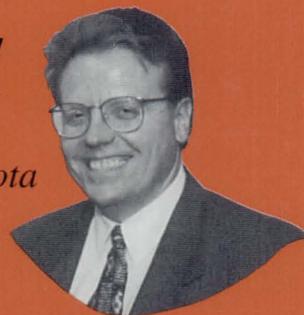




## Matt Tirrell

of Minnesota



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## Puerto Rico - Mayagüez

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*Chemical Engineering Education*  
 Department of Chemical Engineering  
 University of Florida • Gainesville, FL 32611  
 PHONE and FAX : 352-392-0861  
 e-mail: [cee@che.ufl.edu](mailto:cee@che.ufl.edu)  
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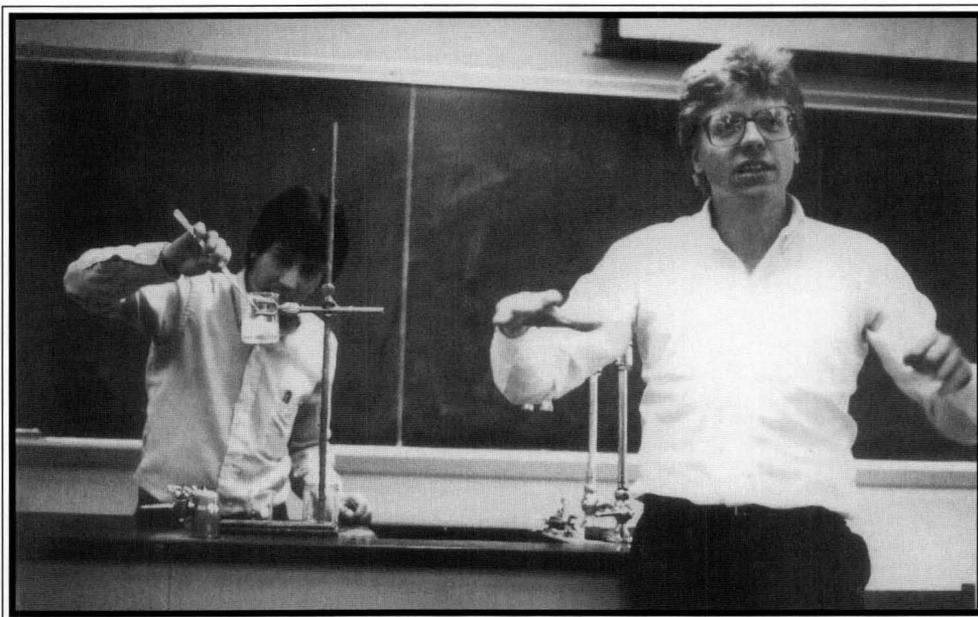
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## Minnesota's MATT TIRRELL



*Matt and teaching assistant Rafael Galvan demonstrating nylon polymerization during a polymer chemistry lecture. Galvan, now at Dow Chemical, coauthored Polymerization Process Modeling with Matt, Neil Dotson (Eastman Chemical), and Bob Lawrence (University of Massachusetts).*

### WRITTEN BY HIS COLLEAGUES

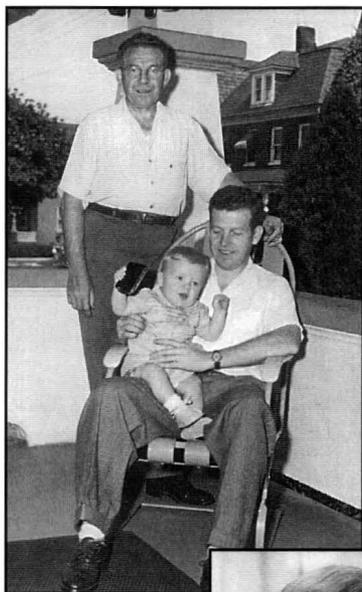
*University of Minnesota • Minneapolis, MN 55455*

In a department that has been home to such chemical engineering legends as Neil Amundson, Rutherford Aris, and Skip Scriven, Matt Tirrell has carved out a niche for himself as a modern-day Renaissance Man. Applying a notably broad knowledge of chemical engineering and materials science to a mulligan stew of engineering research, he is a marked asset to a department emphasizing collegiality and a team-teaching philosophy.

Abundant energy and a gift for organization allow Matt to keep multiple and varied projects moving forward at the same time. After 18 years of making a name for himself, Matt took the reins of the Chemical Engineering and Materials Science Department at the University of Minnesota in

1995, and in so doing he added one more huge responsibility to his shoulders, but he did it without neglecting his other duties as scholar, teacher, mentor, editor, and researcher. His colleagues are justifiably amazed and proud of his diversity and leadership.

Matt was born September 5, 1950, in Phillipsburg, New Jersey, on the Delaware River border with Pennsylvania, and is the oldest of three children. His younger brother, Dave, also developed a strong interest in polymer chemistry and is currently Professor of Chemistry and Chemical Engineering at Caltech. The youngest sibling, Mary, is raising three children in Bangor, Pennsylvania, close to Phillipsburg, and helps in her husband's construction business in addition



◀ *Matthew V. Tirrell, Matthew V. Tirrell, Jr., and Matthew V. Tirrell, III, (our Matt), at 9 months, on the family porch in Phillipsburg, New Jersey.*



▲ *Matt (3) and Dave (9 months). Dave had Matt's support even before he could sit up by himself. Dave followed a similar career path and is now a professor at Caltech.*



*Matt, proud graduate of Belvidere High School in 1968. ▶*

to working hard on the local school board.

Matt's parents were divorced when he was still quite young, and he was largely raised by his mother. His summers were spent at a swimming club, playing golf, and working as a caddie. One of his childhood friends was Jeff Brinker, who is now a ceramist at Sandia and a chemical engineering professor at the University of New Mexico.

Matt entered college at Northwestern University in 1968. While trying to decide the direction of studies he would take, he was swept up in the anti-war protests of the early 70s, with the result that for a short time he considered a life in politics. It's to our benefit that he decided on a more concrete, if no less contentious, field.

While at Northwestern, Matt became interested in polymers during a co-op term spent doing PVC compounding at Cincinnati Milacron. When he returned to campus, he sought out Bill Graessley for a polymer undergraduate research project. (Matt spoke at Bill's retirement from Princeton in May.) After gradu-

## Matt's Mentors

**Joe McHale** (Chemistry, Belvidere High School) excited Matt's interest in chemistry (and his brother Dave's too!) and encouraged him to enter the field.

**Josh Dranoff** (Chemical Engineering, Northwestern) taught in Northwestern's high school summer program between Matt's junior and senior years. He helped Matt see possibilities in chemical engineering as a career. Matt's dad, who was an ME, also encouraged him to consider chemical engineering over chemistry.

**Bill Graessley** (Chemical Engineering, Northwestern) On returning from his Milacron co-op to Northwestern, Matt sought out Graessley to learn more about polymers. Bill asked Matt to set up the first anionic polymerization experiments. He did—in a coke bottle. Matt continued working in Bill's lab when he wasn't co-oping. The position had perks such as a desk—not bad for an undergraduate. Graessley encouraged Matt to go on to graduate school.

**Stan Middleman** (University of Massachusetts) Matt picked polymer science and engineering at University of Massachusetts because of its polymer reputation and because it brought him closer to his chemistry interests. A Northwestern University friend, Bob Weiss was already there. Matt picked Stan as his advisor for the interesting and imaginative research he was doing. Stan was an excellent teacher, a model Matt emulated when he went to Minnesota.

**Skip Scriven and Chris Macosko** (University of Minnesota) Jim Douglas recommended that Matt "go for the best," and he did. Among many things he learned from faculty in his early years at Minnesota include Chris Macosko setting the tone of collaboration and sharing all major equipment and Skip Scriven modeling organization of large quantities of information from seemingly diverse fields.

**Minnesota's five  
"living Heads":**

**Tirrell (1995 - present)**

**Rutherford Aris (1975 - 78)**

**Ken Keller (1978 - 80)**

**Neal Amundson (1950 - 75)**

**and**

**Ted Davis (1980 - 95)**



ating from Northwestern, Matt chose the University of Massachusetts for graduate studies in the Polymer Science and Engineering Department.

In 1977, Tirrell accepted an offer to join the Chemical Engineering and Materials Science Department at the University of Minnesota, and he has been there ever since. When the Department Head, Ted Davis, left to become Dean of the Institute of Technology, Matt became the new Department Head at Minnesota. Along with the usual daily challenges of running a large department (not the least of which is communicating to 30-plus busy, outstanding, and very active faculty), Matt's tenure has the added responsibilities of overseeing a transition to the semester system and planning a building addition.

Matt's leadership style clearly leans toward the inclusive. It is important to him that the faculty be kept fully informed at each developmental stage of major projects. In a tradition started by Neal Amundson, many of the faculty share a large round table during lunchtime, facilitating the exchange of ideas and information. By involving as many faculty as possible in all facets of departmental matters, he helps them focus on the common goal of "how best can we project our unified department to the several external constituencies, *i.e.*, the chemical engineering, materials science, biomedical, polymer chemistry communities, *etc.*"

When prompted, Matt is more than willing to talk about the strengths of his department. He believes that an excellent and caring staff in the office, the shop, the lab, in computing, and in accounting is the backbone of the department. Selfless colleagues, notably Associate Head William Gerberich, the Directors of Undergraduate Studies, David Shores and Wei-Shou Hu (Materials Science and Chemical Engineering, respectively) and of Graduate Studies, John Weaver and Lanny Schmidt, (Materials Science and Chemical Engineer-

ing, respectively) make his job a lot easier. He is grateful for their willingness to manage the huge burden of the semester transition, a project in which "no one wants to invest time, but the outcome of which concerns everyone."

One of the difficult challenges faced by a department head is maintaining connections to his own research community, but Matt has managed quite well in that respect. His research focuses on huge molecules in small spaces, and his work with block copolymers has led to innovations that have allowed oil companies to extract more oil from porous rocks and to create smoother-flowing solutions used in paints, solvents, and toner for copying machines. Later, while leading the polymer program at the Center for Interfacial Engineering (CIE, an NSF-funded academic/industry/government collaboration), several companies with specific research problems expressed an interest in pursuing biomedical applications of polymer research. Having done his PhD thesis on the effect of flow on proteins, Matt jumped at the chance to expand the program. He developed the notion that some of the same ideas used to prevent fine particles in inks and toner from forming clumps could be used in biomedical engineering problems. As a result, part of his research group began working on treating surfaces to improve biological interaction. A new Biomedical Interfacial Engineering arm was added to the CIE, which later developed close contacts with the Biomedical Engineering Center (BMEC) at the Medical School.

Matt is valued as a conduit for interactions between the physical sciences and the medical school at Minnesota. As Prof. Leo Furcht, Head of the Department of Laboratory Medicine and Pathology has put it, "Matt has proved his skill at building consensus among people from many departments who have mutual and conflicting interests. Added to that, he is internationally regarded as a leader and innovator in polymer science, which is critical to the future of bio-

***His research focuses on huge molecules in small spaces, and his work with block copolymers has led to innovations that have allowed oil companies to extract more oil from porous rocks and to create smoother-flowing solutions used in paints, solvents, and toner for copying machines.***

medical engineering.”

Tirrell has a reputation among his graduate students, (38 PhD students and 13 MS students) as a resourceful and caring mentor. His dedication to their education is a result of his pride in his students. He relishes their successes. Matt is known to show remarkable restraint in letting his protégés find their own direction and to think for themselves, guiding them with a gentle hand when they seem to be heading off course. Rasti Levicky, soon to be teaching at Columbia, echoes the thoughts of many of Tirrell's former students when he says, “I learned independence from Matt's being open to what I thought were interesting and important things to do.” Matt has an informal style that encourages students to discuss issues with him, and believing it important to their education, he fosters interactions among the students themselves. He gets them to talk as a way to learn. He also stresses the importance of communication in writing and oral presentations. “If you cannot make your information come across to your audience, you have to question your own understanding of the material.”

It is clear that Matt enjoys his work. In 1992, during a trip to NIST in Washington, DC, Matt, Frank Bates, and graduate student Kurt Koppi (now at Dow Chemical) were trying out for the first time an instrument Koppi had built. They sat down and almost immediately discovered something they hadn't expected—block copolymer orientation *perpendicular* to the flow. They had a great time collecting valuable data on a process that had never been seen before, reveling in the excitement of first discovery. The data was shortly thereafter written up for *Physical Review Letters*, and has become a frequently cited paper.

Matt's goes to great lengths to help his students find interesting jobs after they have completed their studies. They must see something they like about the way he manages his group since a large proportion of them choose academic

### **Tirrell's Former Students and Post-Docs Now in Academia**

Natash Balsara • *Polytechnic University*  
Ioannis Bitsanis • *University of Florida*  
Arup Chakraborty • *University of California, Berkeley*  
Nily Dan • *University of Delaware*  
Angela Dillow • *University of Massachusetts*  
Steve Granick • *University of Illinois*  
Nino Grizzuti • *University of Naples*  
Michael Kilbey • *Clemson University*  
Rasti Levicky • *Columbia University*  
Jaye Magda • *University of Utah*  
Guangzhao Mao • *Wayne State University*  
James Schneider • *Carnegie Mellon University*  
John Torkelson • *Northwestern University*

careers for themselves. They see him working extremely hard, juggling many projects, and doing it well, and it obviously inspires them to do the same. As Kurt Koppi says, “Matt is a terrific mentor. His diverse background spans the whole spectrum of chemical engineering. The depth and breadth of his knowledge helps his students when they are learning to do research, learning to focus their thoughts and to see the overall picture. Matt is able to help them sort out the key features and organize their thought processes to get to the main issues.” In 1981, thanks to the nomination of his students, Matt's

teaching was recognized with a Gordon Starr Outstanding Contribution Award.

Matt has been similarly dedicated to the health of his profession. He has served on the editorial boards of *Journal of Polymer Science*, *Polymer Physics Edition*, *Macromolecules*, *Journal of Chemical Physics*, *Journal of Rheology*, and other idea forums. His most demanding service position currently is as editor of *the AIChE Journal*.

In the course of his career Matt has also earned the recognition of his peers. He has received the NSF Presidential Young Investigator Award, a Guggenheim Fellowship, the AIChE's Allan P. Colburn and Charles M.A. Stine Awards, the John H. Dillon Medal from the American Physical Society, the Alumni Merit Award from Northwestern University, and last year was elected a member of the National Academy of Engineering.

Tirrell's accomplishments have not gone unnoticed by the University of Minnesota. When the University began a capital campaign to increase the school's endowment, part of its program was to increase the number of endowed chairs to help retain accomplished professors. At a youthful 36,

***A gourmet,  
Matt has  
developed a  
flair for  
preparing  
exquisite  
meals. With a  
special  
appreciation  
for French  
Provençal  
and  
Mediterranean  
cuisines, he  
has built a  
collection of  
some 200  
cookbooks  
with recipes  
from around  
the world. . .  
In addition to  
cooking . . .  
[Matt enjoys]  
rugby . . .  
distance  
running . . .  
[and] golf.***

Matt was singled out for the Shell Chair, which Matt has used to enhance the polymer facilities at Minnesota and to nurture his research group.

Attracting and keeping Matt was a shrewd move for Minnesota. Matt has served the University community far beyond the call of duty, an indication of how deeply he believes in the value of education. He has acted on numerous committees, including (currently) the key Faculty Consultative Committee, and has led faculty searches, chaired two separate departments, been a faculty representative to the Senate, and chairman of the faculty club.

Among his many attributes, Matt is a fund-raiser *par excellence*. Both chemical engineering and materials science, and the Biomedical Engineering Center are vastly better off as a result of his efforts. What makes him successful at it? He works hard to



*In light of Matt's reputation as a cook, an invitation to dinner at "Chez Tirrell" is a coveted prize!*

identify possible sources, he addresses himself to links of common purpose between the University department and the funding source, he draws in and ties together disparately skilled colleagues to present cogent possibilities, and he pays attention to the little details that give proposals their air of imminent success. In other words, Matt is comfortable thinking both big and small.

Outside the University, Matt has done volunteer work for the American Civil Liberties Union and has been on the board of directors of a prominent Minneapolis theatre, Theatre de la Jeune Lune. He likes being involved, feeling that he's contributing something to his community.

As hard as he works at his public duties, in private, Matt really cooks. A gourmet, Matt has developed a flair for preparing exquisite meals. With a special appreciation for French Provençal and Mediterranean cuisines, he has built a collection of some 200 cookbooks with recipes from around the world. In addition to cooking, as an assistant professor, rugby was Matt's game, but as an associate professor he turned to more genteel pursuits—distance running. He completed two Twin Cities Marathons and for five years belonged to an afternoon running club. Now, while he has again taken up distance running, he keeps up his health principally through membership in a fitness club and by golfing (in 1995, his best-ball foursome won the department's



◀ *Matt and his wife, Pam, enjoy traveling together. Here, they have just landed in Beijing, China.*

---

*The Tirrell family—Matt with his mother, Lorraine, his sister Mary, and his brother Dave. ▼*



coveted “Amundson Open” title).

Matt also enjoys other sports, such as skiing and biking, but acknowledges that a love of sports *can* get out of hand. He credits his wife Pam for helping him “balance my conventional male tendency to antisocial activities such as sports” with movies and plays. Nevertheless, Matt holds Minnesota Timberwolves season tickets.

Pam and Matt met when she was a writer and editor for University Relations at Minnesota. Matt had won an NSF Presidential Young Investigator Award and Pam was assigned to interview him. We can only speculate that she liked what she saw. Pam grew up in International Falls, Minnesota (“America’s Icebox”) and remembers separate changing rooms for boys and girls on the city’s many ice rinks. She says, “It was tough to play hockey in a skirt, but we did.” Pam has since moved on to work in guest relations at the historic St. Paul Hotel. She and Matt share a restored townhouse near downtown St. Paul, not far from where F. Scott Fitzgerald, and later Garrison Keilor, lived. Pam and Matt have no children, but enjoy visiting with their twelve nieces and nephews.

That Matt maintains continuity in his many interests is all the more remarkable when one realizes how much time he spends in the air. Traveling has played a significant role in Matt’s career, and brings together the two strands of his public and private life. He has been a visiting professor in cities like Bahia Blanca, Guadalajara, Canberra, and Paris. He recently received notification that he’d surpassed one million actual miles traveled (to say nothing of frequent-flier bonus miles), and even this understates the extent of his travels. He often accepts speaking invitations, and his various collaborations require him to take quick trip here and there to keep up with projects. For example, his consulting work with the state and

government consortium, French Petroleum Institute in Paris, takes him back to France at least once a year.

For his effort, there have been numerous returns for Matt. He has seen academic programs started, students graduating, projects being well funded, professional honors and awards coming his way. . . but what higher honor could there be than to have a former graduate student say, as many of Matt’s students do, “When I meet people in the field, I’m proud to tell them I worked with Matt Tirrell.”

As you converse with Matt Tirrell you realize that you are with a unique individual; one with the rare ability to convey ideas in well-crafted complete sentences. Everything Matt says is well considered and easy to follow. This characteristic may be the key to his success in both research and in teaching. “To help myself pay attention in lectures during my sophomore year at Northwestern, I started to think about how I would explain the subject. I feel that this carries over directly to research. Explaining things clearly is intimately connected to doing good research.” As the end of your appointment approaches, you notice Matt cocks his head to check the time on your watch. This busy man does not wear one. With a subtle and not unfriendly gesture, Matt suggests he must be going. □

*Chemical Engineering at the University of*

# ***Puerto Rico***

---

## ***Mayagüez Campus***



*Chemical Engineering facilities at the University of Puerto Rico-Mayagüez.*

**D**uring the last four years, the Department of Chemical Engineering at the University of Puerto Rico-Mayagüez Campus has undergone a major transformation. We developed and implemented a strategic plan that provided specific goals and guidelines for the transformation, with the main goal of the Department being to become one of the top fifty US chemical engineering departments by the year 2002. Our mission is to

*Satisfy the technological needs of Puerto Rico related to chemical engineering.*

This mission will be accomplished by means of teaching, research, and services to students coming from all socioeconomic levels. These students, in turn, will become competitive professionals with a global perspective and with a clear understanding of their social responsibility.

### **OVERVIEW**

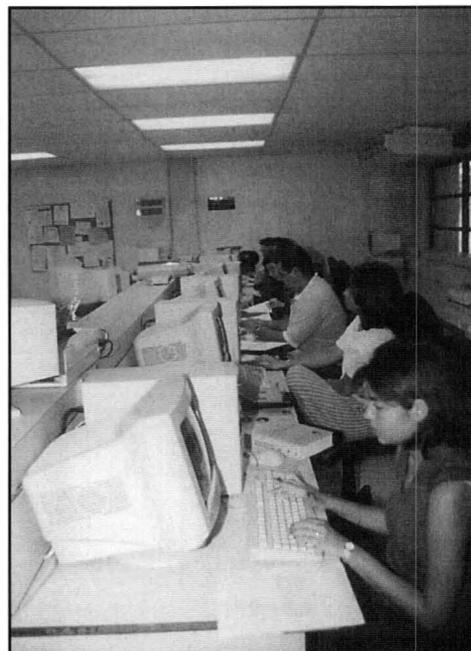
The University of Puerto Rico-Mayagüez is located on the west coast of the island of

*[The] main goal of the Department [is] to become one of the top fifty US chemical engineering departments by the year 2002. . . . This mission will be accomplished by means of teaching, research, and services to students coming from all socioeconomic levels.*

Puerto Rico, about ninety miles from San Juan. The location is relatively close to beautiful beaches as well as other island attractions, such as a tropical rain forest called "El Yunque," a phosphorescent bay located at the town of Guanica, the Arecibo Observatory, and national monuments such as Porta Coeli, which is located at San Germán.

The Department of Chemical Engineering at the University of Puerto Rico saw its first four students graduate in 1930 with degrees in chemical engineering with emphasis on sugar cane refining. In 1948, the University approved the Department's first Chemical Engineering Program with emphasis in other areas, and in 1978, the Department moved to its present location, which is part of the engineering complex at the University. The Department presently has a faculty consisting of 24 professors, of which 18 have PhD degrees and 6 have MS degrees.

The 36,600 ft<sup>2</sup> facility consists of administrative and faculty offices, eight modern classrooms, an amphitheater, ten research laboratories, a pharmaceutical process laboratory, a unit operations laboratory, and two computer centers. There is also an office for the Student Chapter of the American Institute of Chemical Engineers (AIChE) and for Puerto Rico's Institute of Chemical Engineering (IIQPR). As part of the services available to the students, the department has a Student Aid Center (SAC) facility, a non-profit corporation that provides services such as photocopying and supplies.



*Students in the well-equipped computer center at UPR-Mayagüez.*

## UNDERGRADUATE AND GRADUATE PROGRAMS

**Undergraduate Program** • The undergraduate program has an average enrollment of 170 students per year, of which 55% are female. This includes approximately thirty to forty internal and external transfer students per year. The program is ranked among the top ten in the United States based on number of degrees awarded (see Table 1).

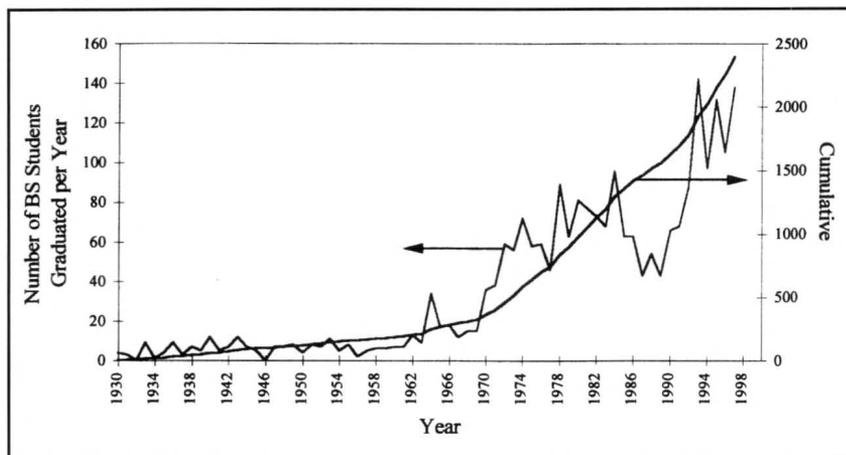
As part of its undergraduate program, the Department offers a Bachelors in Science Degree in Chemical Engineering (BSChE) with several elective courses as options. In the last 68 years, the chemical engineering program at the University of Puerto Rico has graduated more than 2,400 engineers, the largest source of Hispanic chemical engineers in the United States (see Figure 1).

The basic undergraduate curriculum, accredited by the Engineering Accreditation Commission of the Accreditation Board for Engineering and Technology (ABET), requires 172 credits/hours for completion in five years. It includes courses in basic sciences and other branches of engineering to provide the student with a sound, fundamental, scientific, technical, and sociohumanistic education. The students are required to take courses in advanced mathematics, physics, and chemistry during the first two years. At the beginning of the third year of studies, the students start a three-year program dedicated mainly to chemical engineering courses (see Table 2, Section

**TABLE 1**  
Degrees Awarded and Ranking  
(Based on degrees Awarded) from 1990 to 1996

Year	BSChE		MSChE	
	# of Degrees Awarded	Ranking <sup>1</sup> (# of schools)	# of Degrees Awarded	Ranking <sup>1</sup> (# of schools)
1990	66	8 (126)	11	26 (122)
1991	68	8 (120)	7	53 (115)
1992	88	4 (113)	1	99 (108)
1993	142	1 (105)	4	67 (97)
1994	97	7 (124)	8	43 (117)
1995	132	7 (134)	5	83 (127)
1996	105	9 (141)	15	15 (133)

<sup>1</sup> Data obtained from the Annual Report of the American Chemical Society (ACS) Committee on Professional Training (Chemical and Engineering News).



**Figure 1.** BSChE degrees granted from UPR-Mayagüez



*The Department has eight classrooms and one amphitheater to accommodate the 450+ enrolled students.*

1). Also, as part of the BSChE curriculum, the Department offers a number of specialized courses (see Table 2, Section 2). Undergraduates can also take graduate courses as electives (see the section on the graduate program).

The undergraduate research courses offer students an opportunity to obtain first-hand experience in the latest developments in areas such as electrochemistry, photocatalysis, surface catalysis, process control optimization, biochemical engineering, biomedical engineering, and supercritical fluids. Our program also offers several elective course options, in collaboration with other engineering departments, such as environmental engineering, manufacturing engineering, and (in the near future) a biotechnology option.

The manufacturing engineering option is part of the Manufacturing Engineering Partnership (MEEP) created in 1994 by three engineering schools: Pennsylvania State University, the University of Washington, and the University of Puerto Rico-Mayagüez. It is cosponsored by the Procter & Gamble Foundation and aims at providing a proper balance between science and engineering practice in such a way that the students will develop the skills employers value. The courses are supported by a learning factory and laboratory facilities for hands-on activities integrated into the courses and field trips.

The BSChE program has an excellent reputation both on the island and on the mainland. Many prestigious local and US companies, such as Amoco, Kodak, Xerox, Union Carbide, Champion, Pfizer, Abbot, Johnson & Johnson, Pharmacia-Upjohn, ARCO Chemical Co., DuPont, Procter & Gamble, and Merck Sharp & Dohme recruit on our campus (see Table 3). In addition, state government agencies such as the Environmental Quality Board, Aqueduct and Sewer Authority, Solid Waste Management Authority, and the Electric Power Authority recruit our graduates. An average of twenty students per year continue their education with graduate studies.

It should be mentioned that several foundations, such as Procter & Gamble, AMOCO, DuPont, and Sloan provide financial assistance to develop and promote research activities at the undergraduate level.

**Graduate Program** • The graduate program was established

**TABLE 2**  
**Courses Offered**

Standard Courses

- Material and energy balances
- Momentum transfer operations
- Chemical engineering thermodynamics (2 semesters)
- Heat transfer operations
- Kinetics and catalysis
- Mass transfer operations
- Unit operations laboratory (2 semesters)
- Analysis and control of processes
- Process design (2 semesters)
- Mathematical analysis in chemical engineering
- Chemical Engineering electives

Specialized Courses

- Advanced process control
- Air pollution control
- Computer simulation of processes and units
- Equilibrium stage processes
- Microclimate and dispersion of air pollutants
- Industrial waste control
- Introduction to biochemical engineering
- Introduction to biomedical engineering
- Particulate systems
- Pharmaceutical process design
- Plastics technology
- Transport phenomena
- Undergraduate research
- Unit operations in food processing

**TABLE 3**  
**Alumni Profile and Employability**

Academic Year	# of Graduated Students Working in the US <sup>1</sup>		# of Graduated Students Working in Puerto Rico <sup>1</sup>		# of Students Working Toward a Graduate Degree <sup>1</sup>	
	Total	% <sup>2</sup>	Total	% <sup>2</sup>	Total	% <sup>2</sup>
1987-88	8	21.6	6	16.2	7	18.7
1988-89	3	6.8	14	31.8	10	22.7
1989-90	15	18.3	23	28.0	23	28.0
1990-91	16	16.8	31	32.6	27	28.4
1991-92	11	12.6	17	19.5	18	20.7
1992-93	3	2.3	37	28.2	32	24.4
1993-94	1	1.2	32	39.0	16	19.5
1994-95	6	5.0	69	58.0	17	14.3
1995-96	12	11.9	30	29.7	21	20.8
1996-97	13	9.3	30	21.4	25	17.9

<sup>1</sup>Data obtained from the Placement Department, Univ. of Puerto Rico-Mayagüez

<sup>2</sup>Percent taken from the total amount of students graduated that academic year.

in 1972 and offers programs leading to Master in Science (MS) or Master in Engineering (ME) degrees and, in the near future, a program leading to a PhD in chemical engineering. The MS degree (Option 1) requires completion of advanced courses and research in chemical engineering and requires a thesis report plus a final oral examination. Option 2, the ME degree, differs from Option 1 in that the students develop an advanced project; it also requires a final oral examination. The courses offered for these options (see Table 4) cover most of today's top chemical engineering areas.

