities of binary systems in liquids, we can use the Wilke-Chang equation.<sup>[1]</sup> There are also a variety of other empiricisms summarized in the literature.<sup>[4]</sup> Needless to say, these empiricisms, while valuable, are limited in terms of the types of systems that they describe.

An alternative to obtaining the self-diffusivities for fluid mixtures, including those with an arbitrary number of components, is to conduct equilibrium molecular dynamics simulations of the system.<sup>[5-7]</sup> Engineers have been calculating self-diffusivities with this method for a number of years, but using molecular dynamics to obtain self-diffusivities has not yet become a common alternative in chemical engineering transport classes because of the historically extensive computational resources required to conduct the simulations.

In this paper we describe our efforts and our results in incorporating molecular-level simulations into a graduate transport phenomena course. Above all, our philosophy was to provide a utilitarian tool that could be used in a manner analo-

gous to existing techniques, such as the Wilke-Chang equation, to obtain transport diffusivities. Our target audience is the general graduate students in chemical engineering who will not necessarily perform molecular-level simulations as part of their thesis project. In the implementation of this work, we remain keenly aware of constraints due to time, computational resources, money, and target-audience qualifications.

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**Austin Newman** is in the process of completing his degree requirements for a Master of Science in Chemical Engineering at the University of Tennessee. He is working with statistical mechanical models that describe the transport of fluids in nanoporous materials.

**Parag Adhangale** received his BS from the University of Bombay and his MS from North Carolina Agricultural and Technical State University, both in chemical engineering. He is currently pursuing a PhD at the University of Tennessee. His research involves molecular and process simulations of adsorption of multicomponent systems in nanoporous materials.



## BACKGROUND

### Academic Preparation

This transport course is taken in the second semester of the first year of graduate school. The students have already had graduate courses in thermodynamics, advanced mathematics, and fluid mechanics. The advanced mathematics course includes numerical solution of systems of ordinary differential equations (ODEs) and partial differential equations (PDEs).

The course is roughly divided into two components. The first is the generation of transport properties, such as diffusivities. The second component is solution of transport equations, which are most generally systems of coupled parabolic PDEs representing transient material, energy, and momentum balances. Since the students are already equipped to tackle the equations numerically, the course, while demanding practical solutions with numerical values, focuses on conceptual understanding of transport phenomena.

### Molecular-Level Simulation

In an equilibrium molecular dynamics simulation, we select an appropriate potential that describes intramolecular and intermolecular interactions.<sup>[5-7]</sup> A typical potential for the intermolecular interaction of spherical molecules is the Lennard-Jones potential, for which parameters are widely available.<sup>[1-2]</sup> With a potential, we can generate the classical equations of motion, which for  $N$  spherical molecules result in a system of  $3N$  coupled second-order nonlinear ODEs. For the calculation of diffusivities in a bulk fluid,  $N$  is generally in the range from 200 to 1000 molecules. We solve the ODEs numerically, obtaining positions and velocities as a function of time.

By collecting, analyzing (using the Einstein relation for diffusivity), and regressing the trajectories as a function of time, we can obtain mutual self-diffusion coefficients.<sup>[5]</sup> There is one mutual self-diffusion coefficient for each species in the mixture. These coefficients are a function of the thermodynamic state (temperature, density, and composition). They are self-diffusion coefficients because they were calculated from an equilibrium simulation in the absence of macroscopic concentration gradients.

The mutual self-diffusion coefficients provide a quantitative description of each component's mobility in the system, but they are not transport diffusivities (also called Fickian diffusivities). We require transport diffusivities if we intend to use them in Fick's Law in a transport equation (material balance) in order to obtain the solution to an applied engineering problem.

### Irreversible Thermodynamics

The connection between mutual self-diffusivities and trans-

port diffusivities is provided in the framework of irreversible or nonequilibrium thermodynamics. One commonly used equation relates the transport diffusivity to the self-diffusivity via the thermodynamic partial derivative<sup>[8]</sup>

$$D_{ij} = D_{\text{self},i} \frac{c_i \partial \ell n(p_i)}{c_j \partial \ell n(c_j)} \quad (1)$$

Equation (1) contains numerous, potentially serious, assumptions. (Critical discussions of the applicability of the equation are available elsewhere.<sup>[9-17]</sup>) Regardless, Eq. (1) is widely used for lack of an alternative. (One alternative is to perform full-blown nonequilibrium molecular dynamics simulations, which has also been done.<sup>[18]</sup>) For a binary mixture, Eq. (1) yields four diffusivities, which are intended to be used in Fick's law<sup>[13]</sup>

$$\underline{N}_A = c_A \underline{v}_A = -D_{AA} \nabla C_A - D_{AB} \nabla C_B \quad (2a)$$

$$\underline{N}_B = c_B \underline{v}_B = -D_{BA} \nabla C_A - D_{BB} \nabla C_B \quad (2b)$$