The Department's graduate program has generated more than three million dollars in research proposals during the last five years and has obtained funding from agencies and institutions such as the National Science Foundation (NSF), National Institutes of Health (NIH), Department of Energy, Department of Defense, and Sandia National Laboratories. As a result of the research activity, the Departments' faculty gave more than 60 presentations in technical conferences and other activities and submitted almost 40 articles for publication during the 1993-97 period. The Department's research and development areas include biochemical, biomedical, catalysis, reactors, colloids, interfaces, materials, expert systems, control, polymers, composites, thermodynamics, transport, separations, environmental ChE, and energy.

Figure 2 shows the number of students graduated from the Masters program in the years 1974 to 1997.

### PHD PROGRAM

One of the key priorities of the University of Puerto Rico is the development of graduate programs and research activity. As a result of that initiative, the Chemical Engineering Department has developed a strategic plan with the PhD program as one of its primary components. The implementation of the PhD program is critical to reaching the Department's main goal of being among the top 50 US departments. The program has the following objectives:

- To educate the students in how to master and apply scientific methods as a fundamental tool in research.
- To develop the students' capacity to make original contributions to the field of chemical engineering.
- To develop in the students a high sense of social and ethical responsibility, knowing not only the technical and economical aspects of

**The Department's graduate program has generated more than three million dollars in research proposals during the last five years and has obtained funding from [numerous] agencies and institutions . . .**

*their work, but also safety, health, and environmental protection issues.*

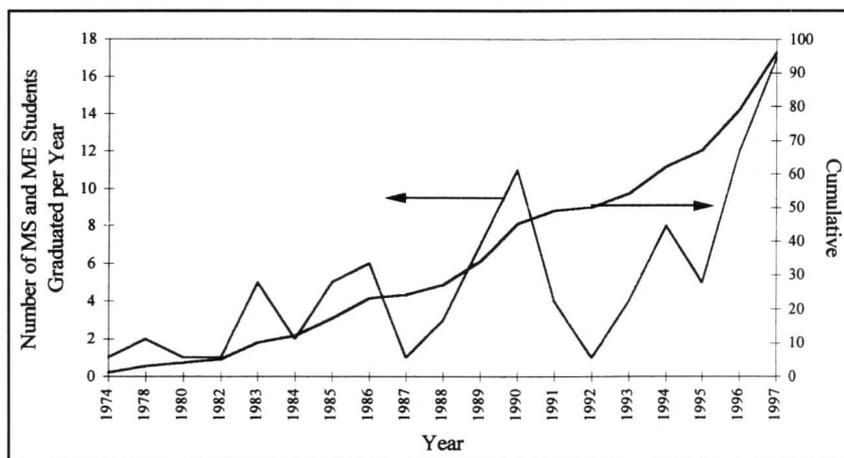
The program will require a minimum of 58 credits/hours for completion. The new courses designed for the PhD that will be added to the graduate courses already developed are listed in Table 5.

**TABLE 4  
Graduate Courses Offered**

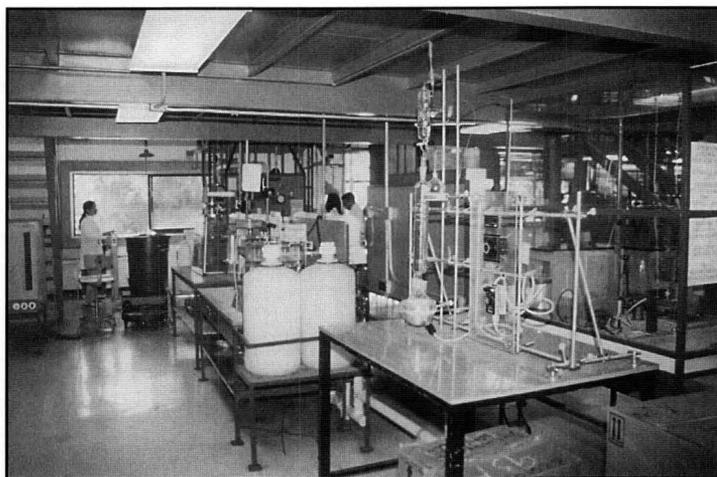
- Advanced heat transfer
- Advanced process control
- Advanced reactor design
- Advanced thermodynamics
- Advanced transport phenomena
- Catalysis
- Electrochemical engineering
- Mathematical methods in chemical engineering
- Numerical methods in chemical engineering
- Chemical process optimization
- Chemical process simulation
- Plant design
- Selected topics in biochemical engineering
- Separation process analysis

**TABLE 5  
PhD Courses to be Added to Curriculum**

- Models for flow systems in chemical reactors
- Atmospheric transport phenomena
- Special topics in heterogeneous catalysis
- Food fermentation and biotechnology
- Special problems at doctoral level
- Finite elements in transport phenomena
- Doctoral seminar
- Doctoral dissertation



**Figure 2. Master's degrees granted by UPR-Mayagüez.**



*The photograph at the left shows the east section of the 3,500 ft<sup>2</sup> unit operations laboratory, and the west section is shown in the photograph below.*



## LABORATORY FACILITIES

The Department has two facilities dedicated exclusively to unit operations, process control, reactor design, and pharmaceutical operations. The laboratory facilities reflect the requirements of the undergraduate program and are fully equipped for their effective use.

The 3,500 ft<sup>2</sup> Laboratory of Unit Operations is equipped with heat exchangers, hydraulic benches, flow-measuring devices, a cooling tower, an absorption tower, distillation columns, chemical reactors, and equipment for digital process control. The facility also has a wet chemistry laboratory equipped with analytical instrumentation such as gas chromatography, high-performance liquid chromatography, UV-Vis spectroscopy, and atomic absorption. These facilities are undergoing major changes to offer the students a state-of-the-art laboratory. Some of the changes include the addition of high-tech chemical analysis instruments, updating and validation of existing experiments, and the creation of new experiments.

As part of the addition of new experiments, the department is planning to develop and install a laboratory module dedicated exclusively to process and manufacturing control using programmable logic controllers and a virtual control room. In addition, the department is evaluating the implementation of experiments in the areas of molecular simulation, micro-chemical systems, and field applications. These developments will give the students first-hand experience in the latest technologies and opportunities available to chemical engineers.

## RESEARCH FACILITIES

The Department's research facilities include ten modern laboratories, an instrumental analysis laboratory, and a computer center. The graduate students also have access to the Central Research Instrumentation Laboratory (managed by the Department of Chemistry), which provides quantitative analysis services for research projects.

The research laboratories are equipped with a total carbon analyzer, a glucose analyzer, gas chromatographs, Fourier transform

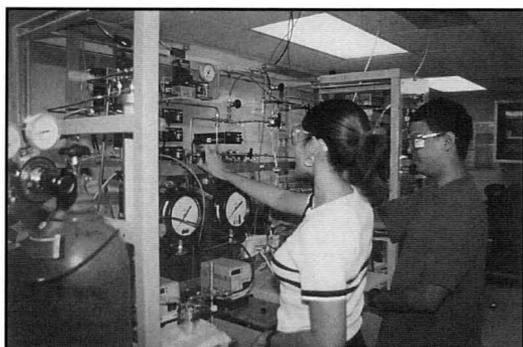
infrared equipment, high-performance liquid chromatographs, a GC-MS, polarographs, an X-ray fluorescence analyzer, spectrometers, a dissolved oxygen analyzer, humidity analyzers, and gel permeation chromatographs. The Central Research Instrumentation Laboratory includes gas chromatography/FT-IR equipment and a nuclear magnetic resonance apparatus.

The Department is designing a 25,000 ft<sup>2</sup> facility that will host the Environmental & Biotechnology Research & Incubator Opportunities Laboratory. This five-million-dollar facility will be used by entrepreneurs and faculty involved in research and development activities. Also, the Department is finishing an area of 2,000 ft<sup>2</sup> that will be used for a research laboratory and an instrumental analysis laboratory. All these initiatives are part of the implementation of the PhD program.

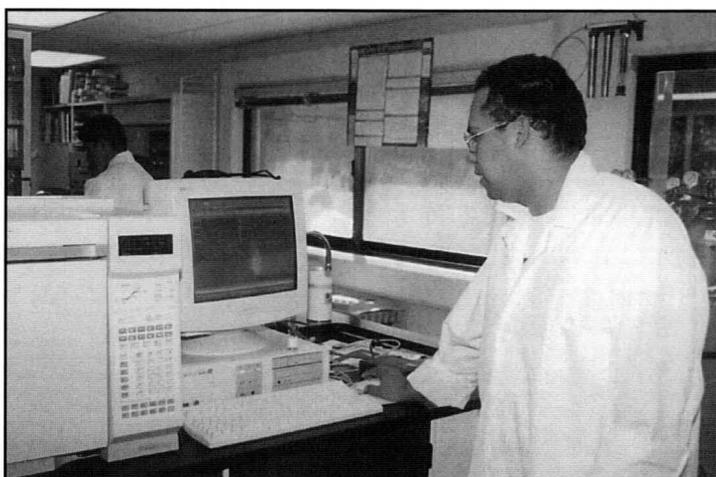
## CHE OUTREACH ACTIVITIES

***Merck Sharp & Dohme Lecture Series*** • The Merck Sharp & Dohme Lecture Series was established by a grant given from the Merck Foundation in 1972. The purpose of the grant is to exchange new technical and scientific developments among those who wish to explore in depth a particular research area in chemical engineering. The grant has allowed our department to invite distinguished scientists and recognized authorities to lecture and has offered our graduate and undergraduate students an unparalleled opportunity to know first-hand these leading scientists and their projects. Most of the authors of textbooks used in our Department have been invited as lecturers in this series. It is one of the longest uninterrupted lecture series in America (25 years).

*Chemical Engineering Education*



***Above is Dr. Nelson Cardona's microcalorimetry laboratory, and below is Dr. José Colucci's environmental research projects laboratory***



***Environmental Symposia*** • As part of the activities celebrated annually in the Department, the Environmental Symposia are an essential part of the strategic plan initiatives to exchange information between the Department, the industrial sector, and the community. Merck Sharp & Dohme cosponsors these seminar sessions from industry and academia on topics related to environmental issues. A poster presentation is given by undergraduate and graduate students.

***Process Design Course*** • The Department has established a partnership with industry to assure that our students complement their academic experience with applied projects. In 1996, the Department modified the Process Design II course, incorporating business experiences into the projects as part of the initiative funded by Procter & Gamble Foundation. The business approach includes assigning real projects or problems from the industrial and governmental sector with emphasis on the development of communication and leadership skills. The final work is presented to representatives of industry and government agencies for their consideration and evaluation.

***Honor Student Activity*** • The Department, in collaboration with the student chapters of AIChE and IIQPR, celebrates the

Honor Students Activity each year. It is dedicated to undergraduate students with a GPA higher than 3.00 (on a 4.00 scale), recognizing their hard work and dedication. The activity consists of an open house, an official ceremony, and a lunch. More than 300 guests come to the event each year.

## **FUTURE INITIATIVES**

The Department is developing several initiatives that will support its intention to serve Puerto Rico. These initiatives include the construction of an Environmental & Biotechnology Research & Incubator Opportunities Laboratory, implementation of the PhD program, a new distance learning program, and development and implementation of a new millennium unit operations laboratory.

Also, the Department is updating the existing computer facilities with the latest software and hardware. One of the initiatives of the Department is to create a multipurpose computer facility in order to integrate the use of computers at all levels in the chemical engineering curriculum. In addition, the facility will support the development of the ME program via videoconferencing.

We have been working to improve our program in order to continue graduating the finest engineers and to solve present and future technical challenges. As the major source of Hispanic engineers in the nation, we are committed to continue these trends for the benefit of our society. We are looking forward to being one of the top fifty U.S. chemical engineering departments by the year 2002!

Additional information about the chemical engineering program can be obtained by contacting

The University of Puerto Rico - Mayagüez Campus  
Department of Chemical Engineering  
PO Box 9046  
Mayagüez, Puerto Rico 00681-9046

Phone: (787) 832-4040, ext. 2568  
FAX: (787) 265-3818

E-Mail: J\_Colucci@RUMAC.UPR.CLU.EDU

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# AN EXPERIMENT IN APPLIED OPTICS

## *Determination of the Kinetics of the Oxidation of an Organic Dye*

P. DELGADO, A. KASKO, J. NAPPI, R. BARAT  
New Jersey Institute of Technology • Newark, NJ 07102

Applied optics is gaining in importance for science and engineering students. A National Science Foundation (NSF) workshop<sup>[1]</sup> recently recommended an emphasis on optics research and education because

*Optical Science and Engineering is an enabling technology—that is, a technology with applications to many scientific disciplines and with the potential to contribute in significant ways to those disciplines.*

This workshop recommended a strong optical component in the undergraduate curriculum of science and engineering students. An interdisciplinary group at New Jersey Institute of Technology (NJIT) has created such an applied optics curriculum.<sup>[2]</sup> It is supported through the Combined Research-Curriculum Development program of NSF and has been very successful.<sup>[3,4]</sup>

Optics should no longer be viewed as a tool of only the physicist. Optical principles, especially as applied to spectroscopy, are obviously important to chemistry students. However chemical engineering students are not usually exposed to optics beyond general undergraduate physics courses. There is a definite need to expose these students to more optics, especially since optical-based sensors for process monitoring are rapidly expanding into the traditional chemical industries.

Optical diagnostics applied to a chemical reactor offer the chance to demonstrate two principles: 1) the determination of reaction kinetics without direct sample analysis of reac-

tants or products, and 2) rapid monitoring for process control.

In this paper we will describe an effective, simple, and inexpensive experiment in applied optics for monitoring the oxidation of an organic dye. Absorption of a laser beam passing through a batch reactor produces data from which overall kinetics are determined. The use of an in-situ laser beam diagnostic avoids the cumbersome, potentially inaccurate, and costly method of direct sampling for optical absorption in an ultraviolet-visible spectrophotometer.

### THEORY AND OBJECTIVES

An organic food color is a complex organic dye with a broad-banded absorption spectrum. In the case of a helium-neon (He-Ne) laser at 632 nanometers (nm), the dye of choice is one with a spectrum with a reasonably strong absorption at the red 632-line, *i.e.*, blue or green. Transmission of the beam through a volume of absorbing dye solution is governed by the Beer-Lambert law<sup>[5]</sup>

$$I_t = I_o \exp(-\sigma CL) \quad (1)$$

where

- $I_t$  transmitted intensity
- $I_o$  incident intensity
- $\sigma$  absorption cross section
- $C$  dye concentration
- $L$  optical path length (distance laser beam passes through dye solution)

Typically, Eq. (1) is rewritten as

$$\mathcal{A} = \ell n \left( \frac{I_o}{I_t} \right) = \sigma CL \quad (2)$$

where  $\mathcal{A}$  is absorbance. Since there is negligible absorption by water at 632 nm,  $I_o$  can be taken to be the intensity of the laser beam exiting the reactor.

The oxidation reaction can be written as



where

**Paglo Delgado, Jr.**, is currently employed by Merck & Company as an analyst. He earned his BS in chemical engineering from the New Jersey Institute of Technology in 1998.

**Anna Kasko** is currently employed by FMC Corporation as a process engineer. She earned her BS in Chemical Engineering from the New Jersey Institute of Technology in 1997.

**Jarod Nappi** is currently employed by Merck & Company as a process engineer. He earned his BS in chemical engineering from the New Jersey Institute of Technology in 1997.

**Robert Barat** is currently an associate professor of chemical engineering at the New Jersey Institute of Technology. He received his PhD in chemical engineering from the Massachusetts Institute of Technology in 1990.

*The [NSF] workshop recommended a strong optical component in the undergraduate curriculum of science and engineering students . . . In this paper we will describe an effective, simple, and inexpensive experiment in applied optics for monitoring the oxidation of an organic dye.*

- A dye  
 B oxidant  
 b overall stoichiometric coefficient indicating the number of moles of B consumed for each mole of A oxidized.

The assumption is that Eq. (3) probably represents an overall stoichiometry, *i.e.*, the dye oxidation occurs via a mechanism of several elementary reactions. Overall reaction kinetics, however, can be determined.<sup>[6]</sup>

The rate of reaction ( $-r_A$ ) can be written as

$$-r_A = -\frac{dC_A}{dt} = k C_A^n C_B^m \quad (4)$$

where

- k overall rate constant  
 $C_A, C_B$  concentrations of dye and oxidant, respectively (mole/cm<sup>3</sup>)  
 n, m overall reaction orders

If the reaction is performed when the concentration of oxidant is in considerable excess over that of the dye (*i.e.*,  $C_A \ll C_B$ ), then  $C_B$  is effectively constant. Equation (4) can then be rewritten as

$$-r_A = -\frac{dC_A}{dt} = k' C_A^n \quad (5a)$$

where

$$k' = k C_B^m \quad (5b)$$

Combining Eqs. (5a) and (2) results in the first working relation needed to model the experimental data:

$$-\frac{d\mathcal{A}}{dt} = k^* \mathcal{A}^n \quad (6a)$$

where

$$k^* = k'(\sigma L)^{1-n} \quad (6b)$$

and is a constant for a given experiment with a specific amount of excess bleach. Taking the logarithm of Eq. (6a) yields

$$\ln\left(-\frac{d\mathcal{A}}{dt}\right) = \ln(k^*) + n \ln(\mathcal{A}) \quad (6c)$$

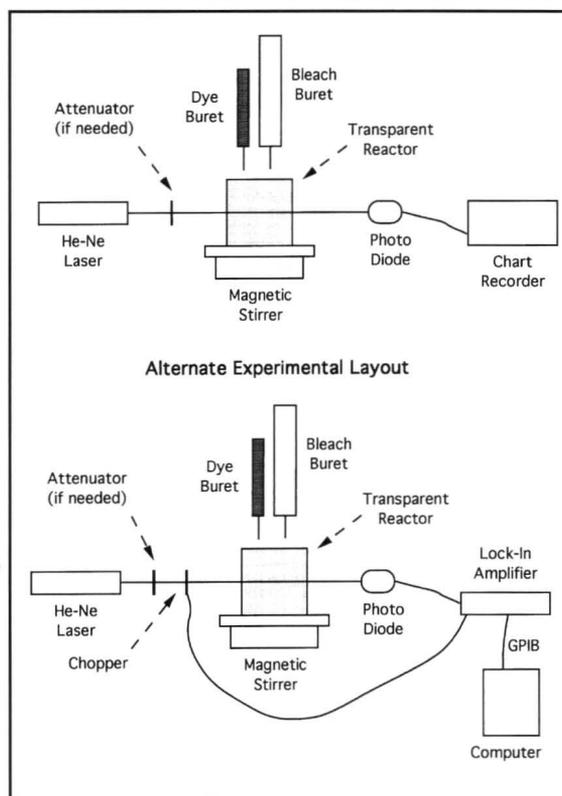


Figure 1. Experimental layout.

Using a differential approach, curves of  $\mathcal{A}$  vs. time are generated from a signal trace. Slopes of these curves, representing the time rate of change ( $-d\mathcal{A}/dt$ ), are determined and then plotted vs. absorbance  $\mathcal{A}$  according to Eq. (6c). The “best fit” slope is the order  $n$ , with intercept giving  $k^*$ .

Alternatively, using an integral approach, two cases can be derived from Eq. (6a) depending on the value of  $n$ . If  $n=1$ , then Eq. (6a) integrates to

$$\ln\left(\frac{\mathcal{A}_0}{\mathcal{A}}\right) = k^* t \quad (7)$$

where  $\mathcal{A}_0$  is the absorbance measured initially with water and dye, but before the oxidant is added. If  $n$  is not equal to 1, then Eq. (6a) integrates to

$$\mathcal{A}^{1-n} = (n-1)k^* t + \mathcal{A}_0^{1-n} \quad (8)$$

Equations (5b) and (6b) are combined to give

$$k^* = k C_B^m (\sigma L)^{1-n} \quad (9)$$

Absorbance data are correlated with either Eq. (7) or (8) to determine the “best fit” reaction order  $n$  and rate constant  $k^*$ .

Whether a differential or integral approach is taken, the series of  $k^*$  values from runs with different volumes of excess bleach are then correlated with bleach concentrations, using Eq. (9) to determine the “best fit” reaction order  $m$ . Taking the logarithm of Eq. (9) yields

$$\ln(k^*) = \ln[k(\sigma L)^{1-n}] + m \ln(C_B) \quad (10)$$

A plot of  $k^*$  vs.  $C_B$  according to Eq. (10) should yield a slope of  $m$  and the rate constant  $k$  to within a constant  $(\sigma L)^{1-n}$ .

## APPARATUS

The schematic for this experiment is shown in Figure 1. The batch reactor can be any transparent container with two parallel flat sides that can serve as windows for the He-Ne laser beam. The container should be appropriate in overall

## Laboratory

size for whatever magnetic stirrer is used. We recommend a Teflon-coated stirring bar. The intensity of stirring should be sufficient to obtain good mixing, yet not so great that it causes a vortex to form and extend into the laser beam path.

The incidence of the laser beam onto the front and back sides of the reactor will generate two back reflections. The reactor should be slightly skewed off-normal to the beam to prevent the back reflections from reentering the laser. Once it is set, care should be taken to avoid moving the reactor relative to the beam. An outline of masking tape around the base of the reactor on the magnetic stirring surface will ensure that the reactor is always in the correct position.

The exiting laser beam is directed into a photodiode or other optical detector. The detector should have a response time much shorter than typical reaction times (see Figure 3). A photodiode is definitely fast enough, in addition to being inexpensive and readily available. Care should be taken to avoid saturating the detector. Placement of neutral density filters (NDFs) or other attenuators in the path of the laser beam before the reactor will reduce the level of light hitting the detector. Detector linearity (*i.e.*, non-saturation) can be checked by ensuring that a 50% drop in detector signal occurs when a 50% NDF is placed before the detector.

The detector signal voltage can be monitored with a chart recorder or other signal detection apparatus (*e.g.*, analog-to-digital data acquisition-equipped personal computer). One configuration currently in use in our interdisciplinary applied optics laboratory course connects the photodiode detector to a lock-in amplifier. The laser beam is modulated with a chopper, and the lock-in amplifier is interfaced to a laboratory computer via a general-purpose interface bus (GPIB).

The bleach and dye reagents can be volumetrically added to the reactor with graduated burettes suspended over the reactor. Water should also be volumetrically added to the reactor.

### TYPICAL EXPERIMENT

In the experiment described in this paper, the reactor is a clear acrylic topless box with a 4x4-in square base and a 5-in height. Durkee Liquid Food Color (blue or green) and household laundry bleach (5.25 weight % NaOCl active ingredient with the balance assumed to be water) are the reagents. The bleach is delivered through a 500-ml burette, which has a sufficiently large bore such that the time to add the reagent was small relative to the reaction time scale. The dye is delivered through a 5-ml burette.

A Spectra-Physics 1-milliwatt helium-neon laser is used in conjunction with an amplified Thorlabs silicon photodetector (Model PDA150). The voltage signal is observed with a chart recorder. A typical simulated trace

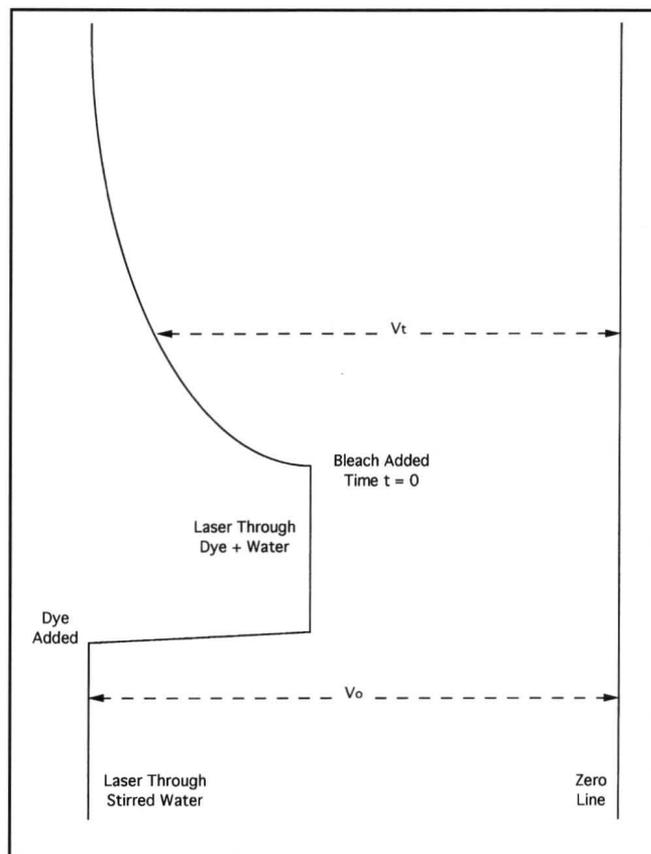


Figure 2. Sample detector signal trace.

is shown in Figure 2. It should be noted that the “zero line” properly corresponds to the detector signal with the laser beam blocked so as to account for any detector voltage offset.

In a typical experiment, 350 ml of water is added to the reactor box (about one-half full) prior to its placement on the magnetic stirrer. Optical alignment of the laser beam, the box, and the detector should be done with the first batch of stirred water. Care should be taken with laser light reflecting

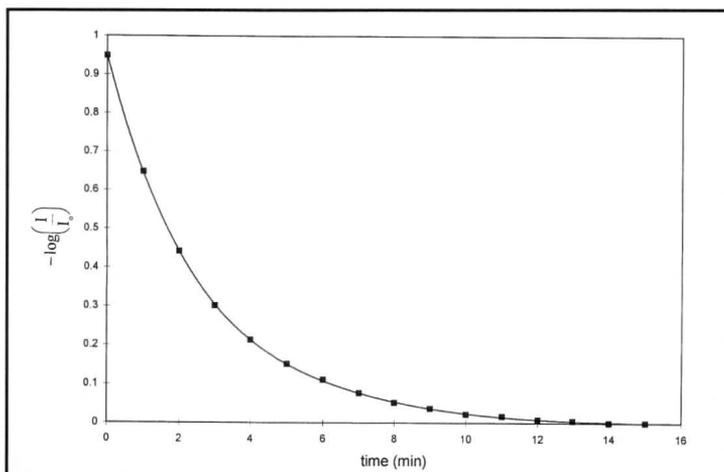


Figure 3. Absorbance vs. time for run #2.

back from various surfaces. Masking tape should be placed around the base of the reactor box to ensure that it would always be returned to the same position so that the optical alignment would not be disturbed.

Detector linearity is then tested. We determined that a total optical density of 1.5 (approximately at 97% intensity reduction) was needed in the path of the laser beam in front of the reactor box.

With detector linearity established, a trace representing  $I_0$  can be recorded. One drop of dye (approximately 0.03 ml) is added to the stirring water. A short delay should ensue to establish a new constant signal trace, which indicates the maximum absorbance. Then, at time  $t=0$ , a fixed volume of bleach (at least 10 ml) is added to the stirred solution. The signal trace is allowed to ascend over time until it reaches an effectively constant value—typically the same value indicative of a clear solution, which indicates a complete reaction. The solution is visibly clear at this point. It should be noted

that the laser light is not absorbed by the bleach, as evidenced by a test made with bleach added to plain water.

It is assumed that a given detector signal voltage,  $v$ , is directly proportional to a given beam intensity,  $I$ , as in

$$v = aI \quad (11)$$

where  $a$  is the constant conversion factor. Equation (2) then becomes

$$\mathcal{A} = \ln\left(\frac{I_0}{I_t}\right) = \ln\left(\frac{v_0}{v_t}\right) \quad (12)$$

where  $v_0$  is the signal corresponding to the laser beam passing through clear, stirred water, and  $v_t$  is the time variant signal corresponding to the attenuated beam as the reaction proceeds. These values are represented on the sample trace in Figure 2.

## DATA ANALYSIS AND RESULTS

The data and results presented in this paper were taken directly from a student group experiment in our senior chemical engineering laboratory course.

Using a differential approach, Figure 3 illustrates a plot of absorbance  $\mathcal{A}$  vs. elapsed time for one drop of blue dye, 20 ml of bleach, and 600 ml of water. Slopes ( $-d\mathcal{A}/dt$ ) were determined graphically. Logarithms of the slopes are plotted vs.  $\ln \mathcal{A}$  (as in Eq. 6c) in Figure 4. The “best fit” slope of 1.03 suggests first-order kinetics in dye concentration.

Using an integral approach for the same run, Figure 5 shows a first-order plot using Eq. (7). The correlation coefficient ( $R^2=0.9948$ ) is sufficiently good to declare the reaction kinetics to be first order in dye concentration.

Table 1 summarizes the results from all the runs. Several other runs were made with different bleach volumes, but always with 1 drop of blue dye and the same starting volume of water. In spite of some fluctuation in the “best fit” order, there is no reason to suspect anything other than first order with respect to dye.

For the case of  $n=1$ , the “lumped” rate constant  $k^*$  reduces to  $k'$ , which is plotted vs. initial bleach concentration in Figure 6 according to Eq. 9. The “best fit” slope of 1.00 shows that the reaction is first order in bleach concentration. The overall rate constant  $k$  is found to be 16.4 liter/mole-minute. An “error” propagation analysis has estimated the uncertainty in  $t_f$  rate constant at 12%.

**TABLE 1**  
“Best Fit” Reaction Order with Respect to Dye Concentration

Run	Volume Bleach	Order n
1	10	1.15
2	20	1.03
3	30	1.03
4	40	1.27

Continued on page 197.

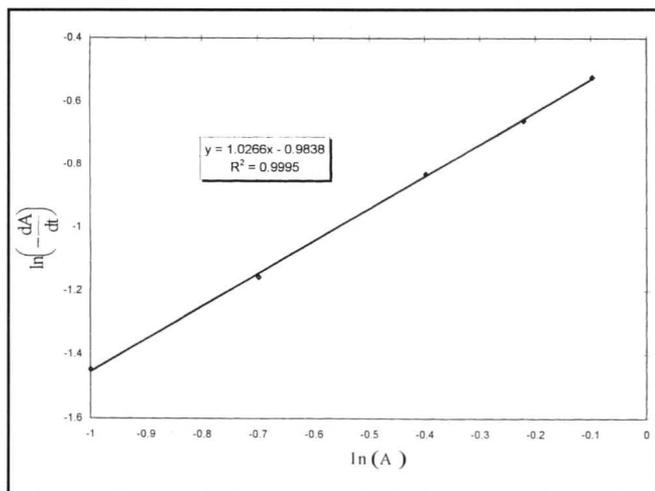


Figure 4. Rate vs. absorbance; differential approach, Eq. 6c.

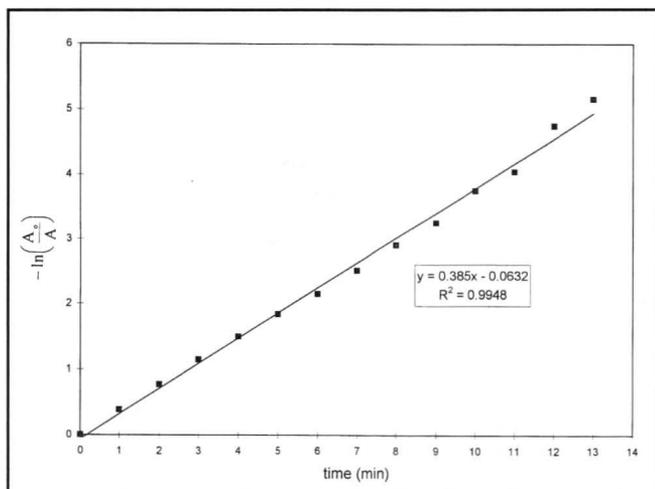


Figure 5. Absorbance vs. time; integral approach, Eq. 7.

# INCORPORATING SAFETY INTO A UNIT OPERATIONS LABORATORY COURSE

JULIA A. KING

Michigan Technological University • Houghton, MI 49931

Chemical process safety is taught at Michigan Technological University (MTU) via two methods: a required junior-level lecture course and integrated into the existing senior-level unit operations course.<sup>[1]</sup> The required junior-level course typically covers industrial hygiene and toxicology, flammability, relief systems, hazard identification, risk assessment, accident investigation, and case histories. After completing this class, the students are ready to apply these topics in the unit operations laboratory, which is the major chemical engineering laboratory experience they encounter.

The unit operations course consists of thirteen different pilot-scale standard experiments (batch filtration, continuous filtration, continuous-stirred tank reactors, cooling tower, flow measurement, fluidization, liquid-liquid extraction, polymer processing, pumping a, pumping b, single-pass heat transfer, shell-and-tube heat transfer, and vacuum drying) and two industrial-scale pilot plants (PSCC, Process Simulation and Control Center, which uses the Honeywell Total Plant Solutions control system), the first being an industrial-scale pilot plant for fractionation of a water-ethanol system, and the second being a PDMS (polydimethylsiloxane) jacketed-reactor pilot plant.

The students are divided into groups of four. The members of each unit operations group remains the same for an entire academic year, and during the year, each group conducts six experiments (or cycles), two of which are the PSCC pilot plants. For each cycle, each group spends one week preparing for their assigned experiment, two weeks in the laboratory conducting their experiment, and one week writing their report.

For each laboratory cycle, one group of students is randomly assigned as the safety committee.<sup>[2]</sup> Safety is the sole duty of this group, and there is a different safety committee for each cycle. This procedure began in 1983 as a method of incorporating safety into the unit operations course. We regard safety as an integral part of the unit operations course,

and student involvement in the program prevents the need for faculty/staff-mandated safety rules. Safety procedures for the unit operations laboratory course are reviewed and approved by the unit operations students, as well as by faculty/staff. This paper focuses on further integration of safety, including using Job Safety Assessments and the Internet, into the existing unit operations course.

## UNIT OPERATIONS COURSE

Most of our chemical engineering faculty are involved in the unit operations course. I was assigned as the faculty member in charge of the safety committee for each laboratory cycle. Typically, the safety committee had been responsible for accident prevention and safety education, including

- Conducting safety audits of the unit operations laboratory before, during, and after the laboratory period
- Distributing "Prevent Accidents with Safety" (PAWS) forms
- Ensuring that each group is familiar with the emergency shutdown procedure for its experiment
- Assisting other groups with safety-related matters
- Conducting the safety meeting for that cycle
- Conducting other safety-related objectives that change from cycle to cycle

Basically, the committee is responsible for the safety of all unit operations students in the laboratory and is assigned to answer (or find the answer) to any safety-related questions



**Julia A. King** is Assistant Professor of Chemical Engineering at Michigan Technological University. She received a BS from Purdue University (1982) and her MS (1987) and PhD (1989) from the University of Wyoming. She has industrial experience from employment at Exxon Baytown Refinery and DuPont/Conoco. Current research interests include polymer and composite materials.

*We regard safety as an integral part of the unit operations course. . . For each laboratory cycle, one group of students is randomly assigned as the safety committee. Safety is the sole duty of this group, and there is a different safety committee for each cycle.*

that the students may have. The safety committee members are assigned a grade based on their performance of these duties. Due to MTU's strong safety culture and required junior-level safety course, the safety committee generally performs its assigned tasks well.

Based on my industrial experience, I led the development of the following enhancements to MTU's already strong safety involvement in the unit operations course:

- Creation of a unit operations laboratory Internet homepage with an emphasis on safety
- Development of a "Safety Inspection Checklist" for the unit operations laboratory
- Revision of the PAWS form to include safety suggestions
- Creation of a PAWS Tracking System that is available on the Internet
- Creation of Job Safety Assessment (JSA) forms for each of the thirteen traditional experiments.

#### INTERNET HOMEPAGE

Everyone is encouraged to visit the Unit Operations Laboratory homepage, located at

<http://www.chem.mtu.edu/classes/uo/safety/chem.htm>

From this page, it is possible to obtain Material Data Safety Sheets (MSDS) via a link to

<http://www.pdc.cornell.edu/issearch/msdssrch.htm>

or to obtain more safety information specific to the unit operations course (Safety Inspection Checklist, PAWS form, PAWS Tracking System, and Job Safety Assessment form). In addition there is a link to "Tips for Safe Lifting Practices" and to "Hygienic Practices to Keep in Mind." These materials have been presented by past safety committees and the class decided they should be placed on the Internet as a reminder to help prevent accidents and to promote good hygiene practices.

#### SAFETY INSPECTION CHECKLIST (SIC)

In the past, the safety committee was responsible for conducting safety audits of the unit operations laboratory. But a formal checklist had not been developed to conduct and record the findings of the audit. Table 1 describes how to complete the SIC, and Table 2 (next page) shows the items listed on the checklist. The actual checklist is designed with a check box for each item for each day of the month.

In order to construct the SIC form, the safety committees studied similar forms from various sources.<sup>[3-5]</sup> The form is divided into two major sections: the first covers general

laboratory items and the second covers safety items related to each individual experiment. The safety committee uses this form at the beginning, during, and at the end of each laboratory period in which experiments are being conducted. Typically, during a month there will be students in the laboratory on six different days.

One SIC form is used for an entire month and is posted by the unit operations laboratory office, and at the end of the month it is filed in the office. If a safety problem is noticed while they are conducting the inspection, the committee attempts to take immediate action to remedy the problem.

**TABLE 1**  
**Safety Inspection Checklist (SIC)**

*The Safety Inspection Checklist was developed to provide the Safety Committee, the faculty, and staff with an organized and effective means for inspecting the Unit Operations Laboratory. It also provides a record of what has been inspected in the past. The inspection is done to ensure that the lab operates in the safest manner possible, that all equipment in the UO Lab is in proper working condition, and to detect and correct any deficiencies in the lab.*

##### **How to Complete the SIC**

- The SIC is divided into two categories: Unit Operations Area and Individual Experiments. The Unit Operations Area of the check list covers items that are not assigned to an individual experiment, such as fire extinguishers, safety showers, ladders, etc, while the Individual Experiments section involves equipment and hazards associated with one particular experiment and includes such things as guards over pumps, gloves worn for changing a die, etc.
- The Safety Committee will fill out the SIC at the beginning and end of the UO Lab day. The checklist is a month-long document with the days of the month indicated at the top. The month and year that the inspection was performed must be filled out if that item is blank on the document. A box associated with each item on the checklist is split in half so that each item can be checked twice—once at the beginning of the day and again at the end of the day. After completing the inspection, the inspector must initial the bottom of the document under the proper day. Once the two inspections have been completed, the SIC is then posted on the chalk board for future inspections. When the month has been completed, the document should be turned over to Tim Gasperich in the UO Lab office for storage and a new SIC can be obtained on disk from Dr. King.
- If any problems arise while performing the inspection, the group must take immediate action to remedy them. If additional assistance is required, the group must inform the appropriate personnel. If there is any equipment missing, a PAWS form should be filled out, and if a safety hazard is noted during the inspection, a PAWS form should be completed and the safety hazard should be corrected as soon as possible.
- *Go to SIC form.*

**TABLE 2**  
**Safety Inspection Checklist**

**UNIT OPERATIONS**

**Emergency Procedures**

- Evacuation routes posted
- All exits and fire doors clearly marked and unobstructed
- Telephones accessible and labeled with emergency numbers
- Eyewash and safety showers clearly marked and unobstructed
- Eyewash inspection up to date with tag
- Safety shower inspection up to date with tag
- Water continued to flow when handle was released
- Eyewash flushed out
- Safety shower flushed out

**First Aid**

- Adequate supplies stocked
- Clearly marked and unobstructed

**Fire Extinguishers**

- Clearly marked and unobstructed
- Inspection up to date with tag
- Correct extinguisher for hazards present

**Personal Protective Equipment**

- Ankle-high boots worn with proper material
- Long pants worn: No loose clothing, hair, or jewelry
- Appropriate eye wear and properly marked
- Safety goggles worn when handling hazardous chemicals
- Hard hat worn at all times; Earplugs worn in designated areas
- Appropriate gloves worn and available
- Dust masks and respirators in UO lab office

**Electrical**

- Left-hand rule used
- Power off to make electrical connections
- Extension cords away from traffic and water
- 3-pronged plugs on cords with ground
- Cords without frays or splices
- Make sure the overhead crane is locked and tagged

**Chemicals**

- Stored in the proper cabinet; Storage cabinets labeled clearly
- Clearly and properly labeled
- Transported properly

**Housekeeping**

- Counters and floors clean and uncluttered
- Ladders in good condition and chained when not in use
- Cylinders labeled, upright, and secure
- Waste containers provided and labeled
- Make sure drain plugs are present
- Drain is accessible

**INDIVIDUAL EXPERIMENTS**

**Batch filtration**

- Agitator locked out when adding slurry to the tank
- Mercury manometer is used
- All valves in proper position when flushing out lines

**Continuous Filtration**

- All guards are securely in place
- Use left-hand rule to turn on power
- Power supply locked out when manually stirring tank

**Continuous Stirred Tank Reactors**

- Cart wheels are kept blocked
- Agitator immersed in solution when starting and stopping
- Valves closed when starting reaction

**Cooling Tower**

- Guard on blower securely in place
- Ear plugs worn for noise level
- Liquid water flowing to heater before starting steam flow

Steam valve closed before liquid water valve

**Flow Measurement**

- Mercury manometer is used
- Pump guards properly secured
- Vent and drain lines before changing orifice

**Fluidization**

- Dust mask worn when screening sand
- Ear plugs worn when using Ro-Tap
- Open valve on air supply slowly

**Heat Transfer**

- Insulated gloves worn when operating steam valves
- Opened steam valves slowly
- Electric timers are away from water
- Stayed clear of steam traps and heater

**Liquid-Liquid Extraction**

- Protective gloves, apron, and goggles worn to handle acetic acid
- Kerosene samples poured back into kerosene barrel after use
- Kerosene pump guard in place
- Sampling valves closed after samples taken

**PDMS Bench-Scale Reactor**

- Goggles, rubber apron, and rubber gloves used to handle KOH
- Red safety can used to weigh and transfer endblock A, 245 fluid
- Pipes and hoses are in good condition and connections are tight
- System inerted with nitrogen at all times
- Experiment run in the hood
- Main gas cylinder valve fully open
- Glassware and thermometer transferred in proper container

**Solvent Recovery**

- Gloves to be worn during sampling
- Take precautions during sampling (i.e., dripping after sampling)
- Check position of valves

**PDMS Jacketed Reactor**

- Goggles, rubber apron, and rubber gloves used to handle KOH
- Red safety can used to weigh and transfer endblock A, 245 fluid
- Pipes and hoses are in good condition and connections are tight
- System inerted with nitrogen at all times
- Main gas cylinder valve fully open
- Glassware and thermometer transferred in proper container
- Face shield worn when adding chemicals to reactor

**Polymer Flow**

- Guards in place and properly installed
- Capillary viscometer pressure no greater than 20 psig
- Tanks not overfilled

**Polymer Processing**

- Insulated gloves worn when changing dies;
- Gloves to be worn during sampling
- Dies fastened correctly
- Heating wires properly attached
- Proper tools used for scraping polymer

**Pumping A**

- Pump guards are in place and properly secured
- Shut down procedure executed properly

**Pumping B**

- Pump guards are in place and properly secured
- Shut down procedure executed properly

**Distillation-Solvent Recovery**

- System inerted with nitrogen at all times

**Vacuum Drying**

- Vacuum pump guard properly secured
- Insulated gloves used to operate steam valves
- Dust mask worn when screening sand
- Ear plugs worn when using Ro-Tap

When it is not possible to remedy the problem immediately, the committee fills out a PAWS form so there will be a record.

**REVISED PAWS FORMS**

The Prevent Accidents with Safety (PAWS) program, initiated at MTU in 1989, is designed to actively and positively involve the students in the safety program. The unit operations students are responsible for their own safety as well as the safety of others working in the area, and any student observing an unsafe act is expected to correct the action before an accident occurs. After correcting the unsafe act, the student completes a PAWS form, which mentions the group that corrected the unsafe act. PAWS points are awarded (positive for safe acts, negative for unsafe acts), and the

group with the most PAWS points each quarter is rewarded with a dinner hosted by the developer of the PAWS program, Dr. A. J. Pintar. Submissions of a “nitpicking” nature are discouraged by not assigning them any points. In a typical cycle, approximately twenty PAWS forms are submitted. Most of them concern personal protective equipment, improper handling of chemicals, and equipment problems. Most PAWS forms are submitted by groups other than the safety committee.

My industrial experience has taught me that people often have good ideas for improving safety, so the PAWS form was modified to encourage students to develop ways for improving safety in the lab as well as to report unsafe acts. In addition, students developed a checklist for common safety concerns. Table 3 describes how to fill out the PAWS form, and Table 4 displays a blank PAWS form.

I also encouraged the safety committees to develop a PAWS Tracking System that could be used to track the forms that were submitted. This system was placed on the Internet so students could view the action that had been taken on their item, could prepare for their next experiment by studying past safety mistakes or concerns observed by

**TABLE 3**  
**Filling Out a PAWS Form**

***Part 1 (Situation Observed)***

1. A situation is observed in the lab that needs to be reported. If you are making a safety suggestion, skip to Part 2.
2. Obtain a PAWS form from the safety committee, Unit Operations Lab Homepage, or the folder located in the Unit Operations Lab Office.
3. Check the line on the PAWS form that describes the situation observed. If none of the lines apply, check “Other.”
4. Make additional comments about the situation in the “Comments” section of the PAWS form. Be sure to include what happened, where it happened, how it happened, and if reporting equipment problems, tell what equipment needs to be fixed. Do not include the name of the person who violated safety procedures; this is not what PAWS forms are for.

***Part 2 (Action Taken/Safety Suggestion)***

1. Report what action, if any, was taken to remedy the safety situation or to record safety suggestions in the “Action Taken/Safety Suggestion” section of the PAWS form. Make sure to record which experiment the suggestion applies to.
2. Sign and date the PAWS form. Include your group number on the form.
3. Place the PAWS form in the box labeled “PAWS Forms” located in the Unit Operations Lab office.

***Safety Committee Duties***

1. Make sure that there are enough PAWS forms for the lab day.
2. Supply each lab group with PAWS forms at the beginning of the lab day. Have more ready in case they are needed.
3. Collect PAWS forms from the box at the end of the lab day.
4. Review PAWS forms.
5. Input PAWS forms into PAWS tracking system.
6. Once the lab cycle is completed and the PAWS forms have been entered into the PAWS Tracking system, give the forms to Dr. Pintar.

*Go to PAWS form.*

**TABLE 4**  
**PAWS Form**

**PAWS**  
**Prevent Accidents With Safety**  
Unsafe Situation Report Form

***Situation Observed***

- Improper protection equipment (hard hat, safety glasses, boots)
- Didn't use goggles while transporting chemicals
- One person moving ladder over 6 feet tall
- Transporting glassware without bucket
- Equipment left unattended
- Equipment problem
- Other

***Comments (where, how, what, experiment name)***

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***Action Taken / Safety Suggestion***

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Signed \_\_\_\_\_  
Lab Group \_\_\_\_\_ Date \_\_\_\_\_

previous groups, etc.

Table 5 shows the PAWS Tracking System items submitted (first page only) for cycle 3 of the 1996-97 academic year. These items include unsafe acts, safety suggestions, equipment problems, etc., related to each experiment. The form also lists who is responsible for remedying the problem and if the item is open or closed ("open" meaning action is still needed and "closed" meaning action has been taken and the item resolved). Open items are discussed with the students, faculty, and staff at the required safety meeting for each laboratory cycle. Each safety committee is responsible for making progress toward "closing" the remaining "open" items.

### JOB SAFETY ASSESSMENT (JSA) FORMS

JSA forms are often used in industry and are typically completed for each "job" conducted in an industrial laboratory. They list each step in the procedure, the potential hazards of each step, the recommended safe procedure to use for each step, and the required personal-protection equipment. Using them as a model, I encouraged the safety committees to develop a JSA form to use for our thirteen traditional unit operations experiments. Table 6 describes how to complete the form and Table 7 shows a blank JSA form, which also includes a safety awareness section (nearest fire extinguisher, eye wash, etc.) and the emergency shutdown procedure.

In the 1996-97 academic year, the safety committees and the groups conducting the experiment believed that the JSA form was useful to complete, could prevent accidents, and should be implemented as a required procedure. Thus, in the 1997-98 academic year, each unit operations group conducting one of the thirteen traditional unit operations experiments had to independently complete a JSA form for their experiment prior to running the equipment. The students do not have access to the JSA forms completed for the experiments in the previous year, but the faculty advisor for each experiment uses a completed JSA form as a guide for evaluating the group's JSA form.

### SUMMARY

Student involvement in safety procedures prevents the need for faculty/staff-mandated safety rules. The students enjoyed working on these safety enhancements to the unit operations course. They were enthusiastic about the projects, they produced high-quality products, safety in our unit operations course has been improved, and our students are better prepared to work in industry as a result of these procedures.

### ACKNOWLEDGMENTS

I would like to thank the entire 1996-97 unit operations class for their participation in the project. I would also like to

**TABLE 5**  
**PAWS Tracking System**

**PAWS INFORMATION FOR EXPERIMENT**  
Cycle 3

Item #	Group #	Experiment Name	Date PAWS form filled out	Unsafe Act/Situation/Suggestion	Action Taken	Person Responsible	Open/Closed	Comments
69	1A	Safety	10/1/96	Open electrical conduit connection on electrical box for heating oven.	Tim Gasperich was informed and he fixed the electrical box.	TPG	Closed	
70	8B	Heat Transfer	10/3/96	Leaky drum for heat exchanger - red gate valve on drum - rusted on bottom near valve created very wet floor.	Labeled and set aside drum, cleaned up floor. Tim Gasperich was informed and he fixed the drum.	TPG	Closed	
71	Dr. Pintar	Safety	12/3/96	Ladders left unchained overnight.	Put chain around ladders.	AJP	Closed	
72	11A	Liquid-Liquid Extraction	12/5/96	Found broken, dirty glassware on floor by liquid-liquid extractor.	Picked up and put in broken-glass container.		Closed	
73	11A	Liquid-Liquid Extraction	12/5/96	Worn sticker on liquid-liquid extractor. H.F. & R. of raffinate stream unreadable.	Sticker replaced and numbers filled in according to kerosene specs. (Traced pipes to kerosene tanks.)	TPG	Closed	

**TABLE 6**  
How to Fill Out a JSA Form

**Job Safety Assessments (JSA)**

*Introduction to Job Safety*

The Job Safety Assessment (JSA) Form provides a faster way of identifying potential hazards in the Unit Operations Laboratory. It acts as a useful reference displaying possible hazards that can occur in each step in an experiment.

*Format of Finalized JSA*

The **first section** is used for identifying each experiment, including the name of the process. Space is provided for the person responsible for filling out the original JSA form. Experimental procedure for a process may change and this could cause a change in the safety hazards associated with that experiment, making revisions necessary. There is a space provided for the person making these revisions, as well as a revision number, revision date, and revision approval by the appropriate faculty. Either Dr. Ellis or David Caspary are the designated persons to approve the revised JSA. Also, the first section contains a portion that shows the necessary personal protective equipment required for the lab. In most experiments, all equipment listed on this form (hard hat, safety glasses, ankle-high books, long pants) are required, but there are exceptions for some experiments.

The **second section** is divided into four columns. The first column contains a detailed sequence of the steps in an experiment, including startup, run time, and shutdown. Potential hazards that can occur at each step of the procedure are listed in the second column. The recommended procedure to prevent these hazards is listed in the third column, and personal protective equipment required for a step is listed in the fourth column.

The **last section** contains the location of safety devices nearest the experiment as well as an emergency shutdown procedure. The safety devices include the nearest fire extinguisher, emergency eye wash and shower, emergency exit, first-aid kit, drain, and telephone.

*Go to JSA Form*

**TABLE 7**  
Blank Job Safety Assessment Form

<b>Job Safety Assessment Form</b>		Unit Operations Laboratory Department of Chemical Engineering Michigan Technological University	
Process Name:	Hazard Level (high medium, low)	Written by: _____	
		Revised by: _____	Revision #: _____
Process Location		Revision date: _____	Revision approved by: _____

**Required Items for Lab:**

Hard Hat | Safety Glasses | Ankle-High Boots | Long Pants

	Sequence of Steps	Potential Hazards	Recommended Safety Procedure	Required Personal Protective Equipment
<b>Startup</b>				
<b>Run Time</b>				
<b>Shutdown</b>				

**Safety Awareness:**

Nearest Fire Extinguisher \_\_\_\_\_  
 Nearest Eye Wash & Shower \_\_\_\_\_  
 Nearest Emergency Exit \_\_\_\_\_  
 Nearest First-Aid Kit \_\_\_\_\_  
 Nearest Drain Plug \_\_\_\_\_  
 Nearest Telephone \_\_\_\_\_

**Emergency Shutdown Procedure**

\_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_

thank Dr. Anton J. Pintar, Dr. Daniel A. Crowl, Dr. Thomas G. Ellis, Mr. David W. Caspary, and Mr. Tim P. Gasperich for their advice.

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# GETTING THE MOST OUT OF A LABORATORY COURSE

AZIZ M. ABU-KHALAF

King Saud University • Riyadh 11421, Saudi Arabia

The laboratory is the proper place for students to apply the theories and principles of chemical processes and unit operations that they have learned in the classroom. It can also be used to simulate industrial practices where the ability to operate plants, to perform original designs, and to modify existing processes is required. Operating a chemical plant requires that the chemical engineer be proficient in problem solving and troubleshooting, and over the years considerable efforts have been exerted to strengthen the links between industry and academia in order to attain that proficiency. Examples include laboratory experiments, practice schools,<sup>[1]</sup> research projects, summer internships in industry,<sup>[2]</sup> co-op projects,<sup>[3]</sup> and others.

This paper will review the current goals of a laboratory course and present the author's experiences in using laboratory time to cover several important topics related to both industry and academia. The subjects that will be discussed are safety procedures, startup and shutdown, troubleshooting, calibration with statistical applications, maintenance, and mathematical modeling and simulation. Different available experiments will be used to achieve these goals.

## LABORATORY OBJECTIVES

Traditionally, a laboratory course emphasizes, through practical sessions, the understanding and application of theories and principles taught in the classroom and presented in textbooks. During the course, the students become familiar with the available process equipment, with instrumental analysis, and with various measurement techniques. They also practice report writing, deal with experimental errors, and learn

to recognize the discrepancy between theory and practice.

A new look<sup>[4]</sup> with new objectives in the chemical engineering laboratory has been suggested, with some of the following objectives:

- *Using the laboratory to develop engineering awareness.*<sup>[5]</sup> Engineering awareness is developed through several applications. Students gain practical experience, acquire skills, and get an idea of the technical difficulties encountered in the design and construction of processing units.
- *Introducing statistical concepts in the experiments.*<sup>[6]</sup> Statistical ideas are incorporated into existing experiments, which are modified through the analysis of data, to introduce certain statistical concepts.
- *Mathematical modeling and simulation.*<sup>[7-10]</sup> A step-by-step method is followed to develop steady-state and dynamical models representing experimental systems. Students are asked to perform analytical and numerical solutions, using available simulation packages.
- *Troubleshooting.*<sup>[11]</sup> Troubleshooting experiments are described to develop the student's ability to diagnose and correct unacceptable process performance.
- *Simulation of industrial work.*<sup>[12]</sup> The procedures used in a typical unit operations lab course are modified to simulate industrial practice. Applied problems and instructions are included.
- *Performing economic evaluations.*<sup>[13]</sup> Estimations of capital and operating costs are performed on typical experiments. Scale-up and economic optimization of an existing plant are considered.

While some of these goals pertain to industrial practice, others reinforce mathematical, statistical, economical, and process concepts. New and/or modified experiments are developed as necessary to meet the goals, and other objectives can be included, such as familiarizing the students with safety regulations, maintenance, and calibration. It is not difficult to achieve all of these goals. The following sections describe our method for meeting the goals within the time



*Aziz M. Abu-Khalaf has educational interests that include developing new objectives and improving the performance of laboratories at the Chemical Engineering Department at King Saud University. Research interests include controlled release systems and corrosion. He can be reached by e-mail at AMKHALAF@KSU.EDU.SA.*

allotted to a typical lab course.

## SAFETY PROCEDURES

Students usually underestimate the importance of safety measures in the lab and occasionally argue about strict safety regulations, particularly when they feel the running experiment is safe. But experiments are not the only source of danger in the lab. For example, danger could come from a pipe carrying hot water or steam to other parts of the lab. To counter this, we emphasize the following items in such a way that they become part of the student's daily practice, both in and out of the lab:

- We familiarize the students with hazard symbols, terms, and abbreviations. Symbols include those on personal protective equipment, dangerous materials, and workplace labels. Terms such as threshold limit value (TLV), hazard rating (HR), lower and upper flammability limits (LFL and UFL), etc., are covered, and the most common abbreviations, such as ACGIH (American Conference of Governmental Industrial Hygienists) and MSDS (Material Safety Data Sheet) are defined. The concepts of fire triangle and tetrahedron are fully explained.
- We teach the students to always be ready for an emergency. We point out the location of emergency outlets, fire extinguishers, in-line showers, and emergency eyewash stations.
- We ask that students wear a lab coat (or apron) during each lab session, and that other personal protective items be used when necessary. For example, the students should wear, as needed, safety eyewear (splash goggles), a face shield, and gloves during distillation and reaction experiments, etc. We ask them to put on dust masks during a solid-handling experiment and anti-noise ear muffs during noisy runs such as a cooling tower tutor.

We also show the students a video tape on safety or refer them to related books.<sup>[14,15]</sup> We give them specific assignments on safety topics and discuss the topics later in a seminar session. In particular, we ask them to compare the safety equipment that is available in the lab with the recommendations in a standard reference. The students can also be asked to prepare data sheets on the specific materials and hazard symbols that will be involved in the experiment they plan to do (references 14 and 16 are very useful in this regard).

Finally, a sheet of safety procedures specific to a certain

*This paper . . . review[s] the current goals of a laboratory course and present[s] the author's experiences in using laboratory time to cover . . . topics related to both industry and academia. The subjects . . . are safety procedures, startup and shutdown, troubleshooting, calibration with statistical applications, maintenance, and mathematical modeling and simulation.*

lab is distributed to the students. It contains general procedures (disposal, proper use of service equipment, gas cylinders, etc.), evacuation instructions in case of fire or chemical spillage, etc. It should also include symbols and abbreviations of equipment and pipelines in the lab.

The lab instructor might also include other topics such as hazard-assessment techniques. The most common is the hazard and operability study (HAZOP), which is a systematic technique for identifying all plant or equipment hazards and operability problems.<sup>[17]</sup>

## STARTUP AND SHUTDOWN

In industry, startup (putting the process and its related equipment into proper operation) and shutdown (when the operation is completely stopped) are related to integrated equipment and interdependent processes. The equipment is often outside the plant and susceptible to weather effects, whereas the lab usually contains small-scale individual equipment with relatively constant ambient conditions.

Startup and shutdown procedures depend on the process, the materials, and the type of equipment being used. The following is a list of common rules used in industry—based on my own experience as a co-op student in a refinery and as a production engineer in other plants. The rules should be emphasized during the lab session.

- Never introduce a cold stream suddenly into hot equipment (such as a heat exchanger). Similarly, a hot stream should not be suddenly introduced into cold equipment.
- Introduce the cold stream first, and stop the hot stream first.
- Any change in operating conditions should be done gradually and should not exceed the listed operating conditions of the specific equipment.
- Make sure that the equipment is gradually, completely, and safely drained and purged.

An effective teaching method is to listen to the students' suggestions and ideas about startup and shutdown and then to discuss with them the significance and implications of the general rules above. This helps them to realize that a sudden change in temperature might cause a thermal or a mechanical stress and result in a bad effect on the equipment. For example, high pressure surges can destroy pressure gauges or other measuring devices or dislocate trays from a distillation column. They will also learn that rapid venting could result in a cooling effect that might freeze the remaining

liquid, and that complete drainage and venting is necessary with flammable materials to avoid the formation of explosive mixtures.

Table 1 is a general guide of the steps that should be taken for startup and shutdown. Since startup and shutdown are transient in nature, they can be modeled mathematically and their behavior can be theoretically predicted.

### TROUBLESHOOTING

Troubleshooting is the ability to characterize or diagnose a problem and to present corrective action to solve it. This ability is essential for people involved with the operation of chemical plants—in particular shift engineers. Abnormal operation can be harmful to operators, to equipment, and to product quality. Corrective action might be constrained by the time and safety of both the employees and the equipment, so a systematic approach should be followed in troubleshooting. This requires a good theoretical background in the process, experience, and engineering sense. A systematic approach requires the presence of enough and reliable (relative to operators and instruments) data and information about the situation, recognizing the problem, choosing the corrective action from the different alternatives, and later feedback. Knowledge-based systems<sup>[18]</sup> are currently used to improve plant operations by using automated diagnosis.