### Traditional ChE Description of Diffusion

Chemical engineers know that the diffusive behavior of a binary system can be completely described by a single diffusivity. Traditionally, we write Fick's law relative to a molar average velocity,  $\underline{v}^*$ , and Fick's law is written (for a binary mixture)

$$\underline{J}_A^* \equiv c_A (\underline{v}_A - \underline{v}^*) = -c D_{\text{BSL}} \nabla x_A \quad (3a)$$

$$\underline{J}_B^* \equiv c_B (\underline{v}_B - \underline{v}^*) = -c D_{\text{BSL}} \nabla x_B \quad (3b)$$

where  $D_{\text{BSL}}$  is the only independent diffusivity.<sup>[1]</sup>

In the course we begin by calculating diffusivities for binary mixtures using the traditional correlations and theories, following the formalism and notation used in Reference 1. In order to compare the diffusivities of molecular dynamics simulations to traditional methods, we must present the diffusivities in Eq. (2) as a single number that can be directly compared to  $D_{\text{BSL}}$  in Eq. (3).

We have derived this relationship for a binary mixture and it is given as

$$D_{\text{BSL}} = x_B (D_{AA} - D_{AB}) + x_A (D_{BB} - D_{BA}) + \frac{1}{c} \left( x_A x_B D_{AA} - x_A^2 D_{BA} + x_B^2 D_{AB} - x_A x_B D_{BB} \right) \left( \frac{\partial c}{\partial x_A} \right) \quad (4)$$

If the fluid is an ideal gas or we make some other assumption in which the density is not a function of composition, then  $(\partial c / \partial x_A)$  is zero. We can use Eq. (4) to obtain a single transport diffusivity for the binary mixture. Since this diffusivity is the same property with respect to the same frame of reference that is generated by traditional methods of estimating

***In this paper we describe our efforts and our results in incorporating molecular-level simulations into a graduate transport phenomena course. Above all, our philosophy was to provide a utilitarian tool that could be used in a manner analogous to existing techniques, such as the Wilke-Chang equation, to obtain transport diffusivities. . . . In the implementation of this work, we remain keenly aware of constraints due to time, computational resources, money, and target-audience qualifications.***

the diffusivity of a binary system (such as the Wilke-Chang equation), we can make a direct comparison.

## A FEASIBILITY STUDY

### Time, Money, and Computational Constraints

Part of the reason that using molecular-level simulations to determine diffusivities isn't as prevalent in chemical engineering classrooms as it could be lies with the perception that the simulations simply require too much computer power. While this was true as recently as the 1990s, it is no longer true. Rigorous molecular-level simulations generating diffusivities (with error bars small enough to permit publication) now take only a few minutes on a several-year-old processor (for example, an AMD Athlon 850 MHz processor). In the example below, we provide specific program clocking. Certainly the impediment is no longer computational resources.

Efficient molecular-level simulations do require a FORTRAN or C compiler. Using a software platform that interprets code rather than compiling it is not an alternative due to the computational efficiency. In our example, we ran the simulations on

- Compaq FORTRAN in the Microsoft Windows environment
- Intel FORTRAN in the Linux environment
- Matlab in the Microsoft Windows environment

We shall show that a software platform that interprets code, rather than compiling it, is about four orders of magnitude slower than a structured code, and is thus not an option. Of the first two choices above, both have advantages. The advantage of the Windows environment is its ubiquity—the disadvantage is that the FORTRAN compilers for the Windows environment are relatively expensive. The advantage of the Linux environment is that both it and the FORTRAN compiler software for it are free.

### Constraints Based on Target-Audience Qualifications

Our target audience are first-year chemical engineering graduate students, including those who do not intend to perform simulations as part of their thesis work. With this in mind, we structured the course to address that audience. Each part of the process that generates the diffusivity (including the molecular-level simulation, the irreversible thermodynamics, and the traditional description of diffusion) is presented

with a pragmatic attitude: we are engineers who need a transport diffusivity; we first want to understand the techniques used to obtain the diffusivity; after we understand it, we want a simple, methodical, (preferably foolproof) algorithm to follow that generates a reliable transport diffusivity that we can use in material balances describing applied engineering systems.