Trouble in industry can be caused by<sup>[19]</sup> such things as misoperation, false alarms, equipment or chemical failure, inadequate equipment design, and process failure. Lab experiments can be effectively used to familiarize students with troubleshooting procedures by designing special experiments for this purpose<sup>[11]</sup> or by using available experiments with problems that occur either naturally or that are created intentionally.

At the conclusion of the course, students should be asked to summarize their experience in the form of a list that other students can benefit from, revise, and extend if possible. In this way, they learn to keep records of all failure and breakdowns as is done in industry. There should be a thorough discussion of the cause and effect of the problem and how to solve it in light of the systematic approach mentioned above. Students should perform the required modifications when necessary. Table 2 gives some examples of typical problems, their cause, and possible corrective actions.

### MAINTENANCE

Maintenance is all important. It keeps plants running, prevents troubles, and identifies the cause of inadequate performance.<sup>[19]</sup> The availability of maintenance software can help an operation to run smoothly.<sup>[20]</sup> When students locate a trouble source, they should participate in the repair and maintenance process. For example, they can dismantle (with the help of technicians) a malfunctioning pump for general

checkup or repair; they can clean a dirty reactor or a packed bed; they can check valves for leakage; and when it is necessary to modify a design, they can do it themselves.

It is important to familiarize students with the important and related terminology of maintenance. This includes planned maintenance, corrective maintenance, routine maintenance, servicing maintenance, running maintenance, and shutdown maintenance. Other suggested projects include

- **Cleaning equipment** such as heat exchangers, cooling towers, coolers in distillation columns, etc. This requires understanding of fouling and scales and the methods of cleaning. The severity of deposits can determine the method to be used: in running maintenance, chemical treatment is applied without the need to dismantle the equipment; for heavier deposits, fluids under high pressure and/or temperature (such as steam) are used. When these methods fail, the equipment must be completely dismantled to remove the adhering deposits. This is known as shutdown maintenance.
- **Water treatment.** This can be accomplished by preventing the formation of deposits by using antifoulants, preventing the reactions that cause deposits by using inhibitors, and using dispersants to prevent coagulation of suspended solids.
- **Noisy equipment.** Fans and other equipment such as mixers should be frequently inspected since friction is a possible source of ignition.

**TABLE 1**  
**Steps for Startup and Shutdown**

- ▶ Discuss with the students the objectives of the experiment, the measurement techniques and instruments, and the materials and the form of energy to be used. Relate the last with the safety section regarding precautions and handling.
- ▶ Ask the students to familiarize themselves with the system, to locate and check all the relevant equipment and valves (all types, including relief valves), and draw a simple but detailed flowchart, with full identification of all relevant parts. On a separate sheet, list all input and output valves and designate them as "open" or "closed" for startup.
- ▶ With the help of the above list, check which valves to open and which to keep closed. Refer to the guidelines given before, particularly if heating/cooling is involved. Make sure that the measuring equipment is ready. While other steps might be specific, when dealing with a reacting system you generally introduce both reactants simultaneously, or add one and then the other, or fill the tank with one reactant and then add the other stream.
- ▶ Follow up the experiment, take the measurements, and keep watching the input and output streams (through flowmeters), the heat source, and the workability of other equipment.
- ▶ Prepare yourself for shutdown. Again, refer to the valve list generated at the beginning of the preparation and to the general guide list.

- Replacing steel pipes in old equipment with plastic pipes.

### CALIBRATION WITH STATISTICAL APPLICATIONS

The objective of calibration is to prepare calibration curves and to apply useful statistical techniques. Examples include constructing calibration curves of conductivity against concentration and recording liquid flow rate with a rotameter. In the case of conductivity, standard solutions are prepared and their conductivity measured by a suitable conductivity meter. The concentration range should cover the actual expected measurements. With a rotameter, an adjustable flow from a suitable pump is passed through the meter and its reading is recorded; then the effluent is measured at certain time intervals. A smooth curve can thus be generated.

Statistical analysis can reveal the presence of errors in the measurements and the propagation of these errors later in the calculation of an unknown sample concentration.<sup>[21]</sup> I recommend that the students perform the following calculations:

- Use linear regression to get the best fit. Calculate the slope and intercept of the calibration line and the percentage fit, which is  $100 (\text{correlation coefficient})^2$ .
- Calculate the residual standard deviation, which is equal to the square root of residual sum of squares divided by residual degrees of freedom.
- Decide whether there is a fixed bias or a relative bias, or both or neither. Fixed bias results in an intercept that is not equal to zero, and a relative bias results in a slope that is not equal to unity.
- Quantify the precision of the prediction of the true concentration of unknown samples.
- Several calibration lines can be collected from differ-

ent groups, and a mean value can be calculated. A t-test can be used by each group to compare its value with this mean. Finally, a repeatability test can be used to check the precision of the test method. Groups will test similar unknown samples and quantify the repeatability as  $r = t \cdot 2s$ , where  $r$  is the repeatability measure,  $s$  is the standard deviation of the readings, and  $t$  is the t-test at a certain confidence limit.

Statistical analysis could also be applied to the experiments themselves, *e.g.*, determining the order of the reaction and the reaction rate constant from a batch reactor run. These values are then used in the continuous reactor calculations. It is appropriate to analyze propagation of errors throughout these calculations and to do some other significant tests on the value of the reaction rate constant.

Other suggested<sup>[5]</sup> calibration projects are a mercury-in-glass thermometer, a thermistor, and type-T and -K thermocouples.

### MATHEMATICAL MODELING AND SIMULATION

Mathematical modeling is the process of describing and approximating actual physical systems using mathematical tools. A real process is mathematically abstracted for purposes of understanding and predicting its behavior. Reducing the experimental effort required to design or optimize the process is another motivation for developing a mathematical model. The model can be checked against experimental data and then reconsidered in order to be more effective and more useful in achieving the required objectives.

The first step in model formulation<sup>[22,23]</sup> usually involves drawing a picture of the system under investigation and selecting the important dependent (responding) and independent (changing) variables, along with the parameters that

**TABLE 2**  
Typical Problems, Causes, Remedies

<i>Experiment</i>	<i>Problem</i>	<i>Possible Cause (Remedy)</i>
Cooling tower	Wet-bulb temperature equal to or greater than dry-bulb temperature of outlet air	<ul style="list-style-type: none"> <li>• False reading (Check measuring devices)</li> <li>• Wick is not wetted (Check water and wick)</li> <li>• Air is blocked (Check air flow)</li> </ul>
	Temperature gradient of water at the bottom section is very small	<ul style="list-style-type: none"> <li>• False reading (Check measuring devices)</li> <li>• Lack of water (Check water flow)</li> <li>• Air is blocked (Check air flow)</li> </ul>
Distillation	Conductivity readings from different trays are not consistent	<ul style="list-style-type: none"> <li>• False readings (Select the correct range at the calibrated temperature)</li> <li>• Incorrect sampling (Cover drawn samples with aluminum foil, cool them to calibration temperature using a water bath, and make sure probe is well immersed in the sample.)</li> </ul>
Reactor	Fluctuated flow, with air bubbles in flow lines	<ul style="list-style-type: none"> <li>• Direct pumping within short distance (Use head tanks. If bubbles are still present, increase the tank height.)</li> <li>• Low level in feed/head tanks (Increase the level of solution in the tanks.)</li> <li>• Back pressure (Check for any resistance to flow.)</li> </ul>

are expected to be important (physical constants, physical size, and shape). The second step is bringing together all applicable physical and chemical information, conservation laws, and rate expressions. The third step requires setting down of finite or differential volume elements, followed by writing the conservation laws. Then an appropriate mathematical solution method is sought with the proper choice of the boundary value of the dependent variables, which finally relates dependent variables to one or more independent variables.

Mathematical modeling seems to be a difficult subject to many students as well as to people working in industry. Dealing with differential equations in industry is sometimes simply avoided and the steady-state simulators are “tricked” into doing the work.<sup>[24]</sup> But, modeling can be made simple and interesting when doing lab experiments, particularly when a team effort is practiced. In industry the team might include specialists such as chemists and statisticians.<sup>[25]</sup> In the lab, students should perform the tasks with the help of the instructor.

I use a CSTR setup<sup>[7-9]</sup> to study startup and shutdown processes. It can be versatile. Students can study second-order or first-order reactions under isothermal or nonisothermal conditions; they can model the dynamics and steady-state behavior of the system; they might consider different approaches to startup and then model them. Other experiments are used to build simple models. For example, in a cross-flow heat exchanger, a model is built to describe the transient heat-transfer process between a heated element of copper and air.

The developed models could be solved analytically and/or numerically; using both approaches is preferable. I encourage the students to use available packages in order to emphasize principles rather than programming. For example, they write a main program and call available subroutines from IMSL, or use MATLAB. Sometimes I ask them to use spreadsheets, which are preferred by industrial people and can be used in a solid-handling experiment to simulate the breakage of a known sample of a solid material.<sup>[26]</sup> I ask the students to solve problems related to the subject of the experiment from their textbooks in an attempt to form a link between lectures and lab work. For example, I ask them to solve problems on transient balances related to crushing and grinding, and to build the model.<sup>[27]</sup>

Data acquisition software can serve as a convenient tool for quickly developing computer simulations of chemical engineering unit operations for use in classroom demonstrations.<sup>[28]</sup> These packages can be used to create virtual unit operations. Simulation is used to avoid some of the disadvantages associated with certain experiments.<sup>[29]</sup> This is useful, for example, when a great amount of time is needed to perform the experiments or when a complex phenomenon such as ion exchange or adsorption is considered.

## DISCUSSION AND CONCLUSIONS

The objective of a lab course is no longer a matter of data collection and the preparation of a full and lengthy report. Many useful things can be extracted from a lab session when the new objectives are properly invested. The list might look lengthy, but this is not a problem as long as the objectives are achieved within the time limit without affecting the scheduled experiments. Safety procedures require one session and should be stressed in every other session. Maintenance and troubleshooting are performed using available experiments. Startup and shutdown are related to every experimental run. Mathematical modeling and simulation should be done in connection with the specified experiment.

Several important points can be drawn from this discussion:

- Industrial work can be effectively simulated in the unit operations lab without affecting the academic approach. This is achieved by stressing subjects such as startup, safety, troubleshooting, report writing, statistical analysis of errors, and modeling.
- The ability to solve problems and troubleshoot is developed by following systematic procedures of safety and of startup and shutdown, and by allowing the students to tackle practical problems and search for corrective solutions.
- Available experiments can be used to achieve the required goals, and when necessary new experiments can be introduced or existing ones can be modified. Students can participate in all of these activities.
- Students realize that simple subjects look difficult when they are not understood or practiced. This is obvious in practicing startup and shutdown procedures. They should be taught to think of applications in order to understand and memorize more easily.
- A worker who understands hazard and safety precautions improves work practice and becomes aware of protection and handling procedures.
- The team effort should not be ignored. It can be practiced by considering troubleshooting, modeling, and analysis.
- Subjects are interrelated. For example, mathematical modeling (in particular, the dynamic type) can help troubleshooting that is usually transient in nature.
- The typical unit operations lab is a fruitful area where many applied subjects can be practiced effectively.

The instructor should make sure that the students understand and grasp the above topics. This could be achieved by discussions during the lab sessions, by oral and written exams, and by asking the students to write short reports as part of a final exam. An experience like the one we have pre-

sented here will, hopefully, give the instructor courage to teach such a course without hesitation.

## ACKNOWLEDGMENT

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## ChE book review

### Mathematical Methods in Chemical Engineering

by A. Varma and M. Morbidelli

Oxford University Press, New York, NY; 690 pgs; \$80 (1997)

Reviewed by

**E. James Davis**

University of Washington

This text follows the Minnesota tradition of applied mathematics in chemical engineering established by Professors Amundson and Aris in that the treatment of the numerous topics is rigorous and vigorous. There is an attempt to complement the mathematical fundamentals with examples arising in chemical engineering, but the balance between theory and application is not uniform throughout the book. The authors naturally lean toward examples from their own research and experience.

The nine chapters cover a wide range of subject matter starting with matrix theory and proceeding to a particularly long chapter dealing with first-order linear ordinary differential equations and stability theory. With respect to Chapter 1, the authors acknowledge their debt to Professor Amundson; that chapter summarizes Amundson's book *Mathematical Methods in Chemical Engineering: Matrices and Their Application*. The first two chapters account for almost one-third of the 690-page book, but Chapter 2 addresses subjects such as Liapunov's direct method and the Hopf bifurcation theorem not covered in typical texts on advanced engineering mathematics. The 135 pages of Chapter 2 include interesting applications such as the analysis of the Belousov-Zhabotinskii oscillatory reaction.

Chapters 3 and 4 are more conventional in their coverage of linear ordinary differential equations and special functions, respectively. A clear presentation of the Green's function for solving nonhomogeneous equations is a plus. The applications included in these chapters are rather lean, and the presentation of orthogonal polynomials such as the Chebyshev and Laguerre polynomials and other special functions is left to problems at the end of Chapter 4 without relevant applications.

The classification of partial differential equations in Chapter 5

Continued on page 219

# A SIMPLE METHOD FOR DETERMINING THE SPECIFIC HEAT OF SOLIDS

K. HELLGARDT, G. SHAMA

Loughborough University • Loughborough, Leicestershire, England LE11 3TU

Specific heat is one of those properties that all undergraduate students of chemical engineering would claim at least some measure of familiarity with, often from close and bloody encounters in the performance of energy balances. Our experience has been that this familiarity rarely extends to methods of determining this important intensive property. Many of the sophisticated methods that have been developed over the last century or so are inappropriate to the repertoire of the first-year laboratory, either because they require elaborate and expensive apparatus and/or because they are time consuming and not easily scheduled into what appears to be that universal period of time (3 hours) devoted to laboratory classes. The interested reader should consult any of the texts on classical calorimetry<sup>[e.g., 1,2]</sup> for a full account of the available methods.

In this paper we describe a simple and inexpensive undergraduate experiment for the determination of the specific heat of solids based on the evaporation calorimeter devised by Dewar in 1904.<sup>[3]</sup> An added advantage of the experiment is that it introduces some important thermodynamic principles in the development of the theory underlying the evaluation of specific heat. To deflect the charge that we may be

over-virtuous in our endeavors, we confine ourselves to a method that will allow the determination of the *average* specific heat of a solid in the range of 80K to 298K.

## BACKGROUND<sup>[4-8]</sup>

The terms “specific heat” and “heat capacity” are often used synonymously. In fact, the term heat capacity is a legacy of the “caloric” theory of heat that Count Rumford essentially laid to rest at the end of the 18th Century. This theory held that heat was a substance that could literally be “poured” from one body to another. We now know that heat cannot be contained within a system, but rather is a manifestation of the interaction of a particular system with its surroundings. The modern concept of specific heat is that it is a measure of the energy changes of a system when energy, in the form of heat, is transferred across its boundaries. Transfers of energy can be conducted under a number of different conditions (*e.g.*, constant pressure or constant volume), each of which can be used to define a specific heat; the concept is further elaborated upon below.

The general change in enthalpy of a system that is in mechanical equilibrium with its surroundings can be obtained with

$$dH = dQ + dW_e + VdP \quad (1)$$

The term  $W_e$  is used to denote all forms of work that may be referred to as “non-P,V work.” *i.e.*, electrical, gravitational, etc. Now, if we assume that there is no non-P,V work done on the system, and heating or cooling occurs at constant pressure, this equation reduces to

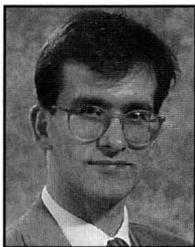
$$dH = dQ \quad (2)$$

Using the relationship

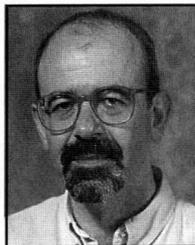
$$dQ = CdT \quad (3)$$

we can then write

$$C_p = \left( \frac{\partial H}{\partial T} \right)_p \quad (4)$$



**Klaus Hellgardt** has been a lecturer in the Department of Chemical Engineering at Loughborough University since 1995. His main research interests lie in the field of heterogeneous catalysis. He obtained his Dipl.-Ing (TH) from the University of Karlsruhe. In 1991 he was awarded an EC Research Training Fellowship during which he completed his PhD and DIC at Imperial College in London.



**Gilbert Shama** has been in the Department of Chemical Engineering at Loughborough University since 1989 and is closely associated with the operation of first-year undergraduate laboratories. He obtained his BSc degree from UMIST, his MSc from Birmingham, and his PhD from Imperial College, London.

which is the definition of the heat capacity or specific heat (at constant pressure). A similar deduction starting from the description of the internal energy of the system  $U$  leads to

$$C_V = \left( \frac{\partial U}{\partial T} \right)_V \quad (5)$$

It can be further shown that the relationship between  $C_p$  and  $C_V$  is

$$C_p - C_V = \left( \frac{\alpha^2}{\kappa} \right) VT \quad (6)$$

Following on from Eq. (4), however, if, at constant pressure, the temperature of a compound,  $S$ , is raised by a small increment  $\Delta T$ , a finite amount of heat needs to be transferred, and

$$Q = \Delta H = n_S C_P^m \Delta T \quad (7)$$

Here,  $C_P^m$  is the molar specific heat and  $n_S$  is the number of mols of compound  $S$ . The specific heat is usually a function of the temperature and approaches zero for very low temperatures (a few degrees Kelvin above absolute zero). In this temperature range, the function  $C_p(T)$ , or  $C_V(T)$  for that matter, is sufficiently accurately described by the theories of Einstein<sup>[9]</sup> and Debye.<sup>[10]</sup> At higher temperatures, the rule of Dulong and Petit<sup>[11]</sup> applies. They observed as early as 1819 that the *molar* heat capacities of elementary solids have values close to 25 J/mol K. The theoretical justification of this law can be drawn from Boltzmann's equipartition theorem. Based on the energy of motion of each oscillating atom in a solid, the internal energy of the system can be described as

$$U = 6 N_A \left( \frac{1}{2} kT \right) = 3 RT \quad (8)$$

Differentiation then leads to the constant value 3 R

$$C_V = 24.9 \text{ J/mol K}$$

Quantization of the vibrational energy of the atoms by Einstein led to an expression for  $C_V$ ,

$$C_V = 3 Rf^2 \quad (9)$$

that could describe the low temperature behavior of the heat capacity. The application of Debye's continuum theory to the vibrational modes of atoms in a solid predicts a cubic law dependency for the specific heat of elemental solids and is a definite improvement over Einstein's work:

$$C_V = \frac{12}{5} \pi^4 R \left( \frac{T}{T_D} \right)^3 \quad (10)$$

***This experiment was designed as a first-year laboratory experiment for undergraduate students in order to familiarize them with the concepts of thermodynamics. Once it is set up, results for a number of different elements can be conveniently obtained and compared.***

In our experiment, various solids are cooled from room temperature,  $T_2$ , to the temperature of liquid nitrogen,  $T_1$ . The *average* molar specific heat between  $T_2$  and  $T_1$  is denoted here as  $\overline{C_P^m}$ . The enthalpy change for a solid immersed into the liquid nitrogen can then be described as

$$\Delta H = H(T_2) - H(T_1) = n_S \int_{T_1}^{T_2} C_P^m dT = n_S \overline{C_P^m} (T_2 - T_1) \quad (11)$$

This change results in the boiling off of  $n_{N_2}$  mols of nitrogen. If the molar heat of evaporation of liquid  $N_2$  is known ( $\Delta H_{N_2}$ ), then  $\overline{C_P^m}$  simply follows from

$$\overline{C_P^m} = \frac{n_{N_2} \Delta H_{N_2}}{n_S (T_2 - T_1)} \quad (12)$$

## EXPERIMENT

A simple evaporation calorimeter was fabricated from two Dewar flasks and additional components mostly comprising standard laboratory items. The entire calorimeter is housed within a PVC container made from a 0.6-m section of 0.2-m diameter PVC pipe, to which is fitted a base plate of 0.4-m diameter. This provides adequate stability for the entire assembly and minimizes the risk of it being knocked over during the experiment. For additional security, we recommend that the PVC container be fastened to the laboratory bench with screws. The large, outer Dewar ("Dewar 2" in Figure 1) has a capacity of 0.5 litre. This Dewar is placed inside the PVC container, and insulating material is poured into the gap between the inside wall of the container and the Dewar. Expanded polystyrene chips of the sort often used in packaging proved to be ideal for this purpose. The smaller Dewar ("Dewar 1" in the figure) has a ground-glass socket at its opening and a capacity of 0.2 liters. The cone closure was modified in our workshop to provide inlet and outlet tubes as shown in the figure. A small glass flask of 50-ml capacity, into which samples are placed, is connected to one branch of the modified cone by clear flexible tubing. A longer length of identical tubing is attached to the other

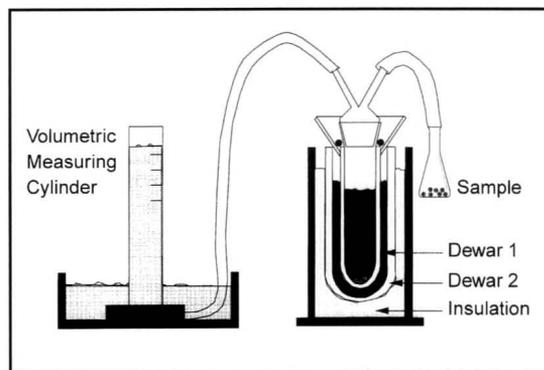


Figure 1. Set-up of evaporation calorimeter.

## Laboratory

branch and is directed to a “beehive shelf” in a large plastic tray filled with water, which serves to collect the nitrogen gas evaporated during operation. A 2-liter measuring cylinder is used for this purpose.

Operation of the calorimeter requires partially filling Dewar 2 with liquid nitrogen. Dewar 1 is then carefully lowered into the large Dewar. (We recommend that a rubber bung be placed at the bottom of Dewar 2 in order to prevent breakage.) Liquid nitrogen is then added to Dewar 1 and care is taken to ensure that the level of liquid nitrogen in Dewar 1 is lower than that in Dewar 2. Approximately 1 g of solid sample is charged into the small glass flask and connected to the cone. This will result in evolution of nitrogen gas, which must be recorded (using a stopwatch) in order to provide a baseline. Once the baseline has been established, the contents of the flask are steadily discharged into the liquid nitrogen, and the volume of gaseous nitrogen evolved is recorded. Once a steady state has been reestablished, the constant evolution of nitrogen is again recorded (second baseline).

### SAFETY

Prior to conducting the experiment, students are briefed on the particular hazards associated with liquid nitrogen and are given eye protectors and insulated gloves. We recommend that students’ handling of liquid nitrogen be minimized and that “bulk” transfers from storage Dewars be carried out by suitably qualified laboratory technicians.

Normally, it will not be necessary to replenish the volume of liquid nitrogen during the course of the experiment once the Dewars have been charged. We employed glass Dewar vessels and encountered no difficulties with their use. (It may be of interest to point out that metal Dewar flasks are also available, and that anyone having particular concerns about breakage may wish to consider using them instead.)

One less obvious hazard associated with the use of liquid nitrogen is the condensation of liquid oxygen from the atmosphere during the experiment. The volume contained in the Dewars of the capacity quoted above are sufficiently small

to minimize this occurrence. As an additional precaution, we fabricated a simple check valve from a truncated plastic filter funnel and rubber “O” ring (see Figure 1) by which the smaller of the two Dewars is suspended inside the outer one.

### ANALYSIS

By extrapolating the volumetric flow rates before and after the experiment, the actual gas volume  $\Delta V$  evolved can be determined (see Figure 2). The value of  $\Delta V$  is the distance between the two baselines at the point where the two areas, A1 and A2, shown in the figure are equal. Using the ideal gas law, the number of mols of evaporated  $N_2$  can be calculated. The partial pressure of nitrogen follows from

$$P_{\text{Air}} = P_{N_2} + P_{H_2O} + P_{\text{hydrostatic}} \quad (13)$$

The atmospheric pressure in the laboratory has to be determined very accurately, and the partial pressure of water at room temperature is taken from the appropriate tables. The correction for the hydrostatic pressure is given by

$$P_{\text{hydrostatic}} = \rho_{H_2O}gh \quad (14)$$

When the heat of evaporation of liquid nitrogen ( $\Delta H_V = 5.56 \frac{\text{kJ}}{\text{mol}}$ )<sup>[12,13]</sup> and the molecular weight of the sub-

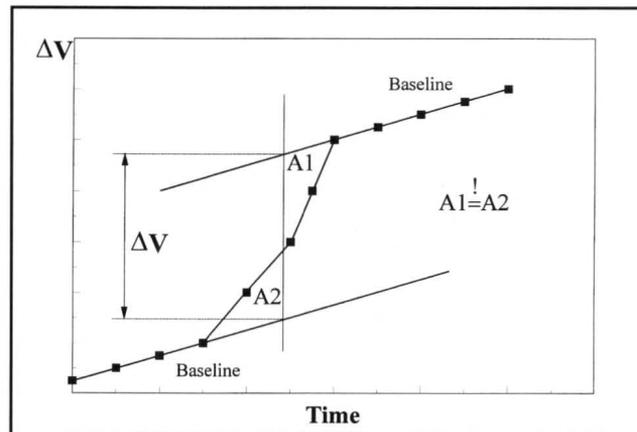


Figure 2.  $N_2$  evolution; determination of the volume of evaporated gas.

**TABLE 1**  
Comparison of Specific Heat Values for Gold, Tin, Silver, Zinc, and Silicon<sup>[14-22]</sup>

Element	Experimental Values [J/mol K]	Data from Literature [J/mol K]
Gold	25.95 [77K - 293K]	25.35 [290K]; 25.42 [298K]; 25.38 [298K]; 19.54 [80K]; 19.63 [80K]
Tin	25.55 [77K - 293K]	26.98 [298K]; 25.32 [298K]; 20.71 [80K]
Silver	23.45 [77K - 293K]	25.28 [290K]; 25.35 [298K]; 25.54 [298K]; 17.91 [80K]; 17.87 [80K]
Zinc	22.85 [77K - 293K]	25.4 [298k]; 25.38 [298K]; 16.86 [80K]
Silicon	13.55 [77K - 293K]	19.99 [298K]; 19.74 [298K]; 5.28 [80K]

stance investigated are known, the heat capacity can be calculated according to Eq. (12).

## RESULTS

We have used the above apparatus to measure the specific heats of gold, silver, silicon, tin, and zinc. The experimental results that we determined are compared with data obtained from various sources in Table 1.

It is clear from Table 1 that the average  $C_p$  values found from our experiments lie somewhere between the values quoted in the literature for the distinct temperature limits of the experiment. The specific heats of all elements considered (with the exception of silicon) seem to obey the rule of Dulong and Petit and are close to  $3R$  as mentioned above.

The somewhat lower value obtained for silicon is due to the fact that the  $C_p$  value for Si approaches lower values at much higher temperatures than is observed for the other metals. This is presumably because the highest frequency for the  $3N$  normal modes of vibration for a silicon crystal is larger than for the other elements due to the intrinsic bond strength.<sup>[5,8,23]</sup>

## CONCLUSIONS

This experiment was designed as a first-year laboratory experiment for undergraduate students in order to familiarize them with the concepts of thermodynamics. Once it is set up, results for a number of different elements can be conveniently obtained and compared. In order to further develop the concepts introduced by this experiment, students could be asked to compare their results with the rule of Dulong and Petit as well as the predictions provided by the theories of Einstein and Debye. The definition of degrees of freedom and their contribution to the specific heats  $C_p$  and  $C_v$  of gases could also be addressed. For especially keen students, the process of achieving very low temperatures by adiabatic demagnetization could be elaborated on.

## NOMENCLATURE

$\alpha$	thermal expansivity ( $K^{-1}$ )
$C_p$	specific heat at constant pressure ( $J\ mol^{-1}K^{-1}$ )
$C_v$	specific heat at constant volume ( $J\ mol^{-1}K^{-1}$ )
$\overline{C_p^m}$	average molar specific heat ( $J\ mol^{-1}K^{-1}$ )
F	frequency factor
g	gravitational acceleration ( $ms^{-2}$ )
h	height (m)
H	enthalpy of a system ( $J\ mol^{-1}$ )
$\Delta H_v$	heat of evaporation ( $J\ mol^{-1}$ )
$\kappa$	compressibility ( $bar^{-1}$ )
k	Boltzmann's constant ( $J\ K^{-1}$ )
n	number of mols (mol)
$N_A$	Avogadro's constant

P	pressure (bar)
Q	heat (J)
$\rho$	density ( $kg\ m^{-3}$ )
R	universal gas constant ( $J\ mol^{-1}K^{-1}$ )
T	temperature (K)
$T_D$	Debye temperature (K)
U	internal energy of a system ( $J\ mol^{-1}$ )
V	volume ( $m^3$ )
$W_c$	non P,V work on system (J)

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# USING PEER REVIEW IN THE UNDERGRADUATE LABORATORY

JAMES A. NEWELL

University of North Dakota • Grand Forks, ND 58202-7101

The value of peer review in developing both critical thinking and student writing skills has been well documented<sup>[1-4]</sup> and is best demonstrated by better laboratory reports. First drafts are often improved because students realize that their peers will be reading their writing.<sup>[5]</sup> Additionally, students are given an opportunity to revise their original report in response to the reviews.

Reviewers benefit by being forced to consider the various elements that result in an effective report. They must be given some guidelines, however. The instructor should provide sufficient structure and guidance to prevent students from giving entirely negative or hierarchal evaluations.<sup>[5]</sup> Providing a structured report sheet for the students to use, similar to a referee report, is advantageous for this purpose (see Table 2).

At the University of North Dakota, peer review has been incorporated into the undergraduate research lab as part of an ongoing effort to develop the oral and written communication skills of our chemical engineering undergraduates.<sup>[6,7]</sup> A student is required to submit a technical journal "article," similar in scope to an extended abstract, based on his or her lab experiment. A copy of the report is then given to some student in the class who has *not* run the experiment. This "reviewer" must learn the details of the experiment, evaluate the technical report, make specific suggestions for revision,



*James A. Newell became an Assistant Professor at the University of North Dakota in 1995. He received his BS from Carnegie-Mellon University, his MS from Pennsylvania State University, and his PhD from Clemson University. His research focuses on high-performance polymers and composites. He was recently named the Dow Outstanding New Faculty Member by the North Midwest section of ASEE.*

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***At the University of North Dakota, peer review has been incorporated into the undergraduate research lab as part of an ongoing effort to develop the oral and written communication skills of our chemical engineering undergraduates.***

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and identify both the strengths and the weaknesses of the report. While the peer review does not affect the grade of the original journal author, the review itself is graded.

Finally, the original report writer receives the peer review along with a faculty review and is given an opportunity to return to the lab to gather any additional data that is required before submitting a revised report in response to the reviews. The revised report is graded separately from the original report.

Each student writes one technical journal article, one peer review, one operations manual, one oral presentation, and one revised final report during the course. Tables 1 and 2 show the handouts given to students and the referee report they are asked to use with their review.

## RESULTS

Peer review was used for the first time in the undergraduate laboratory in the fall semester of 1996, and a noticeable increase in the quality of writing was immediately apparent. The original technical journal reports were better than they had been in previous years.

Although it is difficult to quantify this improvement, it

**TABLE 1**  
**Peer-Review Handout**

Chemical Engineering Lab II  
The Peer Review

### Objective

Almost no journal articles are published in their original form. External readers often can offer new insights and perspectives, detect areas of weak or faulty reasoning, and address ambiguous or incorrect writing issues. Thus, when an editor of a technical journal receives a submission from a researcher, the editor sends the article to another expert in the researcher's field. This peer reviewer identifies strengths and weaknesses of a paper, locates inconsistencies in reasoning or argument, evaluates the technical merit of the paper, and makes two specific recommendations that change the paper. First, the reviewer makes a general assessment of the paper and recommends one of four courses of action. Specifically,

- Publish the paper as is. (This seldom happens.)
- Publish the paper after minor revisions are made.
- Have the author make the suggested major revisions and I'll review it again.
- Do not publish this paper.

Next, the reviewer makes a detailed series of recommendations for improving the paper. These may include, but are not limited to, suggesting additional experiments, requesting additional explanation or analysis, challenging conclusions or premises, and providing proofreading and flow suggestions. The peer reviewer is the guardian of quality for technical journals and his or her role is every bit as important as that of the article author.

### Format

The peer reviewer will submit three copies of the "Reviewer Report" form along with the original journal article and a letter to the journal editor (the professor). Grammatical and typographical errors should be marked directly on the original manuscript. The letter to the editor should include a brief greeting, a statement of purpose (why you are writing this letter), a short summary of your publication recommendation (publish or don't publish), and a brief justification of your recommendation. Regardless of which recommendation you make, you will not be asked to perform a second review of the paper.

The first page of the review provides an area for overall evaluation and specific criticisms and suggestions. Direct questions are asked and explanations for your answers should be included in the comment section, which comprises the rest of the review. The comments should be specific and informative with direct questions, observations, or recommendations being made. Your grade will be based on the following:

- Depth of analysis, including recommendations (50%)
- Demonstration of technical understanding (25%)
- Clarity of expression (25%)

Note: Your peer review will **not** affect the grade of the technical journal article author.

### Miscellaneous Observations

- Criticisms of articles should be constructive in nature. Comments such as "This is awful" will not lead to a better paper (or a better grade).
- In addition to criticizing the article, your review should point out what was good about it.
- It is not enough to say what is wrong; you must also suggest what can be done about it.
- Look for areas that are unclear. Often the author will present useful information, but it will be lost in rhetoric or hyperbole.
- Your suggestions must be reasonable. You could recommend running more trials, but you cannot tell the writer to run 30 or more or to buy more sophisticated equipment.
- While critiquing the paper, consider the things that make a journal article stronger or weaker. Look for these strengths and weaknesses in your own writing.

was unmistakable, and in fact, the truly atrocious papers disappeared altogether. It appears that students are reluctant to give inferior work to their classmates.

Students took the reviewing task seriously. They avoided simple hierarchical judgments and focused on what made the paper either effective or ineffective. They did an outstanding job of identifying grammatical and mechanical problems in the reports, while still identifying strengths and weaknesses in the data analysis.

The final revised reports were substantially better than technical journals from previous years. Grammatical errors were essentially eliminated. More impressively, both the level of analysis and demonstrated technical understanding were much greater.

The forced revision provided important feedback that helped the student improve both the writing and the analysis. The students also spoke of their increased confidence in writing the revised paper.

Additionally, student feedback concerning the peer reviews has been uniformly positive. The students indicate that writing a review led them to recognize weaknesses in their own writing. This improvement in writing skills has been evident in subsequent laboratory classes.

Since these results were presented at the 1997 American Society for Engineering Education conference,<sup>[8]</sup> chemical

**TABLE 2**  
**Review Report Form**

Reviewer Name (1 copy only) \_\_\_\_\_

Title \_\_\_\_\_

Author \_\_\_\_\_

1. Does this article warrant publication in this journal?
  - \_\_\_\_\_ Acceptable in present form
  - \_\_\_\_\_ Acceptable with minor revision, no further review necessary
  - \_\_\_\_\_ Major revision and a second review is required
  - \_\_\_\_\_ Not acceptable (*provide detailed explanation under comments*)
  
2. Is the title satisfactory? \_\_\_\_\_
  
3. Does the abstract adequately summarize the paper? \_\_\_\_\_  
 Could it be more complete or concise? \_\_\_\_\_  
  
*Indicate suggested revision on the manuscript or under comments.*
  
4. Are sufficient references provided? \_\_\_\_\_  
 Are they appropriate and free from obvious omissions? \_\_\_\_\_  
  
*If not, explain.*
  
5. Does the paper present material efficiently? Indicate suggested changes on the manuscript or under comments.
  - (a) Could the clarity or efficiency be improved by changes in the order of the paper? \_\_\_\_\_
  - (b) Should the language or grammar be improved? \_\_\_\_\_
  - (c) Are there portions of the text that could be omitted? \_\_\_\_\_
  
6. Are there errors in factual information, logic, statistical analysis, or \_\_\_\_\_ mathematics?  
 \_\_\_\_\_  
  
*Address these issues in detail in the comments. Suggest improvements.*
  
7. Mechanical errors (*address on manuscript*)
  - \_\_\_\_\_ Figures or tables improperly or incompletely labeled or titled or not cited
  - \_\_\_\_\_ Misuse of references (failure to cite, reference needed and not provided)
  - \_\_\_\_\_ Other \_\_\_\_\_
  
8. Comments  
 \_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_  
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Overall, the use of peer reviews appears to be successful in the undergraduate laboratory.

**SUMMARY**

Student peer reviews seem to be an effective and comparatively simple means of enhancing student writing and data-analysis skills. Key factors in operating an effective peer-review system in the lab include.

- ▷ Providing the student with a template to help focus the review.
- ▷ Grading the reviewer.
- ▷ Making sure the original author revises the paper to address the reviewer's concerns.
- ▷ Keeping the reviewer anonymous.

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## Experiment in Applied Optics

Continued from page 177.

### CSTR CONFIGURATION

An alternative approach to the unsteady-state batch reactor is the steady-state continuous stirred tank reactor (CSTR). The current apparatus could be easily modified by replacing the burettes with delivery reservoirs. Flow meters and pumps (or elevation) would be required. Inlet and withdrawal ports should be fitted onto the transparent stirred vessel. The experiment would still be run with excess bleach.

The theoretical model of the CSTR would begin with a steady-state species balance<sup>[6]</sup>

$$C_{A0} - C_A - k' C_A^n \tau = 0 \quad (13)$$

where

$C_A$  dye concentration in the vessel

$C_{A0}$  dye concentration in the feed

$\tau$  residence time.

Using Eq. (2), the species balance is

$$\mathcal{A}_0 - \mathcal{A} - k' \tau (\sigma L)^{1-n} \mathcal{A}^n = 0 \quad (14)$$

where  $\mathcal{A}_0$  is the absorbance of the reactor feed in the absence of reaction (*i.e.*, a blank run of dye and water without bleach oxidant).

For first-order kinetics ( $n=1$ ), Eq. (14) reduces to

$$\frac{\mathcal{A}_0}{\mathcal{A}} = 1 + k' \tau \quad (15)$$

where a plot of  $\mathcal{A}_0/\mathcal{A}$  vs residence time  $\tau$  would yield the apparent rate constant  $k'$ . The advantage of the CSTR configuration is the application of the laser diagnostic to a steady-state problem. The disadvantage is that large volumes of solutions would be required.

### FINAL THOUGHTS

There are some interesting implications in this study. Since the reaction proved to be first order in dye concentration, the absorption cross section  $\sigma$  was not used (see Eq. 9). This means that an optical calibration to determine  $\sigma$  is not necessary.

The reader may have noticed that this entire analysis was done without knowing the reaction stoichiometry (see Eq. 3). Also, since the reaction is first order in dye, the initial dye concentration is not needed. This is especially convenient since the actual concentration of the dye liquid in the Durkee containers is not known. The label indicates that the dye is manufactured overseas, making inquiries difficult. It has been identified as FD&C Blue No. 1, a complex organic molecule of non-condensed aromatics.

Since the stoichiometry is not known, there is no *a priori*

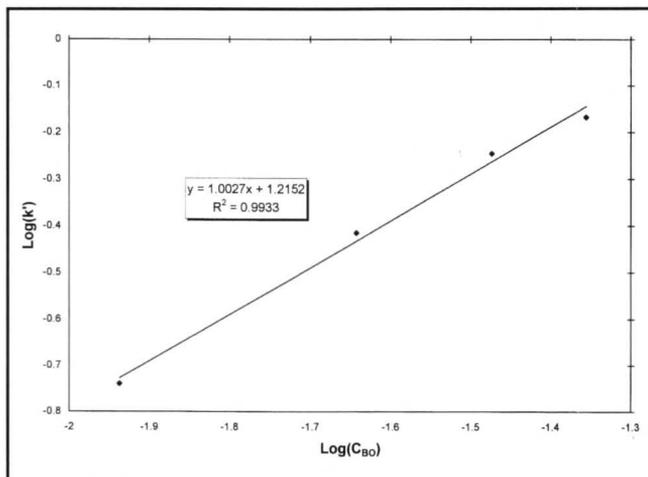


Figure 6. "Lumped" rate constant vs. bleach concentration; Eq. 9.

way to determine how much bleach constitutes an "excess" condition. If insufficient bleach is added, the variation in time of both dye and bleach concentrations must be considered in the kinetic analysis of the absorbance data. If the stoichiometric coefficient  $b$  in Eq. (3) is incorporated into the analysis, its value could be determined as a "best fit" parameter.

Finally, this experiment is effective and relatively inexpensive. An old chart recorder, easily found in any surplus equipment collection, helps to keep the cost down, and glassware should be available in any chemistry stockroom. A small He-Ne laser can be obtained for less than \$100, although the photodiode detector will cost more. The entire experiment can be set up for about \$700.

### ACKNOWLEDGMENTS

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# LOW-COST EXPERIMENTS IN MASS TRANSFER

## Part 4. Measuring Axial Dispersion in a Bubble Column

M.H.I. BAIRD, I. NIRDOSH\*

McMaster University • Hamilton, Ontario, Canada L8S 4L7

The bubble column is one of the most efficient methods of gas-liquid contacting, and it is simple, comprising merely a vertical column and a means of distributing gas into the liquid at the base of the column. Deckwer<sup>[1]</sup> has given a detailed account of bubble columns and their usefulness as gas-liquid reactors as well as mass transfer devices. Bubble columns are often used in organic gas-liquid reactions such as hydrogenation, chlorination, and alkylation. An important application is in the “liquefaction” (hydrogenation) of suspended coal particles at high temperature and pressure.

Bubble columns are often operated countercurrently, with the liquid fed to the top and the gas distributed to the base of the column. The full benefits of countercurrent operation can only be realized if both phases move in plug flow,<sup>[2]</sup> but there is evidence of considerable axial mixing in the liquid phase of bubble columns.<sup>[1]</sup> With axial mixing, the mean driving force for mass transfer is less than it would be in plug flow.<sup>[2]</sup>

The effect of liquid-phase axial mixing on countercurrent mass transfer can be expressed in terms of the Peclet number

$$Pe = UL / E \quad (1)$$

where  $U$  is the superficial velocity of the liquid phase,  $L$  is the active height of the gas-liquid dispersion, and  $E$  is the axial dispersion coefficient. If the Peclet number is greater than 20, plug flow of the liquid can be assumed for engineering design purposes.<sup>[3]</sup> A Peclet number less than about 0.05 will correspond to well-mixed liquid behavior; that is to say the solute concentration is essentially uniform throughout the column. The terms  $U$  and  $L$  are well defined, but the

axial dispersion coefficient  $E$  must often be measured before  $Pe$  can be estimated. Therefore, the measurement or prediction of  $E$  is an important step in the design of a bubble column contactor or reactor.

The axial dispersion coefficient  $E$  is defined in terms of the axial dispersive flux ( $N$ ) of a solute:

$$N = -E \frac{\partial c}{\partial z} \quad (2)$$

Although in this equation  $E$  is analogous to the molecular diffusion coefficient, it is determined by bulk liquid motion such as turbulence, circulation, or motion of bubble wakes. Its value is therefore independent of the molecular structure of the solute. Because of its dependence on bulk fluid motion,  $E$  can be many orders of magnitude greater than molecular diffusion coefficients. Typically,  $E$  is in the range of 1 to 100 cm<sup>2</sup>/s, compared with about 10<sup>-5</sup> cm<sup>2</sup>/s for molecular diffusion coefficients in liquids at ambient temperatures.



**Malcolm Baird** received his PhD in chemical engineering from Cambridge University in 1960. After some industrial experience and a post-doctoral fellowship at the University of Edinburgh, he joined the McMaster University faculty in 1967. His research interests are liquid-liquid extraction, oscillatory fluid flows, and hydrodynamic modeling of metallurgical processes.



**Inder Nirdosh** received his BSc and MSc in chemical engineering from Panjab University (India) and his PhD from Birmingham University (United Kingdom). He joined Lakehead University in 1981, and his research interests are in the fields of mineral processing and electrochemical engineering.

\* Address: Lakehead University, Thunder Bay, Ontario, Canada P7B 5E1

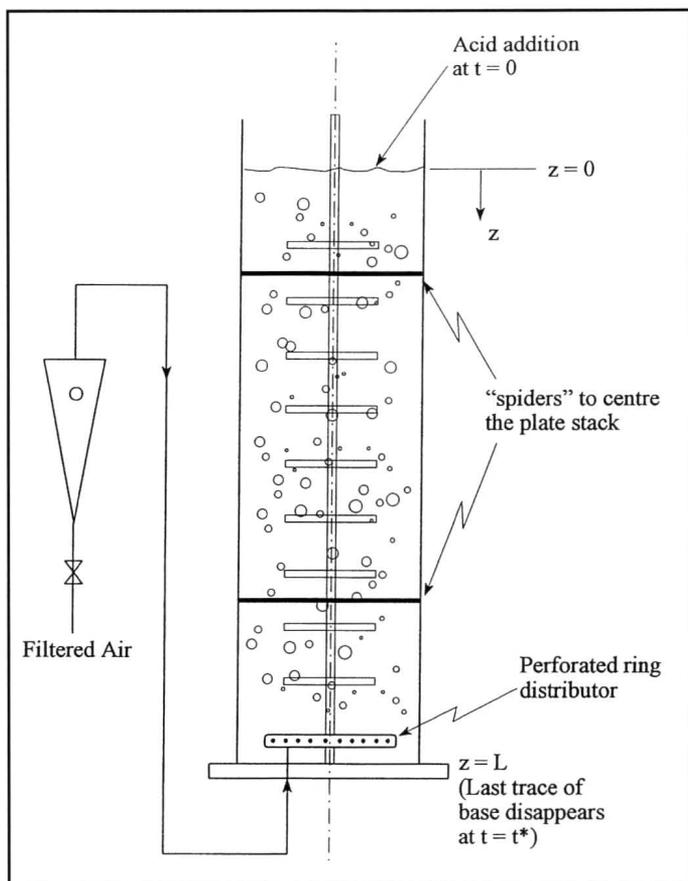
The objective of this experiment is to provide quantitative data on unsteady axial dispersion as well as a visual observation of the turbulent mixing phenomenon in a small laboratory bubble column. The experiment uses an acid-base-indicator system that adds some complexity to the data analysis but eliminates the need for sampling and analysis of liquid at different times and locations.

### MEASUREMENT OF E

Figure 1 shows the experimental bubble column schematically. Axial mixing can be measured by the well-known pulse tracer addition method<sup>[3]</sup> in which the spread of the initial pulse of tracer is determined by the unsteady diffusion equation, assuming that no bulk flow is present:

$$\frac{\partial c}{\partial t} = E \frac{\partial^2 c}{\partial z^2} \quad (3)$$

The conventional tracer method requires sampling the liquid at one point (preferably more than one point) in the column, followed by analysis of the samples. This is too time consuming for most undergraduate experiments. In this experi-



**Figure 1.** Schematic diagram of bubble column showing coordinate system for equations. The baffle stack can be removed for “open column” experiments.

ment, the tracer added is an acid that reacts very rapidly with a base, which is initially uniformly distributed through the liquid in the presence of a suitable indicator. The change in color of the aqueous solution as the pH passes through the neutral point is easily observable, and the movement of the color change through the column can be timed and related to the solution of Eq. (3) so as to give calculated values of E at various conditions.

### METHOD AND THEORY

The column in Figure 1 is initially filled with a dilute alkaline solution at a molar concentration  $c_{b1}$ . We recommend diluting exactly 50 mL of 1.0 mol/L NaOH into distilled water in the column (volume about 40 L), with a few mL of phenolphthalein solution to indicate alkalinity. The concentrated “tracer,” added to the top of the column at  $t=0$ , is a measured volume of 1.0 mol/L hydrochloric acid, which is *more than sufficient* to neutralize the sodium hydroxide. Observation of the column after the addition of acid shows that the red color of the alkaline phenolphthalein starts to disappear at the top of the column; the reaction zone (color change) then moves downward until the last trace of red finally disappears at the base of the column.

The free acid and base mix according to Eq. (3), which is written for each solute, is

Where free acid is present

$$\frac{E}{(1-\epsilon)} \frac{\partial^2 c_a}{\partial z^2} = \frac{\partial c_a}{\partial t} \quad (4)$$

Where free base is present

$$\frac{E}{(1-\epsilon)} \frac{\partial^2 c_b}{\partial z^2} = \frac{\partial c_b}{\partial t} \quad (5)$$

The term in holdup ( $\epsilon$ ) is a correction factor for the volume of gas in the dispersion.

Note that E is the same for acid and base. The acid-base reaction is extremely fast and takes place on a 1:1 mole ratio at a zone where  $c_a$  and  $c_b$  are both very small (pH about 7). The reaction (color change) zone is assumed to be a very thin boundary at which

$$z = z_r \quad (6)$$

$$c_a, c_b \rightarrow 0 \quad (7)$$

$$N_a = -N_b \quad \text{or} \quad -\frac{\partial c_a}{\partial z} = \frac{\partial c_b}{\partial z} \quad (8)$$

The chemical reaction is confined to a very thin zone ( $z \approx z_r$  and  $c_a \approx 0 \approx c_b$ ). At other parts of the column there is no chemical reaction, and therefore Eqs. (4) and (5) do not contain a reaction term. This type of assumption is well

## Laboratory

known in the analysis of gas absorption with instantaneous irreversible reaction.<sup>[4]</sup>

Equations (4) and (5) can be combined in a way consistent with Eqs. (6-8) by creating a concentration variable  $c'$  as follows:

$$\text{For } c_a > 0 \quad c' = c_a + c_{b1} \quad (9)$$

$$\text{For } c_b > 0 \quad c' = c_{b1} - c_b \quad (10)$$

In this way, an equation of the same form as Eq. (3) can be obtained, with  $c'=0$  at  $t=0$  and  $c'_\infty = (c_{a\infty} + c_{b1})$  at  $t = \infty$ .

The standard solution to Eq. (3) in terms of  $c'$  can be shown to be

$$c' = c'_\infty \left[ 1 + 2 \sum_{n=1}^{\infty} e^{-\alpha n^2 \pi^2} \cos\left(\frac{n\pi z}{L}\right) \right] \quad (11)$$

where, in this case

$$\alpha = \frac{Et}{(1-\epsilon)L^2} \quad (12)$$

If the elapsed time is long enough for  $\alpha > 0.1$ , all terms but the first in the series can be neglected, and Eq. (11) becomes

$$c' = c'_\infty \left[ 1 + 2 e^{-\alpha \pi^2} \cos\left(\frac{\pi z}{L}\right) \right] \quad (13)$$

Making the transformation from  $c'_\infty$  by Eq. (9), we find

$$c' = (c_{a\infty} + c_{b1}) \left[ 1 + 2 e^{-\alpha \pi^2} \cos\left(\frac{\pi z}{L}\right) \right] \quad (14)$$

where  $c_{a\infty}$  is the final concentration of acid remaining in the column after mixing has been completed ( $\alpha \rightarrow \infty$ ).

From the point of view of quantitative measurement, the most accurate quantity is the time  $t^*$  it takes for the last trace of red (alkalinity) to vanish at the base of the column. The neutral zone at  $z_r = L$  corresponds to  $c' = c_{b1}$ , and Eq. (14) becomes

$$c_{b1} = (c_{a\infty} + c_{b1}) \left( 1 - 2 e^{-\alpha \pi^2} \right) \quad (15)$$

$$e^{-\alpha \pi^2} = \frac{c_{a\infty}}{2(c_{a\infty} + c_{b1})} \quad (16)$$

This equation is more usefully expressed in terms of  $R$ , the overall acid/base ratio,

$$R = \frac{c_{a\infty} + c_{b1}}{c_{b1}} = 1 + \frac{c_{a\infty}}{c_{b1}} \quad (17)$$

Hence,

$$e^{-\alpha \pi^2} = \frac{R-1}{2R} \quad (18)$$

Taking logarithms and rearranging gives

$$\alpha = \frac{1}{\pi^2} \ln \left( \frac{2R}{R-1} \right) \quad (19)$$

Hence

$$t^* = \frac{(1-\epsilon)L^2}{\pi^2 E} \ln \left( \frac{2R}{R-1} \right) \quad (20)$$

If  $t^*$  and  $\epsilon$  are measured and  $R$  and  $L$  are known,  $E$  can be calculated in a given case. Better still, several experiments can be done under the same conditions of gas flow rate (*i.e.*, same  $E$ ) but with different values of  $R$ . Then the measured values of  $t^*$  can be plotted against  $\ln(2R/(R-1))$  to check for linearity. The slope of the plot will provide an average value of  $E$ .

### APPARATUS

The bubble column used in this project (see Figure 1) is vertical, cylindrical, open at the top, and closed at the bottom. Internal diameter is 8.9 cm and height is 65 cm. The material of construction is clear (methacrylate) plastic. Air is supplied from the 20 psig (230 kPa) line via a rotameter and needle valve. The metered flow of air enters the base of the column via a bubble distributor. A full list of dimensions and operating conditions is given in Table 1. Experiments can be carried out in the absence of column internals, or a stack of baffles (Figure 1) can be placed in the column.

### PROCEDURE AND MEASUREMENTS

Before experiments are begun, a check should be made to ensure that the column is mounted vertically, using a spirit level. Mixing can be affected if the column is tilted away from the vertical.

At the beginning of each experiment, the column is filled to within about 10 cm of the top with distilled water. Then, exactly 50 mL of 1.0 mol/L sodium hydroxide is added. The

**TABLE 1**  
Summary of Experimental Conditions

Column diameter (d) .....	8.9 cm
Column height .....	65 cm
Height of gassed dispersion (L) .....	60 cm (typical)
Number of centrally mounted disk baffles .....	9
Baffle thickness .....	0.75 cm
Baffle diameter .....	5.08 cm
Spacing between baffles .....	5.08 cm
Values of $R$ studied .....	1.05, 1.10, 1.40, 2.00
Values of $u_g$ studied .....	0.83, 1.96, 3.11 cm/s
Gas holdups measured ( ) .....	0.03 to 0.12

alkaline solution is thoroughly mixed by bubbling air for 5 minutes. During this process, about 5 mL of phenolphthalein solution is added to color the solution red. The air flow is started at a desired rate. A volume of stock 1.0 mol/L hydrochloric acid, equal to  $R$  times the volume of 1.0 mol/L sodium hydroxide added earlier, is measured out. It is necessary that  $R > 1$  in order to completely decolorize the solution.

The mixing process is started by quickly adding the acid (within less than one second) to the gas-liquid dispersion. We suggest that a small deflector (*e.g.*, an inverted, 3-cm-diameter, plastic filter funnel) be used so that the acid can be tipped into the column without creating a strong vertical eddy. As the acid is added, a stopwatch is started. The spread of the neutral zone down the column can be observed. It may be possible to measure zone position as a function of time, but the most important measurement is  $t^*$ , the time it takes for the last trace of red color (alkalinity) to disappear from the base of the column. An estimate of error in the  $t^*$  measurement should be made.

A measurement of the gas holdup  $\epsilon$  is required for each gas flow rate. This is done by comparing the height of the gassed dispersion ( $L$ ) with the height of the ungassed liquid ( $L_0$ ),

$$\epsilon = (L - L_0) / L \quad (21)$$

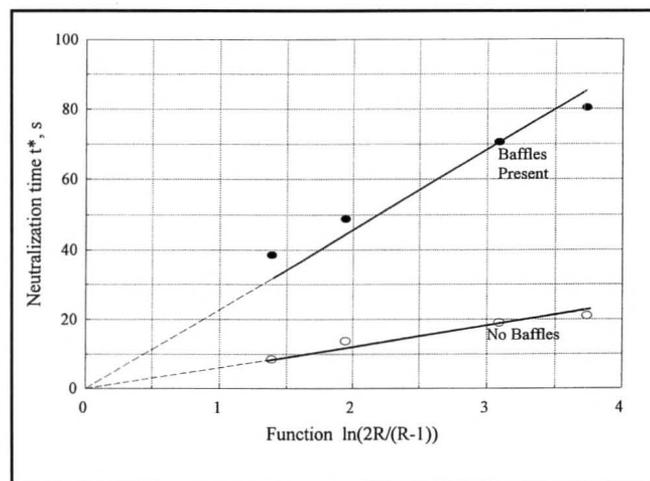
The baffles (5.08-cm diameter) were mounted in a stack on a central support rod that was also equipped with two "spiders" to ensure centering in the column. The baffle stack could be lowered into the column from the open top. The baffle stack is shown in place in Figure 1.

## SAFETY

The student will be handling 1.0 mol/L solutions of hydrochloric acid and sodium hydroxide. The main hazards are possible ingestion or eye damage from splashes. Skin contact is to be avoided, although at the 1.0 mol/L concentration, the skin hazard is moderate. Goggles should be worn; if any acid/base gets on the skin or clothing, wash exposed area with plenty of water immediately after contact. Rinse the apparatus thoroughly with water after each lab day to prevent corrosion damage. It is particularly important to rinse any metal parts that have been in contact with acid or base.

## DATA COLLECTION

On the first day, the column can be operated as an open bubble column without the baffle stack. For a given air flow rate and distributor, the mixing time  $t^*$  should be measured for four values of " $R$ ." We suggest values of 1.05, 1.10, 1.4, and 2.0. Immediately after this, the four data points should



**Figure 2.** Typical data plot of neutralization time  $t^*$  versus function of  $R$  according to Eq. (20). For these data,  $u_g = 0.83$  cm/s.

be roughly plotted as  $t^*$  versus the log function of  $R$  (Eq. 20). If any of the points appear inconsistent, that particular experiment should be repeated.

Then the air flow rate is changed to a new set value, and four more experiments (varying  $R$ ) are done. The sequence is continued until three air flow rates have been covered. A total of twelve experiments is expected, allowing approximately 10 to 15 minutes per experiment. Gas holdup is measured for each gas flow rate.

Then, on the second day, another series of measurements is performed, varying  $R$  and the air flow rate, with the baffle stack in place. This can be shown to give much less axial mixing than in the open column case.

## RESULTS

Figure 2 shows typical data<sup>[5]</sup> on the effects of the chemical ratio  $R$  on the measured neutralization time  $t^*$ . Complete neutralization takes longer as the value of  $R$  approaches unity (*i.e.*, the abscissa function approaches infinity). The data points at the smallest value of  $R$  (typically 1.05) are sensitive to small errors in setting the ratio  $R$ , but it can be seen that the data lie reasonably close to a straight line through the origin. This confirms the assumptions leading to Eq. (20). For a given value of  $R$  the values of  $t^*$  are much greater in the presence of baffles than in the unbaffled condition, which is also to be expected. The slopes of the data plots in Figure 2 are found by linear regression and the value of  $E$  can then be calculated from Eq. (20).

For each gas flow setting studied, and for the presence or absence of baffle plates, a plot of the form of Figure 2 is made, and values of  $E$  are calculated. Figure 3 shows typical

*Continued on page 213.*

# UNIT OPERATIONS LAB

## *Mass Transfer and Axial Dispersion in a Reciprocating-Plate Liquid Extraction Column*

JUNE LUKE, N. LAWRENCE RICKER  
University of Washington • Seattle, WA 98195-1750

The BSChE program at the University of Washington (UW) includes a required 2-quarter lab sequence. The first course emphasizes measurement fundamentals, transport phenomena, statistical analysis of data, and technical communication skills. Experiments are relatively simple.

The second course involves open-ended assignments and the equipment is more complex. Educational goals are to

- Reinforce and integrate the material covered in lecture courses
- Develop students' abilities to plan an experiment, carry it out with good technique, and analyze results in a professional manner
- Refine oral and written communication skills

Students work in teams of three and have three 4-hour lab periods to collect data. A team performs three experiments during the quarter. For each experiment, a designated leader submits a written plan (including a safety analysis) and defends it in a conference with the instructor prior to the first day of data collection. At the end of three weeks, the leader submits a detailed written report, and another team member gives an oral report. The leadership role and other responsibilities rotate from one experiment to the next.