The course is in no way intended to be an exhaustive survey of molecular-level simulation techniques, or of irreversible thermodynamics, or of the numerical solutions of ODEs and PDEs. On the contrary, the course describes a procedure that incorporates each of these elements. As we stated before, the students have obtained enough background during their first semester as graduate students to make this course content feasible.

When discussing molecular dynamics, we present a complete, self-enclosed description of the procedure.<sup>[19]</sup> We discuss only equilibrium molecular dynamics in the microcanonical ensemble, since that is the simplest system to simulate. A “base-case” FORTRAN code for this system is provided and discussed subroutine-by-subroutine in a lecture.<sup>[19]</sup>

## AN EXAMPLE

As a practical example, we work problem 17.A.5 of Bird, Stewart, and Lightfoot.<sup>[1]</sup> The problem asks the students to calculate the quantity,  $cD_{BSL}$ , of an equimolar mixture of ni-

**TABLE 1**  
**Simulation Parameters**

Number of N <sub>2</sub> molecules	108
Number of C <sub>2</sub> H <sub>6</sub> molecules	108
Volume (Å <sup>3</sup> )	1.88153 x 10 <sup>6</sup>
Intermolecular potential	Lennard-Jones
σ <sub>N<sub>2</sub></sub> (Å)	3.667
σ <sub>C<sub>2</sub>H<sub>6</sub></sub> (Å)	4.388
ε <sub>N<sub>2</sub></sub> (K)	99.8
ε <sub>C<sub>2</sub>H<sub>6</sub></sub> (K)	232
Integration algorithm	Gear fifth-order predictor corrector <sup>[22-23]</sup>
Time step (fs)	4
Long-range cut-off distance (Å)	12
Number of equilibration steps	50000
Number of data production steps	500000

trogen and ethane at 288.2 K and 40 atm. In the problem, the student is instructed to solve the problem using (a) an experimental data point and kinetic theory and (b) correlations and kinetic theory. If we obtain the concentration,  $c$ , of the mixture via the Lennard-Jones equation of state<sup>[20]</sup> with standard mixing rules,<sup>[21]</sup> the values of  $D_{BSL}$  are (a)  $3.04 \times 10^{-3} \text{ cm}^2/\text{s}$  and (b)  $2.78 \times 10^{-3} \text{ cm}^2/\text{s}$ .

The students then perform a molecular-level simulation using the parameters given in Table 1. From the simulations, they obtain self-diffusivities. They use Eq. (1) to generate transport diffusivities from the self-diffusivities, and they use the Lennard-Jones equation of state to provide the thermodynamic derivatives in Eq. (1). They use Eq. (4) to obtain a single transport diffusivity for the binary system.

Following this procedure, the students obtain a value of  $D_{BSL}$  of  $2.98 \times 10^{-3} \text{ cm}^2/\text{s}$ , which is nicely bracketed by the two estimates obtained via traditional means. A summary of the results of the molecular-level simulation that generated the self-diffusion coefficients, as well as the thermodynamic partial derivatives obtained from the Lennard-Jones equation of state and used in Eq. (1), are provided in Table 2.

Two notes of explanation are in order for Table 2. The temperature and pressure in the molecular dynamics simulation do not exactly match those stipulated in the problem. Because this is not a course in molecular simulation, we limit ourselves to simulating in the microcanonical ensemble, which is the simplest ensemble. In using the microcanonical ensemble, we fix the number of molecules of each species, the total system volume, and the total energy. Since the problem asks for the diffusivity at a given temperature and pressure, we estimate the density that corresponds to the requested T and p, using the Lennard-Jones equation of state. We then equilibrate at that density, maintaining a constant temperature with velocity scaling. For data production, we run in the microcanonical ensemble, which fluctuates about the set temperature, because there is no driving force pushing the temperature to another value.

Second, we see that  $D_{N_2, C_2H_6}$  is negative. It is acceptable to have a negative diffusivity in a Fick's law of the form of Eq. (2). This simply indicates that, all other things being equal, nitrogen would diffuse up the ethane gradients. This negative term, however, is roughly five times smaller in magnitude than the positive  $D_{N_2, N_2}$ , which yields a net positive transport diffusivity.

If we were to assume that the molar volume was not a function of composition, an assumption which is true for, among other systems, ideal gases, then the latter term from Eq. (4) would drop out and we would have a numerical value of  $D_{BSL}$  equal to  $3.07 \times 10^{-3} \text{ cm}^2/\text{s}$ , as compared to the value from the complete version of Eq. (4), which was  $2.98 \times 10^{-3} \text{ cm}^2/\text{s}$ . The effect of that term is to lower the diffusivity from a more ideal case.

In Table 3 we provide the CPU usage for our three cases on an AMD Athlon 850 MHz processor. Clearly, either of the FORTRAN cases makes this calculation a very reasonable homework problem, requiring less than 8 minutes of CPU time. We have solved a system of 648 (3 dimensions x 216 molecules) second-order

**TABLE 2**  
Simulation and Equation-of-State Results

<u>Molecular Dynamics Results</u>		<u>Equation-of-State Results</u>	
T(K)	293	T(K)	288.2
p(atm)	39.7	p(atm)	40
$x_{N_2}$	0.5	$x_{N_2}$	0.5
$c(\text{molecules}/\text{\AA}^3)$	$1.148 \times 10^{-3}$	$c(\text{molecules}/\text{\AA}^3)$	$1.148 \times 10^{-3}$
$D_{\text{self}, N_2} (\text{cm}^2 / \text{s})$	$3.445 \times 10^{-3}$	$\frac{c_{N_2}}{PN_2} \frac{\partial p_{N_2}}{\partial c_{N_2}}$	1.1025
$D_{\text{self}, C_2H_6} (\text{cm}^2 / \text{s})$	$2.333 \times 10^{-3}$	$\frac{c_{N_2}}{PN_2} \frac{\partial p_{N_2}}{\partial c_{C_2H_6}}$	-0.2150
$D_{N_2, N_2} (\text{cm}^2 / \text{s})$	$3.798 \times 10^{-3}$	$\frac{c_{C_2H_6}}{PC_2H_6} \frac{\partial p_{C_2H_6}}{\partial c_{N_2}}$	2.3916
$D_{N_2, C_2H_6} (\text{cm}^2 / \text{s})$	$-7.405 \times 10^{-4}$	$\frac{c_{C_2H_6}}{PC_2H_6} \frac{\partial p_{C_2H_6}}{\partial c_{C_2H_6}}$	0.7850
$D_{C_2H_6, N_2} (\text{cm}^2 / \text{s})$	$2.392 \times 10^{-4}$	$\frac{\partial c}{\partial x_{N_2}} (\text{molecules}/\text{\AA}^3)$	$-4.1060 \times 10^{-4}$
$D_{C_2H_6, C_2H_6} (\text{cm}^2 / \text{s})$	$1.832 \times 10^{-3}$		
$D_{BSL} (\text{cm}^2/\text{s})$	$2.98 \times 10^{-3}$		

**TABLE 3**  
CPU Usage

(The Matlab time is projected for a simulation of 550,000 steps, using the fact that a simulation of 20,000 steps used 179,360 seconds of CPU time. All codes were run on an AMD Athlon 850 MHz processor.)

<u>Software</u>	<u>Operating System</u>	<u>CPU Usage (Seconds)</u>
COMPAQ Visual FORTRAN 6.5	Windows XP Professional	443
Intel FORTRAN Compiler 5.0	Red Hat Linux 7.1 with Kernel 2.4.2-2	324
Matlab 5.1	Windows XP Professional	$4.932 \times 10^6$

ODEs over 550,000 time increments (2 nanoseconds of data production—more than enough time to establish a self-diffusivity for this system) in 8 minutes.

In this demonstration, we computed the transport diffusivity of a high-density gas that could be adequately described with traditional methods, but there is nothing in the simulation code that limits it to a binary mixture, which therefore greatly expands the capabilities of molecular-level simulation.

## CONCLUSION

We have presented work describing the practical use of molecular-level simulations to determine diffusivities in a course targeted at the general audience of first-year chemical engineering graduate students. We have shown how the simulation techniques can be used to directly complement traditional methods for obtaining diffusivities. We have provided an algorithm by which students can generate transport diffusivities that can be used in material balances that describe practical engineering applications. In the implementation of this work, we have shown that it is computationally feasible to include numerical simulations in the classroom. We have also shown that it is a financially modest approach for chemical engineering departments.

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## NOMENCLATURE

$c$	total molar concentration
$c_i$	molar concentration of component $i$
$D_{\text{self},i}$	self-diffusivity of component $i$
$D_{ij}$	Darken transport diffusivity
$D_{\text{BSL}}$	single independent diffusivity for a binary system
$J_A^*$	flux of component $i$ , relative to molar average velocity
$N_i$	flux of component $i$ , relative to laboratory frame of reference
$p$	total pressure
$p_i$	partial pressure of component $i$
$T$	temperature
$v_i$	velocity of component $i$
$v^*$	molar average velocity
$x_i$	mole fraction of component $i$

$\epsilon_i$  intermolecular potential well-depth of component  $i$

$\sigma_i$  collision diameter of component  $i$

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