We have recently developed a multifaceted experiment on an important unit operation (liquid-liquid extraction). A typical assignment asks a team to characterize one or more of the following:

- Equilibrium solute distribution between two liquid phases as a function of solute concentration
- Mass transfer coefficients (or HTUs) for steady-state extraction in a reciprocating-plate column as a function of operating conditions
- Residence-time distribution and the influence of axial dispersion on column efficiency

In this paper we will describe the experiments briefly, explaining how they fit in with the educational mission of the course.

### EXPERIMENTAL EQUIPMENT

Our liquid-liquid contactor is a standard Karr<sup>[1]</sup> reciprocating-plate column (see Figure 1). The mass transfer zone is a glass tube, 2.5 cm ID, 2 m long. It contains 36 perforated stainless steel plates (approximately 60% open area) spaced at 5-cm intervals on a central stainless shaft. An electric motor makes the shaft oscillate vertically at frequencies of 0-180 cycles/minute (displayed on a meter and easily varied during operation). The vertical stroke length is 0-5 cm (variable, but constant for the duration of a run). We bought the column, drive system, and internals as a package from the Chem-Pro Equipment Company.

Kerosene is the dispersed phase (a 40-liter stainless steel reservoir allows runs of several hours). It passes through a rotameter and enters as large droplets at the bottom of the column. Smaller droplets form as the kerosene flows upward through the reciprocating plates in the contacting zone. Droplets coalesce above the aqueous inlet location, and the kerosene flows by gravity to a collection vessel.

A feed of tap water passes through a rotameter, enters the column about a foot below the top, and flows downward by gravity, eventually leaving at the bottom. With the drain



**June Luke** received her BS degree in chemical engineering from the University of Washington in 1997. She is currently a first-year graduate student at the University of Delaware. This past summer she worked as an intern at Hercules, Inc., where she studied polymerization reactions employing microwave energy.



**N. Lawrence Ricker** received his BS from Michigan, and his MS and PhD from Berkeley, all in chemical engineering. He worked as a systems analyst for Air Products and Chemicals before joining the University of Washington's department in 1978, where he is currently Professor of Chemical Engineering. His research specialty is process simulation and control.

valve of Figure 1 closed, the exiting water flows upward through flexible tubing to a tee, then back down to a collection vessel. The location of the tee (adjusted by a sliding clamp) controls the water/kerosene interface location inside the column. The section above the tee provides an emergency overflow line and a vent

A 6-mm sampling port with a rubber septum allows either tracer injection or removal of an internal sample at the water feed entry point. A conductivity meter (Omega CDTX-81, 0-200  $\mu\text{S}/\text{cm}$ ) monitors the conductivity of the exiting water phase. We added a zone of 5-mm glass beads between the kerosene inlet and conductivity meter to promote plug flow in that region. Otherwise, flow is laminar and Taylor dispersion biases the measurement of the residence-time distribution. The conductivity meter provides an analog output to a microcomputer.

### PHASE EQUILIBRIA

The system n-butylric acid/kerosene/water offers the following advantages:

- ▶ Butylric acid concentrations can be measured accurately by titration, even at high dilution. Use of a dilute solute simplifies analysis of mass transfer experiments and minimizes chemical consumption and waste-disposal problems. Dilute aqueous solutions of butylric acid and its salts may be sewered. Other acids could be used, but butylric is one of the few having a distribution coefficient of order unity in a nonpolar organic. This makes it easy to avoid a pinch of operating and equilibrium lines in mass transfer experiments.
- Butylric acid's strong, unpleasant odor is a disadvantage; good ventilation is essential.
- ▶ Kerosene is inexpensive, insoluble in water, and reasonably safe and odorless. Nearly all of it can be recovered and recycled. The lack of a known molecular weight forces students to think about the choice of

*... the challenge is to work within the constraints of the lab, obtain consistent, credible results, understand their limitations, and communicate it all effectively. Some students appreciate this and rise to the challenge immediately.*

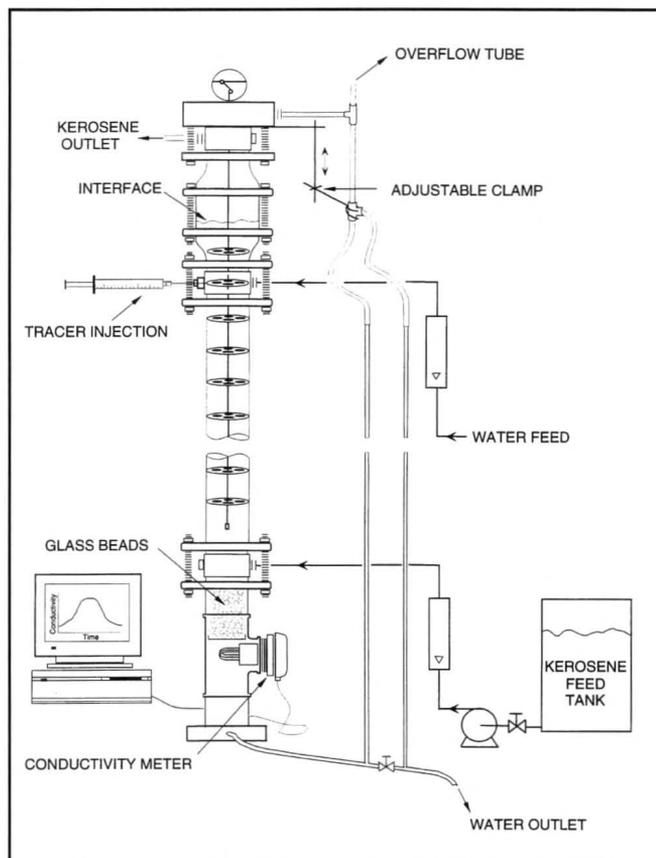


Figure 1. Standard Karr Reciprocating-Plate Column.

the basis for equilibrium and mass-transfer calculations. One could easily substitute a pure hydrocarbon, however.

- ▶ Distribution coefficient data are unavailable in the literature; they must be measured to determine mass transfer driving forces. We provide the students with published data for the analog system butylric acid/hexane/water, however. This gives them a basis for comparison and allows them to estimate appropriate solvent/feed ratios for extraction runs.
- ▶ Results are insensitive to variations in ambient temperature in the lab, avoiding the need for temperature control.

**Measurement of Solute Distribution** • This bench-top experiment seems simple, but it requires careful planning and execution. Mixtures of the three chemicals equilibrate in a suitable container at room temperature. Analysis of samples from one or both phases follows. Students must choose overall mixture compositions such that equilibrated phases have solute concentrations

in the correct range (*i.e.*, as expected in mass transfer experiments). Other considerations include the agitation protocol, time needed to reach equilibrium (we suggest at least one-half hour), and whether it is necessary to measure the solute concentration in both phases. An alternative is to measure one and estimate the other by mass balance. We ask the students to perform an error analysis that compares these alternatives.

Example data appear in Figure 2. The empirical relationship  $y=0.20x^{1.82}$  fits well over the range  $x=0$  to 2 wt. % butylric acid in the aqueous phase,  $y=0$  to 0.8 wt. % butylric acid in the kerosene phase. Heinonen and Tommila<sup>[2]</sup> observed similar nonlinear behavior for n-butylric acid/hexane/water, attributing it to the dimerization of butylric acid in the nonpolar organic phase.

Team leaders usually assign one member to this task,

## Laboratory

which can run in parallel with mass transfer experiments. Study of the full composition range is a significant effort, however. The instructor might instead provide data from a previous group's report, asking the current team to verify some aspect of it. A variant is to provide two or more old reports (good and bad), forcing the team to separate the wheat from the chaff.

**Titration** • Analysis of aqueous samples for butyric acid content is straightforward. We titrate with aqueous NaOH (usually 0.5 N). A phenolphthalein indicator gives a sharp endpoint. For organic samples, one approach is to add the sample to a beaker containing water and phenolphthalein, then slowly titrate with NaOH while stirring vigorously (using a magnetic stir bar). The butyric acid transfers to the aqueous phase where it reacts to form sodium butyrate, which is insoluble in kerosene. Mass transfer is slow, however, so the endpoint is less obvious. An alternative is to equilibrate the sample with an excess of aqueous NaOH, then titrate the unreacted NaOH with aqueous HCl. Another is titration with NaOH in a suitable organic solvent, such as methanol. This requires a pH meter to detect the endpoint.

### MASS TRANSFER EXPERIMENTS

A typical assignment asks the team to measure the overall height of a transfer unit (HTU) as a function of shaft oscillation frequency. The feed is kerosene with a specified concentration of butyric acid (usually less than 1 wt. %), and the solvent is tap water. We also specify the shaft stroke length and the kerosene feed rate. The team must select the water rate(s) and determine the region of operability. The main constraint is flooding, which occurs at high feed rates or high oscillation frequency. Another is phase inversion, *i.e.*, a transition from water-continuous to kerosene-continuous operation. It is also important to avoid a pinch of the operating and equilibrium lines. Otherwise the calculated HTU value is very uncertain.

Students find that running the equipment is non-trivial. The minimum HTU is usually close to the flooding point, where small changes in operating conditions (especially insufficient attention to flow control) can have dramatic effects, easily seen within the glass column. It usually takes a team one full lab period to develop the skill needed to collect useful data in this region. To reduce frustration, we instruct them to avoid flooding conditions in early experiments.

We emphasize the importance of steady-state operation, suggesting that they measure the outlet aqueous butyric acid concentration—the easiest to titrate—periodically until the value is essentially constant, then analyze a sample from the kerosene raffinate to check mass-balance closure. It takes about one-half hour (or turnover of four column volumes) to reach steady state after a change in operating conditions.

Figure 2 shows a typical operating line for the measured

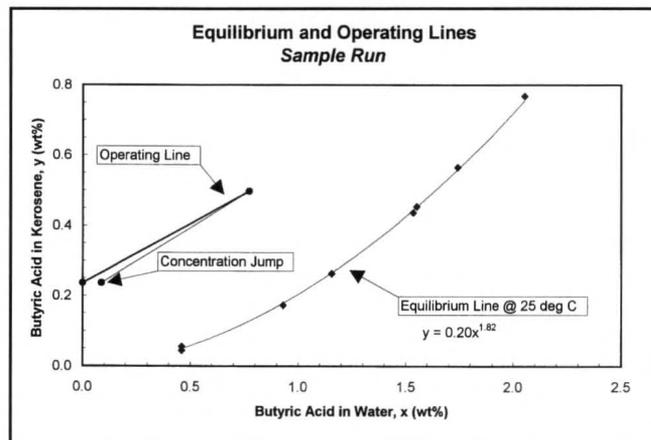


Figure 2.

concentrations of inlet and outlet streams under the assumption of plug flow in two immiscible phases, and dilute operation. Other operating conditions were oscillation frequency = 110 cycles/minute, kerosene feed = 3.0 g/s, and water feed = 1.1 g/s. Calculation of the overall number of transfer units (NTU) would be trivial if the equilibrium line were straight.<sup>[3]</sup> With a curved equilibrium line, however, students must review the theory carefully, which enhances their understanding.

For the case shown in Figure 2, the NTU is 0.83, giving an HTU of 225 cm. Although the HTU decreases with increasing frequency as expected, the values remain well above the 5-25 cm reported in the literature.<sup>[1]</sup> This motivates the assignments for the follow-on teams, who are asked to determine the reason for the large HTUs. Possible variations (other than changes in the chemical system) are the stroke length, tray spacing and design, and choice of the dispersed phase (water-dispersed operation is poor with stainless trays, however). Axial dispersion can also affect liquid extraction performance,<sup>[4,5]</sup> suggesting a study of this possibility.

### AXIAL DISPERSION EXPERIMENTS

There are two ways to check the extent of axial dispersion. The more direct way is to analyze samples from within the column. For example, if one expects strong axial dispersion in the continuous phase, there should be a discontinuity in the continuous-phase concentration at the feed location (a "concentration jump," as shown in Figure 2).

Good technique is needed to remove a representative internal sample. Significant amounts of the dispersed phase may be entrained, and the students must decide how to deal with this. Figure 2 shows that the jump was rather small in the sample run; the corresponding HTU is 220 cm, a decrease of only 2% from the plug-flow value.

The alternative is to measure the residence-time distribution (RTD). This has been advocated in *CEE* previously for gas-liquid contactors.<sup>[6]</sup> Several texts provide good back-

ground on calculational methods and interpretation.<sup>[7,8]</sup>

The continuous phase is most prone to axial dispersion. To measure the RTD, a student injects about 1 ml of  $\text{KMnO}_4$  dye tracer into the aqueous (continuous) phase at the feed point (Figure 1). The pulse is easy to follow visually, and the concentration transient at the outlet can be analyzed quantitatively using the conductivity meter.

The  $\text{KMnO}_4$  is insoluble in kerosene, so it is possible to measure the continuous-phase RTD during normal counter-current operation. We have found, however, that entrained kerosene droplets can interfere with conductivity measurements. The main problem is development of an insulating coating on the probe surface. Students can mitigate this by operating far from the flood point (to minimize entrainment), making baseline corrections on conductivity measurements and cleaning the probe periodically—but this is inconvenient. Thus, we usually assign a study of RTD in the absence of kerosene. Variables are then the water feed rate and the degree of agitation.

An alternative would be to measure dye concentration via UV-vis spectroscopy, which should be less sensitive to the presence of kerosene. We have not tried this yet because our measurements show that the presence of the dispersed phase has little impact on the RTD in our 2.5-cm column. This would not be the case in general.

The students use the measured RTD to calculate a Peclet number at each condition. Peclet numbers can be related to the mass transfer results using the equations developed by Sleicher,<sup>[5]</sup> which provide a correction to the assumption of plug flow. Laddha and Degaleesan<sup>[4]</sup> (pp. 125-127) illustrate the calculations in detail. For the conditions of the sample run, assuming plug flow in the dispersed phase, the observed continuous-phase Peclet number leads to a correction of only 2%, *i.e.*, essentially the same as the correction based on the measured concentration jump.

## DISCUSSION

For our 2.5-cm reciprocating-plate column, axial dispersion increases with increasing plate oscillation frequency and decreasing feed rate, but is never a dominant factor. Continuous-phase Peclet numbers are of order 30 or greater under most conditions. The presence or absence of the dispersed phase has only a small effect. These observations are in agreement with those described in the literature.<sup>[9]</sup>

This forces students to look elsewhere to explain the large HTU values found in mass-transfer runs. It is instructive to follow up with a more polar-dispersed phase having a density closer to water and a lower interfacial tension (*e.g.*, MIBK), which exhibits much lower HTUs. It would also be interesting to run RTD experiments in a column with a much lower length-to-diameter ratio where axial dispersion would

be more significant.

We occasionally ask a team to quantify flooding behavior. It would be logical to do this prior to mass-transfer experiments. Useful information on expected behavior is available in the literature.<sup>[10]</sup>

Student reaction to the RTD experiments has been very positive. They appreciate the visualization of axial dispersion and the automated collection of conductivity data, which makes calculation of the RTD easy. They enthusiastically vary operating conditions over a wide range, check repeatability, etc.

They are less pleased with the phase-equilibrium and mass-transfer experiments. Most complaints concern the odor of butyric acid and the tedium of multiple titrations. We could change the solute, but butyric acid has important advantages, as noted previously. Odor can be reduced, but is difficult to eliminate. Automated titration would increase student productivity and morale.

In general, we want the students to have some hands-on responsibilities in each experiment. In contrast to their *a priori* expectations, the point is not to demonstrate perfect (or even good) agreement between the textbook and reality, nor is it to see modern industrial equipment and instrumentation in action (although such exposure is certainly worthwhile). Rather, the challenge is to work within the constraints of the lab, obtain consistent, credible results, understand their limitations, and communicate it all effectively. Some students appreciate this and rise to the challenge immediately. Others grumble throughout the quarter, but judging by alumni surveys, their frustration with the course often turns to praise once they have graduated.

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# Random Thoughts . . .

## THE NEW FACULTY MEMBER

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

**T**hink back to your experience as a new faculty member. If you conjure up mainly memories of a happy time of exciting new opportunities suddenly open to you—new collegueships, new intellectual challenges, etc.—it's probably been quite a while since you were a new faculty member.

If you think a little more about it, you may start to recall the hurdles you had to jump over to start a research program—writing proposals and trying to get them funded, attracting and learning how to deal with graduate students, and having to churn out a large number of refereed papers while you were still trying to figure out how to do research. You may remember the incredibly time-consuming labor of planning and teaching new courses and the headaches of dealing with bored classes and poor student performance and possibly cheating and poor ratings and a host of other problems you never thought about when you were a student. And you may recall sitting through endless departmental faculty and committee meetings, wondering how you could manage to squeeze in some time for your family and yourself on top of everything else you had to do. Learning to cope with all those conflicting demands on your time and energy was probably not a fun-filled experience for you. Few faculty members ever receive guidance on how to be a faculty member, and it can take years to figure it out by trial-and-error.

Entry into the profession is if anything harder now than it used to be. Even institutions that historically emphasized undergraduate education are pushing their new faculty members to build strong funding and publication records in their first three years, and most institutions still do little or nothing to help the newcomers make the transition from graduate student to assistant professor. The stress on the new faculty members can be debilitating, and those who survive often do so at a severe cost to their personal relationships and/or health.

Robert Boice, head of a faculty teaching center at SUNY—

Stony Brook, has spent many years studying faculty members in their first 3-4 years and has summarized his observations in *The New Faculty Member*.<sup>[1]</sup> This column outlines some of his main points.

Common characteristics of the typical new faculty members Boice observed are that they

- ❶ *spent far less time on scholarly writing (proposals and papers) than was needed to meet promotion and tenure criteria for their institutions*
- ❷ *admitted to going to class overprepared (with more material than they could reasonably cover in the allotted time) and rushing to complete everything, often at the expense of active student participation. Many spent nearly 30 hours per week on class preparation*
- ❸ *equated good teaching with good content*
- ❹ *taught defensively, doing whatever they could to avoid student complaints. They were primarily concerned that students would complain about*



**Rebecca Brent** is Associate Professor of Education at East Carolina University. She received her BA from Millsaps College, her MEd from Mississippi State University, and her EdD from Auburn University. Her research interests include applications of simulation in teacher education and writing across the curriculum. Before joining the faculty at ECU, she taught at elementary schools in Jackson, Mississippi, and Mobile, Alabama. She received the 1994 East Carolina University Outstanding Teacher Award.

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



content errors

- received student evaluations that fell well below their expectations and blamed the results on external factors (invalid rating systems, poor students, unfavorable class times and sizes)
- experienced a sense of loneliness and lack of collegial acceptance, and had difficulty establishing productive contacts with colleagues who could provide guidance and support

Not all new faculty members fit this description. Boice identified 5–9% of new faculty as “quick starters,” who in their first 2-3 years turned out enough proposals and papers to put them in fine shape for promotion and tenure. They also scored in the top quartile of peer and student ratings of teaching and self-ratings of their enjoyment and comfort levels as teachers. Unlike the majority of their colleagues, the quick starters

- spent three hours or more per week on scholarly writing
- integrated their research into their undergraduate classes
- did not spend major amounts of time on course preparation (after their first semester, they averaged 1–1.5 hours of preparation per lecture hour)
- lectured at a pace that allowed for active student participation
- regularly sought advice from colleagues, averaging four hours a week on discussions of research and teaching

The main differences between typical new faculty and quick starters are the latter group’s abilities to balance conflicting demands on their time and to quickly establish productive networking with colleagues. Boice has developed a “balance program” to help new faculty members do those things. Participants in the program commit to these guidelines:

1. Limit classroom preparation to a maximum of two hours per hour of lecture.

This target is extremely difficult for many professors, but those who manage to reach it find that they can still cover what they want to cover, appear more relaxed to their students, and are better able to maintain a pace that encourages active student involvement in class.

2. Spend 30-60 minutes a day on scholarly writing.

New faculty often feel they must have long unbroken stretches of time to write, but the demands of an academic career seldom allow this luxury. Writing for a set time daily leads to steady productivity and fewer feelings of anxiety over failure to meet scholarly productivity expectations.

3. Spend at least 2 hours a week on discussions with colleagues focused on teaching and research.

(Periodic meetings over lunch are convenient for such networking.) It is difficult for most new faculty members to meet this commitment, but doing so pays big dividends. Good contacts provide ideas and sometimes tangible assistance in getting a research program off the ground and/or improving teaching success.

4. Keep daily records of work time expenditure.

Recording helps new faculty self-monitor how well they are meeting Commitments 1–3.

5. Integrate research interests into lectures.

Doing so leads to greater enthusiasm for teaching as well as recruitment of students as research assistants.

Boice found that faculty going through this program initially resisted its requirements, particularly the one about limiting lecture preparation time, but after five weeks they began to look and feel more like quick starters. Regular meetings with a facilitator or mentor were instrumental in helping them stay with the program. Once they attained the standards set out in the plan, they reported greater efficiency and a higher level of comfort in their teaching.

*The New Faculty Member* offers a variety of useful suggestions for supporting new faculty. We recommend it to administrators, mentors, faculty developers, and anyone else concerned with helping new faculty members attain the levels of research productivity and teaching skill for which their potential was recognized when they were hired.

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1. Robert Boice, *The New Faculty Member*, San Francisco, Jossey-Bass (1992). For additional discussions of problems faced by new faculty members and ways their departments can support them, see the Random Thoughts columns “Teaching Teachers to Teach: The Case for Mentoring,” *Chem. Engr. Education* 27(3), 176-177 (1993) and “Things I Wish They Had Told Me,” *Chem. Engr. Education*, 28(2), 108-109 (1994). □

All of the *Random Thoughts* columns are now available on the World Wide Web at [http://www2.ncsu.edu/effective\\_teaching/](http://www2.ncsu.edu/effective_teaching/) and at <http://che.ufl.edu/~cee/>

# THE PRACTICAL SIDE OF CHEMICAL ENGINEERING

## *At The University of New Brunswick*

GUIDO BENDRICH, TODD S. PUGSLEY

*University of New Brunswick • Fredericton, New Brunswick, Canada E3B 5A3*

In an attempt to better prepare our students for their life after graduation, the Department of Chemical Engineering continuously seeks ways to expose the students to the practical aspects of chemical engineering. Factory tours and laboratory exercises present students with early opportunities to experience the world of chemical engineering during their first and second years.<sup>[1]</sup> After studying several of the chemical engineering core courses (material and energy balances, heat and mass transfer, fluid mechanics, and thermodynamics), the students are given the opportunity to apply what they have learned to real industrial problems through an industrial project course known as "Practice School," and during their senior year, their practical experience is extended during a Plant Design course. This paper describes the industrially oriented approach taken in both the Practice School and Plant Design courses.

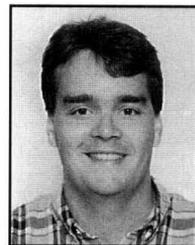
### PRACTICE SCHOOL

Practice School projects can be considered as an introduction to the concepts of industrial design. They generally accent the application of material and energy balances and thus tend to be relatively basic from a design point of view. But within the scope of their project, the students are expected to develop a detailed design solution. This industry-sponsored endeavor allows the students to become familiar with many aspects of an engineer's working life. Almost all students participate in this course (a limited number, however, exercise the option of preparing a report on a departmentally approved research topic).

#### *Course Logistic*

A two-week project in selected industrial process plants is scheduled after the spring examination period (the last week

**Guido Bendrich** joined the Department of Chemical Engineering at the University of New Brunswick after spending some nineteen years in various industrial settings throughout the world. He obtained his PhD from McMaster University in 1992. His teaching and research interests are in industrial plant design, cost estimation, plastics processing, developing communication skills, and education.



**Todd Pugsley** received his PhD from the University of Calgary in 1995 and was a Post-Doctoral Fellow at the Technical University Hamburg-Harburg (Germany) for six months before joining the Department of Chemical Engineering at the University of New Brunswick in 1996. His research interests are gas-solid fluidization and reaction engineering.

in April to the first week in May). Groups of third-year students (jointly supervised by a faculty member and a professional engineer employed by the company) are assigned to engineering projects to be carried out on industrial process units. While working in the plant, the students are introduced not only to the problem at hand, but (perhaps of equal importance) also to the various aspects of real-life engineering, including time management and teamwork. The students are also encouraged to take very detailed notes while working in the plant.

At the end of the two-week period, the group presents their results orally and submits a preliminary typewritten report to the company representatives. The students are then expected to work during the summer months on the final solution to the design problem. Although the group members tend to disperse to summer employment during this time, they are able to stay in effective contact through electronic mail, fax,

and telephone. The combination of detailed plant notes and continued communication throughout the summer months is critical when the students return for the fall semester since, at that time, the results of their work are documented in the form of a final comprehensive report that must be submitted by the end of September. The following outline shows the typical content of the comprehensive report.

- **Introduction to the Design Problem** *This section presents a brief introduction to the industry and the assigned task.*
- **Theory** *A detailed discussion of the governing equations and principles is given in this section. The knowledge gained in the core courses is essential to providing a concise description of the relevant theory.*
- **Results** *The data taken at the plant are presented in this section.*
- **Data Analysis** *An in-depth data analysis leads to the final design. Simulation software packages may be of assistance to the students in the final design. Working with industry on a viable solution to one of its problems also entails an economic evaluation of the final design.*
- **Conclusions and Recommendations** *Suggestions for the implementation of the final design and the possible continuation of future studies are put forward to the company.*

To complete the requirements of the course, each Practice School group is required to present its work in a 15-minute oral presentation scheduled during the month of October. Invitations to visit the department and attend the presentation are extended to the companies that participated, to the other engineering departments, and to the public.

### **Suitable Practice-School Projects**

When the Practice School course was initiated in 1970, all of the projects were supplied by a lead-smelting company in

**... students are given the opportunity to apply what they have learned to real industrial problems through an industrial project course known as "Practice School," and during their senior year, their practical experience is extended during a Plant Design course.**

the northern region of the Province. At that time, enrollment in the department was less than it is now; today, we have as many as thirty-five students for whom we must find suitable projects each spring. With groups of three or four at each industrial location, this translates into a need for ten or more projects every year. As a result, students now work in industries from across the Province, and we rely heavily on the industrial contacts of the individual faculty members to obtain the necessary projects.

The industries that participate in the Practice School welcome the opportunity and, in many cases, have come to depend on the work that is done by the students every year. Many of the problems that our students work on are problems for which the typical process engineer in these plants does not have the time. Examples are projects involving process water balances or balances on components of waste streams around sections of the plant.

As might be expected, certain projects lend themselves better to the Practice School structure than others. Because of the student's relatively short stay at the industrial site, the projects must be well defined by the company, with clear objectives that can be met in two weeks. Also, it is important that any equipment provided by the company for a sampling campaign or for laboratory analysis be in working order and ready to use on the students' first day at the plant. Furthermore, we have observed that projects that allow the students to work independently (*i.e.*, limited dependence on plant personnel for assistance in sample collection or laboratory analysis) are most desirable. Table 1 lists the most recent Practice-School topics in which we

**TABLE 1**  
**Recent Practice-School Projects**

<i>Industry</i>	<i>Project Title</i>	<i>Objective</i>
Integrated wood pulp and chemical production facility	Design of an HCl vacuum scrubber for the electrochemical plant	Eliminate the environmental and operational hazards associated with the filling process of concentrated HCl into tank trucks
Integrated wood pulp and chemical production facility	Sodium chlorate filter replacement and an alternative method for sodium hypochlorite removal	1) Design of an economically feasible separation process for the removal of sodium chlorate. 2) Develop a system for the complete removal of sodium hypochlorite from one of the plant's product streams.
Crude-oil refinery	Desalter waste minimization	Determine the desalter impact on the effluent unit.
Lead-concentrate mining operation	Residence time distribution and grade recovery of the lead-upgrading circuit	Evaluate the performance of the lead upgrading cells using a CaCl <sub>2</sub> tracer.

have been involved as faculty supervisors.

## Conclusion

Practice School is one of the first steps our students take in becoming acquainted with the industrial environment. Although the actual time spent in the plant environment is only two weeks long, the program ensures that essentially all of our undergraduate students have some industrial exposure by the end of their third year. During this two-week period and the subsequent report-writing stage, students have an opportunity to put the theoretical knowledge they have gained and the skills they have developed to practical use. They build confidence in themselves and in their ability to apply what they have learned to solve industrial problems. These Practice School projects ease the students into the senior year of the chemical engineering program.

## PLANT DESIGN

One approach to the senior Plant Design course is to make use of prepackaged (and sometimes outdated) case studies. The instructor might have twenty such cases to choose from, and the course is essentially run as any other lecture. But is this approach in the best interest of our customers, the students? Engineers who have gone through a “traditional” (chemical) engineering education tend to agree that additional practical components should be added to the curriculum and especially to the senior design project. The expression “plant design” should immediately imply industrial applications;<sup>[2]</sup> consequently, industry should be involved in the design course. Working with practicing engineers on relevant industrial problems and not just trying to fulfill their degree requirements gives students a great sense of achievement and satisfaction.

The Plant Design course, as our department defines it, is a capstone course in which our senior undergraduates use their knowledge to work on an industrially relevant problem. Over the years, close ties between New Brunswick companies and our department have been established. Through personal contacts, the department seeks to obtain industrially relevant design problems for our students, while the industries are interested in obtaining solutions for their design problems. If successful, the students and the industrial partner will benefit from this cooperation. The various steps involving the successful completion of an industrially sponsored design project are described below.

## Course Logistics

During initial meetings between the industrial sponsor and the course instructor, the design project’s topic and scope are established. The company designates an engineer to supply relevant project information such as process and instrumen-

tation diagrams, flow sheets, and plant operating data. Recent design topics supplied by industry have ranged from “Design of a Sodium Chlorate Plant” to “From PET to the Soft Drink Bottle.”

At the beginning of the term, the class is divided into design teams (comprised of three to four members each) that are required to solve different design problems. As the individual groups begin working on the design problem, they are concurrently being introduced to the concepts of group dynamics,<sup>[3]</sup> hierarchical plant design,<sup>[4]</sup> design of experiments, and scale-up procedures. The steps taken to arrive at an optimized solution of a design problem are:

- **Formulation of the Project Parameters** *Pertinent materials, such as P&ID, flow sheets, and any other information relating to the design problem, are given to the students during the first lecture. One reason for identifying the process specifications is to make sure that there are no surprises for either the students or the company upon completion of the project. Where possible, a plant tour during the second week helps the students learn more about the plant operation and assists them in establishing contact with the company engineer.*
- **Literature Review and Generation of Alternative Solutions** *A thorough search of the existing literature, as well as application of relevant design and manufacturing codes, helps the design teams minimize design errors and maximize their efforts. Exercises to encourage the lateral thinking process, the background of the students in the field of engineering, and the knowledge gained from the literature search will yield alternative design solutions.*
- **Development of Gantt Chart** *The management of design projects within the constraints of the university environment, i.e., the heavy course load for students, is easier said than done. The plant design course environment is very turbulent and is composed of numerous design team meetings, section report writing, conflict resolution, planning, and communication with the various parties involved. It is extremely important for the students to learn about time management. A bar (Gantt) chart developed by each design group assists everyone in keeping the projects focused.*
- **Development of the Conceptual Design** *After the preliminary process flow diagrams have been developed, an engineering panel comprised of two practicing engineers reviews the initial conceptual designs. The panel arrives at a “go/no-go” decision.*

Certain recommendations may be put forward by the panel to enhance the proposed design. If the engineers should arrive at a no-go decision (which has not happened yet, perhaps due to the students' intensive practical preparation through practical laboratory exercises,<sup>[1]</sup> practice school, and PEP), the students would be asked to revise their design and report back to the engineering panel.

- **Execution of the Design Calculations and Assessment of Performance** Computer simulations are an invaluable tool for an engineer. Simulation programs such as CMOLD, HYSYS, and FLUENT are used by the design teams to accomplish their design tasks more efficiently. Many design problems, however, still cannot be adequately simulated. Therefore, experimental work or hand-computations are frequently necessary to obtain the required design specifications. The students must also keep safety aspects foremost in their minds throughout the design stage.
- **Optimum Economic Design** In almost every design case there are several technically equivalent design solutions. The optimum size can often be obtained only by cost comparison of different schemes. There is a tendency to evaluate a parameter as being the optimum factor. This sub-optimization may result in an increase in the overall process equipment cost. Care must be taken to study the overall system and its economic implications. The students are required to evaluate their design solution from an economic perspective.
- **Preparation of Specifications** The use of specification sheets is mandatory, but due to time constraints, they need not be fully completed. These sheets are the basis for the company in the continuation of the design projects.

Ultimately, a final report summarizing the work done on the project must be submitted. The report's content follows a format similar to that described by Seider and Kivnick.<sup>[5]</sup>

**Proper  
planning  
and  
preparation  
will  
alleviate the  
“culture  
shock”  
experienced  
by a  
graduate  
engineer  
when  
accepting a  
position in  
industry.  
The Plant  
Design  
course  
presents an  
excellent  
opportunity  
for students  
to learn  
more about  
the language  
and customs  
of  
professional  
engineers.**

The individual groups are then required to present their final design at the Annual Industrial Chemical Engineering Conference. The conference, which is organized by the chemical engineering student body, attracts attendees from the university, industry, and government. It is intended to hone the presentation/public speaking skills of the students, to present the design solutions to the participating companies, to allow the graduating students to “rub shoulders” with decision makers and perhaps to discuss employment opportunities, and to develop new university/industry relationships as well as bolster existing ones.

### **Conclusion**

While this plant-design concept has been successful, it should be pointed out that the notion of an industrially oriented plant design course is not new. Articles by Seider and Kivnick<sup>[5]</sup> and Rockstraw, et al.,<sup>[6]</sup> have discussed both this concept and their affiliations with local companies. Our effort is different because, while New Brunswick is a highly industrialized province, there is no single industry in close proximity to the University with which we have been able to develop a close, continuous relationship. Rather, projects come from various companies each year.

It is interesting to note that our involvement with industry through the Practice School has led to projects for Plant Design. The most recent example is the sodium chlorate plant-design project mentioned above, which grew out of the sodium chlorate filter and sodium hypochlorite removal Practice School projects. Furthermore, several national and international companies currently support our effort to educate students in a more practice-oriented way. Information technologies have made it possible for the students to work on design problems that are not available in our local area.

### **GENERAL OBSERVATIONS**

Students enjoy working on an industrial design project and feel pride in that a part of their work will be implemented in an industrial operation. When this course concept was first introduced, some students commented:

*“I can't design a plant addition for a company; I don't have enough experience to un-*

*dertake this task."*

*"Is this for real?"*

After the students had time to think about the underlying objectives, the comments were more along the line of:

*"Finally I am not working for the wastebasket anymore."*

*"Thank you for introducing us to the world of practical engineering."*

Although the student comments have been positive, there is always room for improvement. In industry, chemical engineers seldom work on a project by themselves; different disciplines are needed to ensure the successful completion of a project. There will be electrical engineers, mechanical engineers, civil engineers, chemical engineers, architects, and business people working side-by-side.

In the 1997-98 academic year, mechanical engineering students will also participate in the Plant Design course, creating a more realistic design environment. A design project involving the local aquaculture industry was carried out in the fall of 1997. It involved interactions with the biology department and was quite successful.

Expanding the design course to involve other disciplines, however, creates some problems that need to be addressed. Of particular concern is the issue of prerequisites. For example, mechanical engineering students do not take courses dealing with separation processes or reactor design, which are both Plant Design prerequisites for our students. During the course of a design project, process economics and safety and environmental concerns have to be considered simultaneously. Having recognized that these subjects are inseparable, starting in 1998-99, we will introduce a new full-year design course to more adequately cover them. The new course will represent the amalgamation of the Plant Design and Process Economics and Safety courses.

Proper planning and preparation will alleviate the "culture shock" experienced by a graduate engineer when accepting a position in industry. The Plant Design course presents an excellent opportunity for students to learn more about the language and customs of professional engineers. Our hope is that our students' transition to industry will be considerably eased.

## **ON TO THE THIRD PARADIGM OF CHEMICAL ENGINEERING**

Wei<sup>[7]</sup> observed that two paradigms have shaped the field of chemical engineering throughout this century. In the 1920s, the first paradigm of unit operations was developed. Then, with the publication of *Transport Phenomena*, by Bird, Stewart, and Lightfoot<sup>[8]</sup> in 1960, came the more analytical and fundamental second paradigm. In a recent article, Landau<sup>[9]</sup> states,

*"It is my opinion . . . that we need a change in direction toward more relation to practice and to industry, which perhaps might constitute the third paradigm."*

Elsewhere in the article, Landau comments,

*" . . . I believe chemical engineering's third paradigm, if there is one, is to return the discipline closer to the practices in industry, and to strengthen its interdisciplinary ties. . . ."*

While the first two paradigms were indeed revolutionary, the next paradigm should not be. As discussed by Douglas,<sup>[10]</sup>

*"As we extend chemical engineering into new application areas, we will need experts in each of these paradigms."*

Whether or not one accepts the notion of an emerging third paradigm, we do feel that our Practice School and Plant Design courses are effective approaches to preparing chemical engineers for their future in the profession. We emphasize practical, industrially oriented projects and are promoting an interdisciplinary structure. The students are also firmly grounded in the fundamentals of chemical engineering and the basic sciences. The positive feedback obtained thus far from the students encourages us to continue thinking of new and innovative approaches for improving the existing courses.

## **ACKNOWLEDGMENT**

The authors wish to thank Robin Chaplin and Derek Lister for their invaluable suggestions during the development stage of the plant-design course. Also, Jules Picot provided us with his first-hand recollection of the early days of the Practice School. The most recent Practice School projects would not have been possible without the coordination efforts of Mladen Eic.

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## Experiment in Mass Transfer

Continued from page 201.

final data<sup>[5]</sup> on the effect of  $u_g$  on  $E$ , with and without baffle plates. Also shown for comparison on Figure 3 is an equation that has been suggested in the literature<sup>[6]</sup> for axial dispersion in unbaffled bubble column,

$$E = 0.35(gu_g)^{1/3}d^{4/3} \quad (22)$$

We can see that the unbaffled column data (open circles) are in the same order of magnitude as predicted by Eq. (22), showing the same trend of a slight increase in  $E$  with respect to gas velocity. In the presence of the baffles,  $E$  is greatly reduced and the values go through a shallow minimum with respect to  $u_g$ . The tendency of  $E$  to increase at the lowest values of gas velocity is thought to be due to the formation of trains of gas bubbles following a preferred path up one side of the baffles, resulting in a downflow of liquid on the other side.

### GENERAL REMARKS

This experiment can be carried out in as little as one three-hour laboratory period, although two such periods are better for a thorough comparison between the results with and without baffles. The experimental work is not highly demanding, although students must be careful to measure solution volumes accurately, and necessary safety precautions must be followed. It is preferable that prepared standard 1.000 mol/L solutions of acid and base be used; these are available in 20 L quantities from most scientific suppliers.

Students should be encouraged to use computers to examine the time-dependent concentration profiles in the column by means of Eq. (11). Numerical examples can also be developed to confirm the stated assumption leading to Eq. (13), namely that only the first term in the series is important when  $\alpha > 0.1$ .

As a further exercise, the eddies of color at the neutralization zone can be videotaped in close-up mode. Playing these

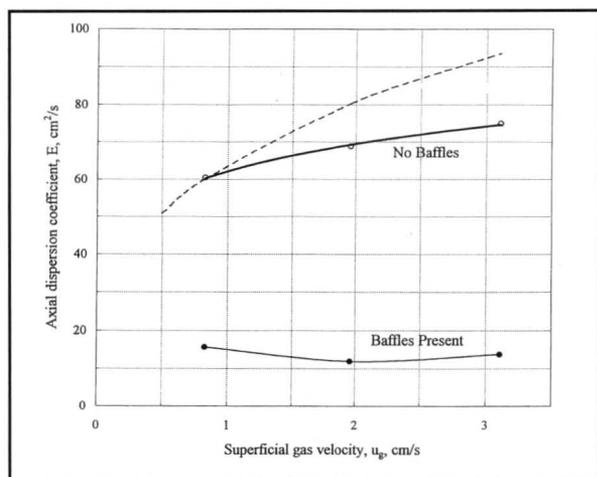


Figure 3. Axial dispersion coefficients plotted versus  $u_g$ , with and without baffles. Dashed line denotes Eq. (22)

back at slow speed provides a good visualization of the highly random nature of turbulent axial dispersion.

Our experience over a period of about eight years has shown that this experiment provides students with good insight into axial mixing. The present method offers two advantages over more classical "trace injection," such as salt or dye. First, the complexities of sampling/analysis of the tracer are diminished, allowing more data to be obtained in a given period, and second, the sharp color change boundary allows students to directly observe the mixing process.

### ACKNOWLEDGMENTS

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### NOMENCLATURE

$c$	concentration, mol m <sup>-3</sup> or mol/L
$c'$	concentration variable defined by Eqs (9) and (10), mol m <sup>-3</sup> or mol/L
$d$	internal diameter of column, m
$E$	axial dispersion coefficient m <sup>2</sup> s <sup>-1</sup>
$g$	acceleration due to gravity, ms <sup>-2</sup> (=9.81)
$L$	depth of gas/liquid mixture, m
$L_0$	depth of ungasged liquid, m
$n$	term in expansion series
$N$	flux, mol m <sup>-2</sup> s <sup>-1</sup>
$Pe$	Peclet number
$R$	ratio (mols acid added) to (mols base added)
$t$	time, s
$t^*$	time for neutralization at $z=L$ , s
$U$	superficial liquid velocity, m s <sup>-1</sup>
$u_g$	superficial gas velocity, m s <sup>-1</sup>
$z$	axial distance, m (measured downward, see Figure 1)

#### Greek Symbols

$\alpha$	dimensionless time, see Eq. (12)
$\epsilon$	gas holdup (fraction)

#### Subscripts

$a$	free acid
$b$	free base
$I$	initial value
$\infty$	as $t \rightarrow \infty$
$r$	reaction zone

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# CASE STUDY PROJECTS IN AN UNDERGRADUATE PROCESS CONTROL COURSE

B. Wayne Bequette, Kevin D. Schott, Vinay Prasad, Venkatesh Natarajan, Ramesh R. Rao  
*Rensselaer Polytechnic Institute • Troy, NY 12180-3590*

In recent years, there has been an on-going argument that engineering students need more open-ended problems, more team projects, more written memos, reports, and oral presentations, more practical problems, and more interactive learning (rather than complete dissemination of course material by lecturing) in their undergraduate education.

At Rensselaer Polytechnic Institute we try to include all these factors in our process control course. The focus of this paper is on a case study project performed during the latter half of the semester. We will cover not only the project, but also a background description of the Rensselaer curriculum, the introductory material for the project, the venues used for distributing course material, future teaching efforts, and a summary.

## BACKGROUND

There are roughly 80-90 BS degrees granted in chemical engineering at Rensselaer each year, while there are approximately 30 environmental BS degrees granted. A num-

ber of courses in the curriculum (material and energy balances, dynamic systems, chemical process control, unit operations laboratory I and II) are taught to both the chemical and the environmental students.

A distinguishing characteristic of the Rensselaer curriculum (in addition to the fact that both chemical and environmental engineering take many of the same courses) is that we have had separate courses in dynamics and control for over a decade. Another is that the dynamics and control courses are taught during the junior year. One advantage of teaching these courses at that time is that students tend to take more of a process-systems engineering viewpoint in the senior courses (reactor design, separations processes, process design, lab I and II).

The process dynamics course covers more material in more depth than the "front end" of a typical single course in dynamics and control. Particular emphasis is given to numerical methods for the solution of algebraic and differential equations, with MATLAB as the numerical analysis pack-

**Ramesh R. Rao** received a BE in chemical engineering from Annamalai University and a Masters from the Indian Institute of Technology, Kanpur. Before joining Rensselaer Polytechnic Institute to pursue a PhD, he spent two years as a research engineer at the Tata Research Design & Development Centre, Pune. His current research interests focus on model predictive control applications in chemical and biomedical engineering. (Far left)

**Venkatesh Natarajan** received his Bachelor of Technology from the Indian Institute of Technology, Bombay, and his MS from Rensselaer Polytechnic Institute, both in chemical engineering. He is pursuing a PhD at Rensselaer, where his research involves the scale-up and optimization of ion-exchange biochromatographic systems. (Second from left)

**Vinay Prasad** obtained a Bachelor of Technology from the Indian Institute of Technology, Bombay, and an MS from Kansas State University, both in chemical engineering. He is now pursuing his PhD at Rensselaer, and his research interests lie in process design, analysis, and control, with a focus on batch chemical processes. (Second from right)

**B. Wayne Bequette** is Associate Professor of chemical engineering at Rensselaer Polytechnic Institute. He received his BS from the University of Arkansas and spent several years as a process engineer at American Petrofina before obtaining his PhD from the University of Texas, Austin. His teaching and research interests are in process control, design, and biomedical engineering. (Right)

**Kevin D. Schott** received his BS in chemical engineering from the University of Massachusetts and his MS in electrical engineering from Rensselaer Polytechnic Institute. He has several years of experience with Monsanto and is completing his PhD at Rensselaer. His research involves multiple-model and gain-scheduling approaches to nonlinear control. (Not pictured)



age. State space models receive much attention. Also, phase-plane analysis and an introduction to nonlinear dynamics and chaos is provided. A textbook for this course has been published by Prentice Hall.<sup>[1,2]</sup>

## INTRODUCTORY MATERIAL FOR PROCESS CONTROL

A major advantage of the two-course sequence in process dynamics and control is the proper coverage that can be given to the topic of process control. Process control is taught in the spring of the junior year, immediately after the students have taken process dynamics. After a concise review of modeling and dynamics, we are able to leap into important issues of control-system design. The topics covered in the course are

- Motivation
- Review of process modeling for control
- Introduction to feedback control
- Direct synthesis and open-loop “control”
- Internal model control (IMC)
- IMC-based PID control

*The process dynamics course covers more material in more depth than the “front end” of a typical single course in dynamics and control.*

- Introduction to frequency response
- Frequency response for control-system design
- Control using multiple measurements
- Implementation issues
- Decentralized control
- Multivariable control
- Case-study problems in multivariable control

Each of the topics, including characteristic homework problems, is summarized in Table 1.

When we first taught this course, we also introduced discrete control-system design, and in some years we included model-predictive control (MPC). Our philosophy now is to cover less material, but to provide more depth. Since our course is taught during the junior year, students often select a senior project in control or take a reading course in ad-

**TABLE 1**  
Process Control Course Topics

**Motivation and Introduction to Control** Fairly standard material on economic, safety, and environmental incentives is presented. Simple examples, such as “taking a shower” and surge drum level control are discussed extensively in the lectures. Issues include objectives, measurements, manipulated inputs, disturbance inputs, continuous vs. batch (and semi-batch) and feedforward/feedback. As a homework problem, the students select a favorite activity and analyze it in detail from a control perspective.

**Review of Process Modeling for Control** This section is much shorter than in a standard course since the students completed a dynamic-systems course during the previous semester. Both fundamental and input/output models (obtained by step tests) are reviewed. An example homework problem is to develop a nonlinear model for a series of gas surge drums. The students form a state-space model via linearization, find transfer functions, and simulate the open-loop system using SIMULINK.

**Classical Feedback Control (PID)** The concept of PID control (in various forms) is presented, and the effect of the tuning parameters is discussed and illustrated by example. Traditional methods such as Cohen-Coon and closed-loop Ziegler-Nichols are covered. A typical homework assignment is a continuation of the previous modeling and simulation assignment (gas drums, for example), again using SIMULINK for closed-loop simulation. The students are encouraged to explore the robustness of their control-system designs.

**Direct Synthesis and Open-Loop “Control”** One issue stressed in this section is that, because of inherent performance limitations (right-half-plane zeros, time-delays), one cannot arbitrarily select any desired closed-loop response and yield a physically realizable (or internally stable) controller. We show how the open-loop control system design approach evolves to the internal model control structure when one accounts for disturbances and model uncertainty.

**Internal Model Control (IMC)** The IMC procedure is a major focus of the course and distinguishes the course text from other undergraduate

texts. Factorization of the model, inversion of the “invertible” portion of the model to form the ideal controller, addition of a filter for realizability, and tuning for robustness are all covered.

**IMC-Based PID Control** We show how to rearrange the IMC structure to the standard feedback structure, often resulting in a PID algorithm. The design procedure for open-loop unstable systems is also detailed. The control of a biochemical reactor at an open-loop unstable point is used as a homework problem.

**Frequency Response for Control-System Design** One of the main motivations for covering frequency response is that gain-margin and phase-margin concepts lead to a better understanding of robust control-system tuning. A typical homework problem involves steam drum level control.

**Control Using Multiple Measurements** Here we introduce feedforward and cascade-control design. Again, steam drum level control is often used for the homework problem. At this point in the semester, the students usually have a week with a lighter load because of student government elections. During this week we normally take a tour of the campus boiler house, pointing out the various control loops; it is clear to the students that an operator would not be able to operate the boilerhouse without feedback control.

**Implementation Issues** Important practical issues, such as variable scaling, proportional gain, installed valve characteristics, are covered in this section of the course.

**Decentralized Control** The relative gain array is introduced as a tool to help select variable pairings for decentralized multivariable control structures; distillation control problems of various sizes are used as illustrative examples. Students implement these techniques in their case studies.

**Multivariable Control** There is little time to provide detailed treatment for full multivariable control design. Usually, static and dynamic decoupling are covered; sometimes, multivariable IMC is also covered.

vanced control where we cover digital control and MPC.

## COMMUNICATION

A number of excellent process-control textbooks are currently available, but each lacks some of the features of the soon-to-be-published text,<sup>[3]</sup> such as

- In-depth coverage of the IMC procedure
- Connections between open-loop design and IMC
- IMC design for open-loop unstable systems
- Focus on MATLAB and SIMULINK

The course enrollment is typically large (roughly 120 students), which somewhat limits the type of faculty/student interaction that can occur in lectures, although we try to motivate as much discussion as possible by using a “Phil Donahue” approach. There are three 50-minute lectures per week, a 50-minute recitation by a teaching assistant, and a weekly computer lab for solving homework problems. Lectures contain a mix of analytical derivations and simulation results (the lecture hall is equipped with a workstation, a PC, a VCR, a computer/video projector, and two overhead transparency projectors).

Homework assignments are given weekly and are solved in groups of three; typical assignments are discussed in Table 1. The students are expected to provide a one-page written memo summarizing the results of the assignment. Working in groups improves the students’ interaction skills and enables more complex problems to be solved, and providing a written memo improves their communication skills. The homework assignments constitute 30% of the course grade. We place a high weighting on the homework assignments because we feel that students learn more about dynamics and control through interactive simulations (combined with analytical solutions) than analytical solutions alone.

MATLAB is the software package used for numerical analysis and simulation. The students have been introduced to MATLAB in the process-dynamics course, and it is sometimes used in the chemical engineering thermodynamics course. One of our first assignments directs the student to complete a tutorial review of MATLAB.

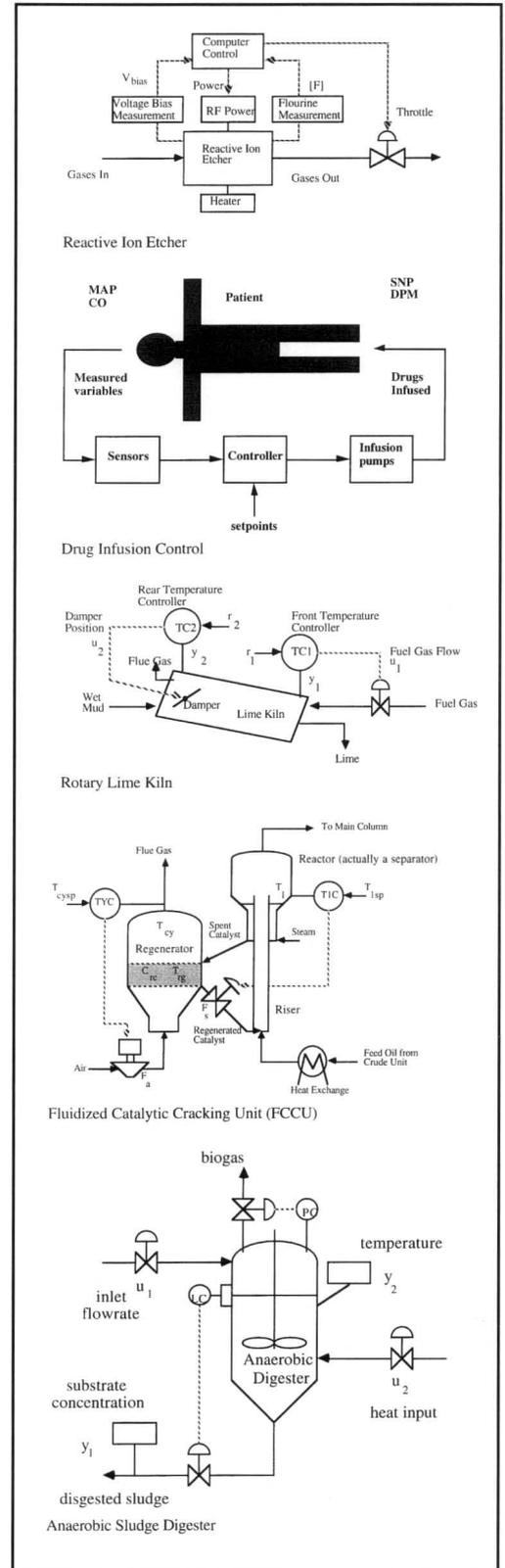
Rensselaer has an extensive network of roughly 500 workstations (IBM RS6000 and Sun SparcStations), with a site license for MATLAB/SIMULINK (as well as many other packages). We reserve a computer lab with thirty workstations for three nights a week. The lab is staffed by the instructor or a teaching assistant.

The course homepage is used as an additional venue for distributing material. Summaries of lecture notes, practice problems for exams, and tutorial modules in hypertext form, are made available on the course homepage. It can be found by linking to “Courses” from

<http://www.rpi.edu/~bequeb>

**TABLE 2**  
Control Case Studies

Mixing Tank (tutorial example)	Evaporator
Dowtherm Heater	Solution Copolymerization
Reactive Ion Etcher	Fluidized Catalytic Cracking Unit
Drug Infusion System	Wet Grinding Circuit
Rotary Lime Kilm	Anaerobic Sludge Digester



**Figure 1.** Case study instrumentation diagrams.

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***The projects are more open-ended than typical undergraduate assignments, provide more experience working in a group environment, and further develop written and oral presentation skills. . . . The case studies give [the students] the opportunity to “tie it all together” and to understand each component of a control-system design project.***

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An electronic newsgroup is used to answer common questions or to post notes about the lecture material. Rather than responding to many individual e-mail questions, a single posting to the newsgroup saves faculty and TA time. Also, it gives the students the capability of posing questions that can be answered by other students (this feature is not used as often as we would like).

The written examinations are fairly standard. Three one-hour exams (45% of the course grade) and a three-hour comprehensive final exam (25% of the course grade) are required. It would be nice to give some exams on the com-

puter, but thus far it has been too big of a challenge to organize for 120 students.

### CASE STUDY PROJECTS

In a typical semester, for the final course project we allow the students (in groups of three) to select from at least five different case studies on multivariable control. A breadth of applications are covered, from biomedical to classical chemical processes (see Table 2). Since the students are allowed to select from a variety of problems, they are more motivated and able to attach physical significance to the problem they study. During the most recent offering of the course, we decided to revise the case-study concept, placing more emphasis on it.

During the last half of the (spring 1997) process control course, the students worked in three-person teams on multivariable control projects that they selected from a choice of five systems: reactive ion etcher; drug infusion; rotary lime kiln; fluidized catalytic cracking unit (FCCU); and anaerobic sludge digester. Control diagrams for each of these case studies are shown in Figure 1. Each project was advised by a different member of an instructional team.

The students were given a brief description of each project. They selected their own teams of three students each and chose a project (project advisors were not designated until after the groups were selected). Each project included many phases typically associated with a control design project: literature review, model development and process identification, control structure selection and controller tuning for SISO systems, multiple SISO loop tuning, and decoupling. This approach gives the undergraduate student a sense of what an industrial control problem involves, including working in a project-team environment with a project advisor. It also gives the graduate students and teaching assistants experience in advising and teaching and reinforces many control-system concepts.

To illustrate the case study, we will use the reactive ion etcher example. The control diagram is shown in Figure 1 and suggested references are in Table 3. Descriptions of all case studies can be obtained by linking to “Educational Material” at the homepage found at

<http://www.rpi.edu/~bequeb.>)

#### ● Literature Review (1 week)

Students are given a brief description, with control instrumentation diagrams, for each of the projects. They form groups of three and perform a concise literature review to

**TABLE 3**  
**References for Five 1997 Case Studies**

General references for reactive ion etcher (suggested to the students)

- Bagwell, T.A., T. Breedijk, S.G. Bushman, S.W. Butler, S. Chatterjee, T.F. Edgar, A.J. Toprac, and I. Trachtenberg, “Modeling and Control of Microelectronics Materials Processing,” *Comp. Chem. Eng.*, **19**(1), 1 (1995)
- Lee, H.H. *Fundamentals of Microelectronics Processing*, McGraw-Hill, New York, NY (1990)
- Sze, S.M., *VLSI Technology*, McGraw-Hill, New York, NY (1988)
- Wolf, S., and R.N. Tauber, *Silicon Processing for the VLSI Era*, Lattice Press, Sunset Beach, CA (1986)

The model we use is modified from

- Rashap, B.A., M. Elta, H. Etemad, J.P. Fournier, J.S. Freudenberg, M.D. Giles, J.W. Grizzle, P.T. Kabamba, P.P. Khargonekar, S. Lafortune, J.R. Moyne, D. Teneketzis, and F.L. Terry, “Control of Semiconductor Manufacturing Equipment: Real-Time Feedback Control of a Reactive Ion Etcher,” *IEEE Trans. Semicond. Manuf.*, **8**(3), 286 (1995)

Models for drug infusion, lime kiln, FCCU, and an anaerobic digester are presented in

- Yu, C.L., R.J. Roy, H. Kaufman, and B.W. Bequette, “Multiple-Model Adaptive Predictive Control of Mean Arterial Pressure and Cardiac Output,” *IEEE Trans. Biomed. Eng.*, **39**(8), 765 (1992)
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- Alatiqi, I.M., A.A. Dadkhah, A.M. Akbar, and M.F. Hamouda, “Comparison Between Dynamics and Control Performance of Mesophilic and Thermophilic Anaerobic Sludge Digesters,” *Chem. Eng. J.*, **55**, B55 (1994)

provide background material on the unit operation of interest and the industry where this process is dominant. They write a concise memo, which is evaluated by the project advisor.

### Model Development (1 week)

A SIMULINK file, developed by the project advisor, is provided for each group. The open-loop diagram for the reactive ion etcher is shown in Figure 2. The actual model for the etcher is shown, in *unmasked* form, in Figure 3. Notice that constraints, time-delays, and noise are included. To develop a model that will be used for control system design, the students perform open-loop step tests. Example results are shown in Figure 4.

The groups provide a short memo (with plots and transfer functions attached), summarizing the modeling results. The advisor evaluates the memo and makes suggestions for additional modeling studies, if necessary.

### SISO Controller Design (1 week)

In this phase, the groups perform independent SISO control design, usually pairing the loops based on physical considerations. They use one or more of the techniques covered in the course (IMC-based PID is the most popular choice). The groups prepare a short written report describing their results. It is important here that the project advisor catch obvious mistakes before the groups close both loops simultaneously.

### MV-SISO Controller Design (1 week)

Here the groups use the relative gain array (RGA) to gain insight about variable pairing and how independently designed loops need to be retuned when both loops are closed. Failure sensitivity is considered very important in this phase; if one loop fails (is opened or saturates), the other loop should not go unstable. Advisor comments on the memo report assist the groups in preparing the final written report.

### Final Written Report (1 week)

This is a formal written report with the structure of a typical technical paper. Much of the material can be gathered (with some rewriting) from previously written memo reports. Most groups also take the time to perform “full” multivariable control studies, such as static and/or dynamic decoupling.

### Oral Presentation (1/2 week)

Each group prepares a fifteen-minute oral presentation (plus five minutes for questions) that is evaluated by the project advisor and at least one other evaluator. This gives the students a chance to enhance their oral presentation skills. Also, it is much easier for the project advisor to see what the students really learned from the experience and to provide immediate feedback.

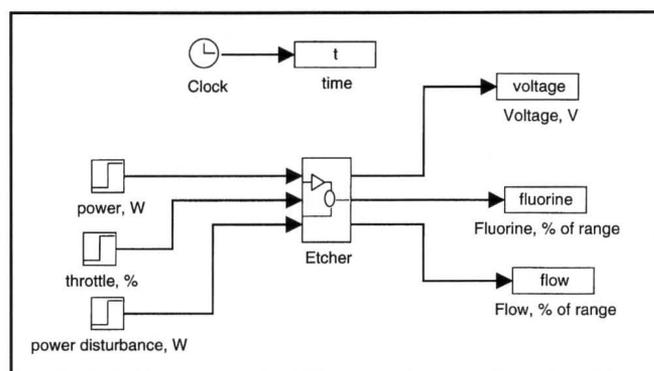


Figure 2. SIMULINK diagram for open-loop tests.

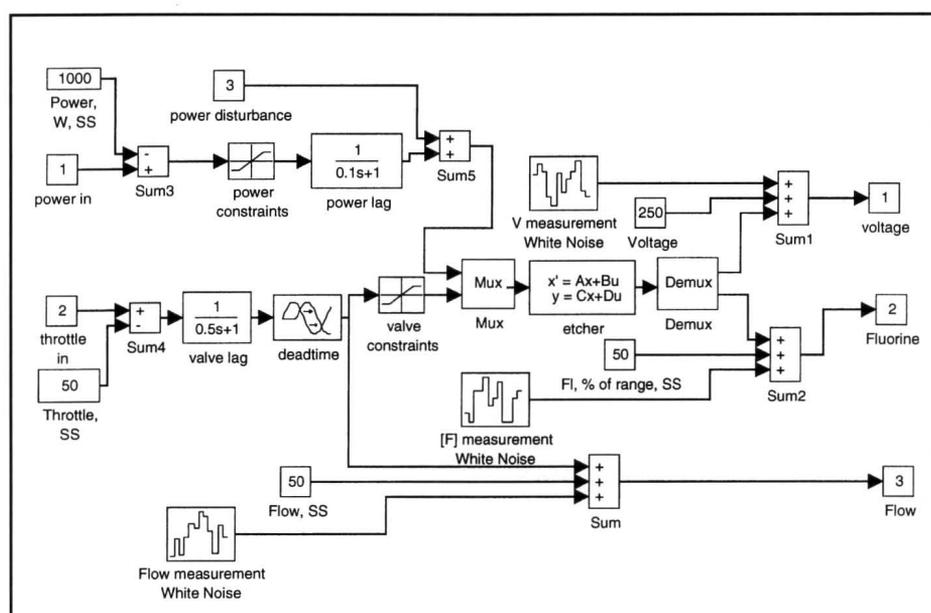


Figure 3. Etcher unmasked.

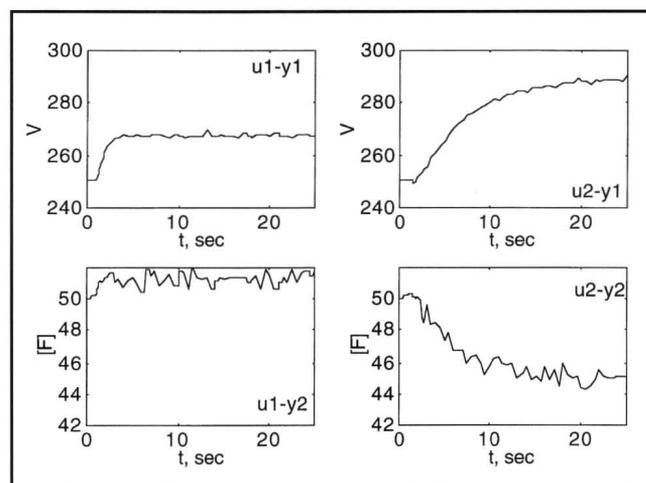


Figure 4. Step responses.

## GENERAL COMMENTS

We found that many students have no idea how to perform a literature review. Often, an internet search was conducted using a web-crawler (Alta Vista or a similar program). Approximately one-half of the literature reviews consisted of a rambling essay about motivation or previous work, with no specific citations of the literature. We asked a number of groups to revise their literature review.

Clearly, our case studies in multivariable control require a lot of effort and coordination of all members of the instructional team. It is important to have a robust simulation set-up for the students to perform their initial identification tests. It is also important to provide rapid feedback. Groups generally turned in their memo reports on Friday, and we usually evaluated them and returned them to the students on Monday.

Comments from the undergraduate students have generally been favorable. The case studies give them the opportunity to "tie it all together" and to understand each component of a control-system design project. It should also be noted that the role of the case-study advisors shifts during the projects, ranging at various times from boss to intelligent co-worker to all-knowing judge and inquisitor.

## FUTURE TEACHING EFFORTS

Currently, the control course has been taught in a fairly traditional lecture/recitation/computer-lab format, with three lectures and one recitation per week. The recitation typically covers the assignment for that week or reviews a recent exam. Students are also expected to participate in one computer laboratory session per week.

There is a move in the Rensselaer curriculum toward "studio" or "workshop" learning, where students meet twice a week for two-hour sessions with a faculty member and one or two teaching assistants. The idea is for the students to learn interactively by solving problems rather than by passively listening to lectures. Rensselaer is currently renovating or constructing a large number of classrooms to fit the studio format, with student workstations (not just computers) where students can interact and solve problems in groups. The instructor or teaching assistant can give "mini-lectures" as groups encounter common stumbling blocks or can provide more background material as needed.

Since the dynamics and control sequence is taught during the junior year, it offers an excellent opportunity to consider process control implications in the process-design course. We plan to do this as process-flowsheeting packages begin to have dynamic extensions that are relatively easy to use.

## SUMMARY

We have presented an approach to using case-study projects in a process control course. The projects are more open-ended than typical undergraduate assignments, provide more experience working in a group environment, and further

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develop written and oral presentation skills. In addition to the learning experience for the undergraduates, we have found that the teaching assistants, the graduate students, and the instructor also learn from the approach.

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## BOOK REVIEW: *Mathematical Methods*

*Continued from page 189*

takes a fairly classical approach, and the authors dig into first-order partial differential equations in Chapter 6 with relish. They offer a particularly thorough treatment of the subject replete with examples of waves, shocks, and weak solutions. This is obviously a favorite topic of the authors, and many chemical engineers dealing with packed bed or chromatographic separations will find meaty bones to chew on in Chapter 6.

Fourier and Hankel transforms are covered in Chapter 7, but the applications to the vibrating circular membrane and semi-infinite strips and cylinders are not particularly stimulating for the chemical engineer. The applications of Laplace transforms in Chapter 8 are probably of greater relevance to chemical engineers.

Although the references at the end of each chapter are not extensive, they are well thought out and direct the interested reader to more comprehensive treatments of the subjects. The variety of mathematical tools useful to chemical engineers is reasonably well covered, and the authors point out that they felt it necessary to exclude complex variables, statistics, and numerical methods. It would have been reasonable to include a short summary of similarity analysis because similarity solutions are so often encountered in fluid mechanics and heat and mass transport processes. An instructor may wish to supplement the book with examples of similarity analysis.

Some of the chapters are beyond the abilities of many undergraduates, but chemical engineering graduate students would profit greatly by working through the entire nine chapters. I plan to use this text in my graduate course in mathematical methods applied to chemical engineering, replacing Hildebrand's widely used book *Advanced Calculus for Applications*, because it is necessary to supplement Hildebrand's book with chemical engineering applications. Varma and Morbidelli do this well and at a cost that is reasonable.

One finds that the book has been carefully proofread, for it is difficult to find typographical errors. The figures are simple and uncluttered, and they are entirely adequate to illustrate the relevant mathematics. There is a good set of problems at the end of each chapter, and many chemical engineering applications are incorporated in these problems.

The rigor and sophistication of this book go well beyond the few competing texts that claim to be advanced mathematics for chemical engineers, and I can add my humble imprimatur to those of Professors Amundson and Aris who encouraged the authors to write this book. □

# TEACHING ANTIWINDUP, BUMPLESS TRANSFER, AND SPLIT-RANGE CONTROL

SERENA H. CHUNG, RICHARD D. BRAATZ

University of Illinois at Urbana-Champaign • Urbana, IL 61801-3792

Providing fast and smooth transitions during discrete process changes is of high industrial importance. For example, in polymerization, production runs for a particular polymer are typically of limited duration, and the reactor conditions must be modified to produce a different grade or type of polymer. Another type of discrete process change occurs when a controller output saturates. *Reset windup* is said to occur when the controller continues to integrate the error signal during saturation, causing large overshoots and oscillations.

Discrete process changes also occur during *split-range control*, in which different manipulated variables become active in different operating regimes. Split-range control is useful when more than one manipulated variable is required to span the whole range of setpoints.<sup>[1-3]</sup> Controllers that provide smooth transitions during discrete process changes are said to provide *bumpless transfer*.

Although industrial control systems must be designed to

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*... students are rarely taught in their undergraduate process control courses how to address such [discrete process change] problems. This paper serves to close this [educational] gap...*

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handle such discrete process changes, students are rarely taught in their undergraduate process control courses how to address such problems. This paper serves to close this gap in the education of undergraduate chemical engineers. The paper is distributed as a reading assignment to students in the undergraduate chemical process control course at the University of Illinois, and the material is discussed during the lecture immediately after the students have covered feedforward, ratio, and cascade control.

First, the students are introduced to the process model of a laboratory apparatus for collecting permeation data for thin polymer films.<sup>[4]</sup> The temperature must be controlled to very high accuracy for the apparatus to provide accurate measurements of diffusion coefficients. The students are taught to control the process using multiple digital Internal-Model-Control-Based Proportional Integral Derivative (IMC-Based PID) controllers in the velocity form.

For homework, the students are required to derive the control algorithm, to simulate closed-loop responses using different controller-tuning parameters, and to propose and discuss potential improvements (see Table 1 for the homework assignment). The students are also required to compare the closed-loop response of their best controller to that obtained by a default controller that was implemented on the real apparatus.<sup>[5]</sup> Although this paper focuses on IMC-Based PID control, the homework assignment can be readily modified to teach other controller design methods.

**Richard Braatz** received his BS from Oregon State University and his MS and PhD from the California Institute of Technology. After a postdoctoral year at DuPont, he became an assistant professor of chemical engineering at the University of Illinois. His main research interests are in the modeling and control of complex systems.



**Serena Chung** received her BS in chemical engineering from the University of Illinois, Urbana-Champaign in 1998 and plans to pursue a PhD in chemical engineering. Her current research interests are in the modeling and control of crystallization.

The advantages of using this control problem for training students are

- The process dynamics and performance specifications are based on a real system.
- The two operating conditions are substantially different (there are significant changes in time delay, gain, and time constant).
- A practical control algorithm is provided that can be easily implemented in a process control laboratory or in industry.
- A MATLAB program simulating the process and the classical control algorithm is available via the Internet.<sup>[6]</sup>

## PROBLEM STATEMENT

Precise control of the temperature,  $T$ , of a sample containing a thin polymer film is required to provide accurate measurements of the diffusion coefficient.<sup>[4]</sup> The manipulated variable is the power to a heating tape that surrounds the polymer sample. Heat sinks allow the temperature of the sample to be reduced quickly. For temperatures below 30°C, the heat sink is distilled water, and for higher temperatures, the heat sink is gaseous nitrogen. The advantage of the gaseous-nitrogen heat sink over the liquid-water sink is that

it allows a wide range of temperatures to be covered by only manipulating the heating power. The distilled-water sink provides a more stable response for temperatures under 30°C.

The heat sinks are at room temperature, which is approximately 21°C with slow variations up to  $\pm 1^\circ\text{C}$ . For each heat sink, temperature responses to step changes in heating power were taken at a variety of operating conditions along the desired temperature trajectory in order to estimate the importance of nonlinearity. The process responses were linear for each heat sink, with the transfer functions given by

$$P_1(s) = \frac{1.0 e^{-2.4s}}{9.5s + 1} \quad (1)$$

for the gaseous-nitrogen heat sink ( $T > 30^\circ\text{C}$ ), and

$$P_2(s) = \frac{0.068 e^{-1.4s}}{1.7s + 1} \quad (2)$$

for the liquid-water heat sink ( $T < 30^\circ\text{C}$ ), where the time constants,  $\tau_i$ , and time delays,  $\theta_i$ , are measured in minutes, and the process gains,  $K_i$ , are measured in  $^\circ\text{C}/\%$  power. The heating power is constrained between 0 and 100%. At steady state, the sample is at room temperature when the heating power is turned off.

The goal of the closed-loop system is to smoothly ramp the temperature from stable operations at 120°C to 25°C (see Figure 1a). For reproducible collection of diffusion data, the temperature must stay within 0.5°C of the setpoint 70 minutes before and 50 minutes after the ramp, and within 1.5°C throughout the ramp. The control algorithm must provide bumpless transfer between the radically different process

**TABLE 1**

**Homework Assignment  
Antiwindup, Bumpless Transfer, and Split-Range  
Control**

(The textbook referred to in Problem 2 is Ref. [1], Handout A is Ref. [5], Handout B is this paper.)

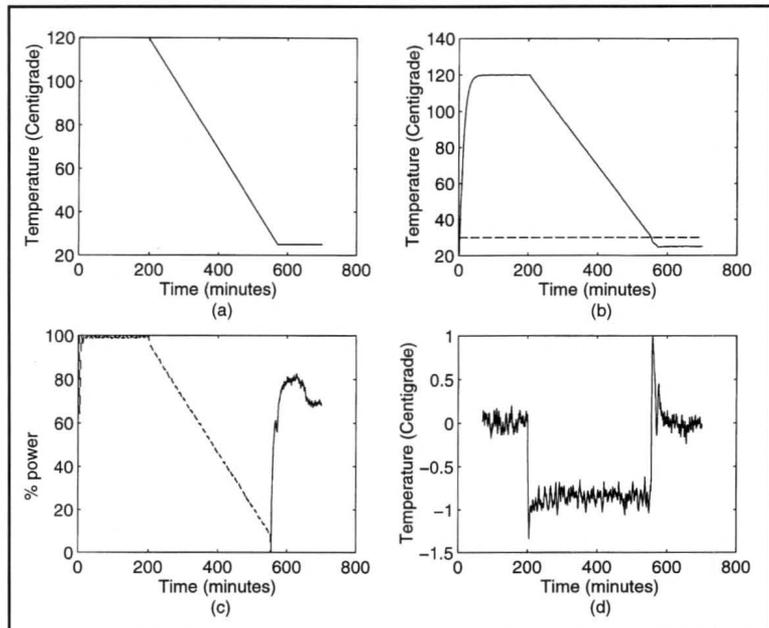
**Problem 1.** In Handout B, derive Equations (7) and (8) from Equation (6).

**Problem 2.** Draw a block diagram for the split-range control problem described on page 583 of the textbook. Describe the differences and similarities between this control problem and the control problem described in Handout B.

**Problem 3.** Use Netscape to download the MATLAB program `bump.m` from <http://brahms.scs.uiuc.edu/~erp/lssrl/software>. This program implements the two IMC-based PID controllers and the process models described in Handout B. Implement several values of the IMC tuning parameter  $\lambda$ , and select the  $\lambda$  that gives the best overall performance. Justify your selection.

**Problem 4.** Implement the IMC-tuning parameters listed in Equation (20) of Handout A in the MATLAB program. Select  $\lambda$  to give the best overall performance. Compare the performance for this controller with the best performance reported in Problem 3. List conditions for which the IMC tuning parameters in Handout A are expected to provide superior performance. Propose and discuss modifications that could improve your best control algorithm.

**Problem 5.** Compare your best closed-loop response to that in Figure 1 of Handout B. Discuss.



**Figure 1.** (a) Setpoint; (b) closed-loop temperature tracking (—) and transition line between heat sinks (---); (c) power output from the nitrogen (---) and water (—) heat sinks; (d) difference between setpoint and controlled variable.

behaviors, Eqs. (1) and (2), that result when the temperature crosses 30°C, while satisfying the constraints on heating power. This control problem is referred to in industry as a *split-range control problem*.<sup>[1]</sup>

## CONTROL ALGORITHM

One strategy is to design an Internal-Model-Control (IMC)-Based Proportional-Integral-Derivative Controller (PID) with a filter for each process transfer function, implement the controllers in digital velocity form, and switch controllers when the heat sinks are changed. Figure 2 is the block diagram of the system. The continuous-time transfer function for an IMC-Based PID controller is<sup>[7-9]</sup>

$$k(s) = K_c \left( 1 + \tau_D s + \frac{1}{\tau_I s} \right) \frac{1}{\tau_F s + 1} \quad (3)$$

where

$$K_c = \frac{2\tau + \theta}{2K(\lambda + \theta)}; \quad \tau_I = \tau + \frac{\theta}{2}; \quad \tau_D = \frac{\tau\theta}{2\tau + \theta}; \quad \tau_F = \frac{\lambda\theta}{2(\lambda + \theta)} \quad (4)$$

The IMC tuning parameter  $\lambda$  provides a trade-off between speed of response and the robustness of the closed-loop system to measurement noise and inaccuracy in the model.

The time domain expression for the controller is

$$\tau_F \frac{du}{dt} + u(t) = u(0) + K_c \left( e(t) + \tau_D \frac{de}{dt} + \frac{1}{\tau_I} \int_0^t e(\tilde{t}) d\tilde{t} \right) \quad (5)$$

where  $e$  is the difference between the setpoint  $r$  and measured variable  $m$ . To avoid *derivative kick*,<sup>[2]</sup> the derivative of the error  $e=r-m$  is replaced with the derivative of the measured variable  $m$  to give

$$\tau_F \frac{du}{dt} + u(t) = u(0) + K_c \left( e(t) - \tau_D \frac{dm}{dt} + \frac{1}{\tau_I} \int_0^t e(\tilde{t}) d\tilde{t} \right) \quad (6)$$

By approximating the integral by a summation and the derivatives by a first-order backward difference, and rearrang-

ing, we arrive at the control algorithm in digital form

$$u_n = \frac{u_0}{1 + \tau_F / \Delta t} + \frac{\tau_F / \Delta t}{1 + \tau_F / \Delta t} u_{n-1} + \frac{K_c}{1 + \tau_F / \Delta t} \left( e_n - \tau_D \frac{m_n - m_{n-1}}{\Delta t} + \frac{\Delta t}{\tau_I} \sum_{k=1}^n e_k \right) \quad (7)$$

where

$\Delta t = t_n - t_{n-1}$  sampling time

$u_n$  value of the manipulated variable (% Power) that is held constant between times  $t_n$  and  $t_{n+1}$

$m_n, e_n$  defined similarly.

Writing Eq. (7) for the  $n-1$  sampling instance and subtracting gives what is referred to as the velocity form of the algorithm:

$$u_n = u_{n-1} + \frac{\tau_F / \Delta t}{1 + \tau_F / \Delta t} (u_{n-1} - u_{n-2}) + \frac{K_c}{1 + \tau_F / \Delta t} \left( e_n - e_{n-1} - \tau_D \frac{m_n - 2m_{n-1} + m_{n-2}}{\Delta t} + \frac{\Delta t}{\tau_I} e_n \right) \quad (8)$$

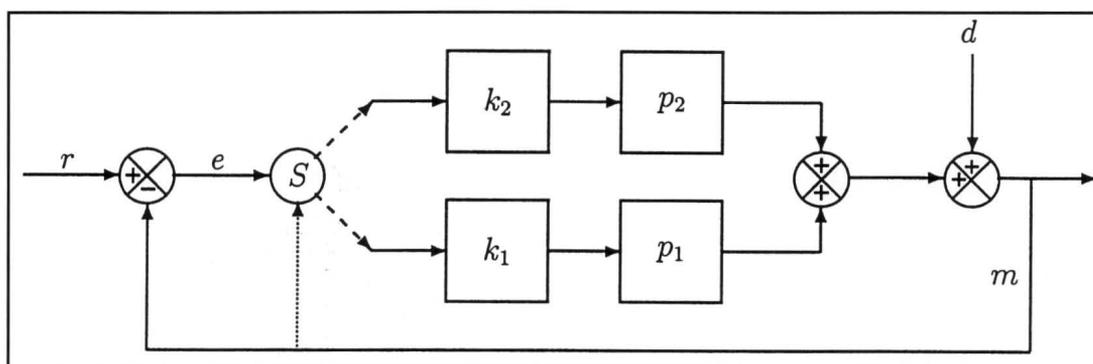
The main advantage of implementing the controller in this form is that it will not integrate the controller error when the manipulated variable reaches a constraint (for example, 0 or 100% power). For this reason, the controller will also perform better during transitions between different operating conditions—that is, it will provide *bumpless transfer*. The sampling time was selected as  $\Delta t = 0.1$  minute, which is consistent with well-known rules-of-thumb.<sup>[1]</sup> The IMC tuning parameter was selected to be  $\lambda = 1.0$  minute to give fast uniform closed-loop response throughout the temperature ramp. Disturbances on the output were modeled as integrated white noise, given by

$$d_0 = \beta \gamma_0 \quad (9)$$

and

$$d_k = d_{k-1} + \beta \gamma_k \quad (10)$$

where the  $\gamma_k$ 's are normally distributed random numbers.



**Figure 2.** Block diagram. The setpoint signal is  $r$ , the error signal is  $e$ , the measured temperature is  $m$ , and the effect of the disturbances on the temperature is  $d$ . The selector  $S$  switches between the controllers  $k_1$  and  $k_2$ , depending on the value of the measured temperature.

The coefficient  $\beta$  was set to 0.013, to be consistent with the open-loop step tests for the apparatus.<sup>[4]</sup>

## CLOSED-LOOP RESPONSE

A simulation of the closed-loop temperature response to programmed step and ramp trajectories is shown in Figure 1 (the program producing the plot is available from the World Wide Web<sup>[6]</sup>). The simulated response is very similar to the experimental response shown in Figure 3.6 of Drake.<sup>[4]</sup> If disturbances had been better modeled as entering the process input, then the alternative IMC-Based PID controllers derived in [5,7] would provide improved performance. A slightly more complex IMC controller would be used [7,9] if zero offset in tracking the ramp had been required.

## CONCLUSIONS

The model of a polymer-film-diffusion apparatus was used to teach the design of controllers that can handle discrete process changes. An available MATLAB code<sup>[6]</sup> demonstrates that two digital IMC-Based PID controllers, implemented in velocity form that switch during transitions between operating regimes, provide high performance for this problem. This paper and the MATLAB program are provided with the hope it will encourage teaching the design of such controllers in undergraduate courses in process control.

## ACKNOWLEDGMENTS

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## CHEMICAL ENGINEERING THERMODYNAMICS

by Y.V.C. Rao

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Reviewed by

Thomas E. Daubert

Pennsylvania State University

This beginning intermediate text is a welcome addition to the limited number of texts appropriate to entry-level chemical engineering courses. While the major emphasis of the book is for use in the classroom, employment by more advanced students and practitioners is suggested and is justified by the breadth of material included.

Each chapter of the book begins with a set of learning objectives that is more helpful than the usual one-or-two paragraph introduction informing the reader of a chapter's content. At the end of each chapter, a quantitative summary reviews the material, including the important definitions and equations. A set of review questions (primarily qualitative but sometimes requiring a calculation) and a set of problems pertinent for class use complete each chapter.

The fourteen chapters of the book proceed logically from basic definitions and concepts to more complex topics, but do not become lost in esoteric arguments of little use to undergraduates. Chapters 1 and 2 give the basic definitions of both thermodynamics itself and primary concepts such as systems, processes, properties, energy types, and equilibrium, together with the units used for thermodynamic calculations. Review questions and problems support the text in prompting the student to make sure they understand the material.

Chapter 3, on PVT relations of fluids, discusses real fluids together with ideal gases as a preparation to their use for later application to calculations using the first and second laws. The selection of relations includes the progression of cubic equations from van der Waals to the various modified Redlich-Kwong equations, as well as the virial equation and Pitzer corresponding states. The selection is in line with current industrial use and what I myself would recommend.

The first law treatment is classical, beginning with calculations of various types of processes for ideal and nonideal gases as well as steam. Treatment of control mass and control volume analysis for transient flow processes is much more thorough, but also more understandable than most treatments. Standard thermochemical calculation methods are also included.

The second law treatment in Chapter 5 is again classical, with a good comparison of heat engines and heat pumps and methods for calculation of entropy. Control volume analysis and efficiency calculations are brief, but unusually clear.

In Chapter 6, the mathematical analysis of the state principle, the criteria for equilibrium, the Gibbs-Duhem equation, and the derived energy properties, in my opinion, need not be as difficult as they are presented. This is the only chapter that absolutely needs its summary for understanding and relevance.

Relations among properties and their manipulation by Jacobians

Continued on page 237

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 which elucidate difficult concepts. Please submit them to Professor James O. Wilkes (e-mail: wilkes@engin.umich.edu) or Mark A. Burns (e-mail: maburns@engin.umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

# AN INTRODUCTION TO PROCESS FLEXIBILITY

## *Part 2: Recycle Loop with Reactor*

W. E. JONES, J.A. WILSON

*University of Nottingham • Nottingham, NG7 2RD, England*

An earlier article<sup>[1]</sup> discussed teaching flexibility via a simple heat-exchange problem. Heat exchange is a convenient starting point for flexibility teaching because the equations and resulting calculations are easy to handle. Other process operations can rapidly become complex and a rigorous treatment very demanding.<sup>[2]</sup> Hence it is pleasing to find that a potentially complex recycle loop with reactor can be simplified to provide a thought-provoking, process-flowsheet-based exercise that emphasizes understanding of the system's operation.

It is important to stress, even with simplification, that the recycle loop is still a much broader example than that for heat exchange, making the exercise more suitable as a basis for project work or a discussion question. One of the authors first became interested in the problem when attempting to explain the operating bounds of an ammonia or methanol synthesis loop during the course of final-year design projects. The reactor used in this exercise is a simpler design than commonly found in ammonia and methanol plants, but the exercise still illustrates many of the issues that make design and operation of such process systems so interesting.

### BACKGROUND

The exercise considers a reversible exothermic reaction taking place in the gas phase over a catalyst in an adiabatic

reactor. The reactor is part of a recycle loop where product is separated from the reactor effluent and unreacted feed is recycled (see Figure 1). It is well known that when designing recycle loops, an economic optimum exists for reactor conversion that balances reactor size against the combination of product separation load and circulation rate.

Having chosen the design conversion, the circulation rate is an immediate consequence in order to meet the required



**Warren Jones** holds BSc and PhD degrees in chemical engineering from the University of Nottingham and is a registered Chartered Engineer. He has a wide-ranging interest in both front-end process and detailed plant design, developed initially through nine years of experience with a major engineering and construction company. Teaching responsibilities include several design courses, and engineering thermodynamics.



**Tony Wilson** holds BSc and PhD degrees in chemical engineering from the University of Nottingham. With industrial and consulting experience in process control and batch process engineering, and with active research in both fields, he coordinates the department's research in computer-aided process engineering and is responsible for process control teaching at the undergraduate level.

production. The choice of reactor operating temperature is also important and may be optimized by the designer as part of the reactor size-separation load/circulation rate trade-off.

In the case of reversible exothermic reactions, selection of

a relatively low temperature permits a higher conversion, but this must be balanced against a slower rate of reaction leading to a large catalyst inventory. The design conversion for reversible exothermic reactions often approaches quite closely the upper bound imposed by thermodynamics.

Finally, the temperature will increase through the catalyst bed, but a single temperature value is needed to characterize operation; for this we will use inlet temperature. It is assumed that reactor inlet temperature can be adjusted independently.<sup>[1]</sup>

For a flexibility study, the catalyst inventory and other equipment will be fixed; we are interested in investigating how the plant will perform under alternative operating conditions.

From the earlier discussion, two obvious parameters to characterize operation are circulation rate and reactor inlet temperature. As noted before, the reactor inlet temperatures can be adjusted to maximize production for fixed circulation rate (illustrated in Figure 2a.<sup>[3]</sup>).

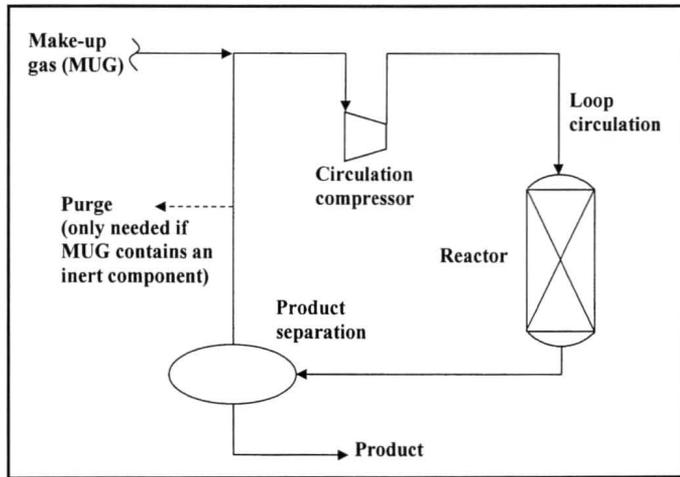


Figure 1.

To the left of the maximum, increasing inlet temperature improves the rate of reaction, leading to more production. But as the temperature increases, the deteriorating equilibrium conversion imposed by thermodynamics “bites,” and production peaks. Operation at the optimum inlet temperature ensures that the minimum circulation rate to meet production is being used; we assume the optimum temperature to be selected in each case.

A typical industrial example is more complex and involves four additional considerations:

- Catalyst deactivation
- Producing circulation around the loop
- Loop pressure
- Presence of an inert component in the make-up gas

The catalyst can be deactivated in several ways.<sup>[4]</sup> Here, we are more interested in the overall effects of deactivation than we are in the details of one particular mechanism, so we adopt a simple model—namely, uniform deactivation throughout the catalyst inventory. The normal response to loss of production through catalyst deactivation is to raise the reaction rate by increasing the inlet temperature. For reversible exothermic reactions, however, this action further limits the conversion, and unless the circulation rate is also increased, the production target will not be met.

The effects of catalyst deactivation are demonstrated in Figure 2b, which compares performance at beginning-of-run (BOR) and end-of-run (EOR). Note particularly that the BOR circulation rate is

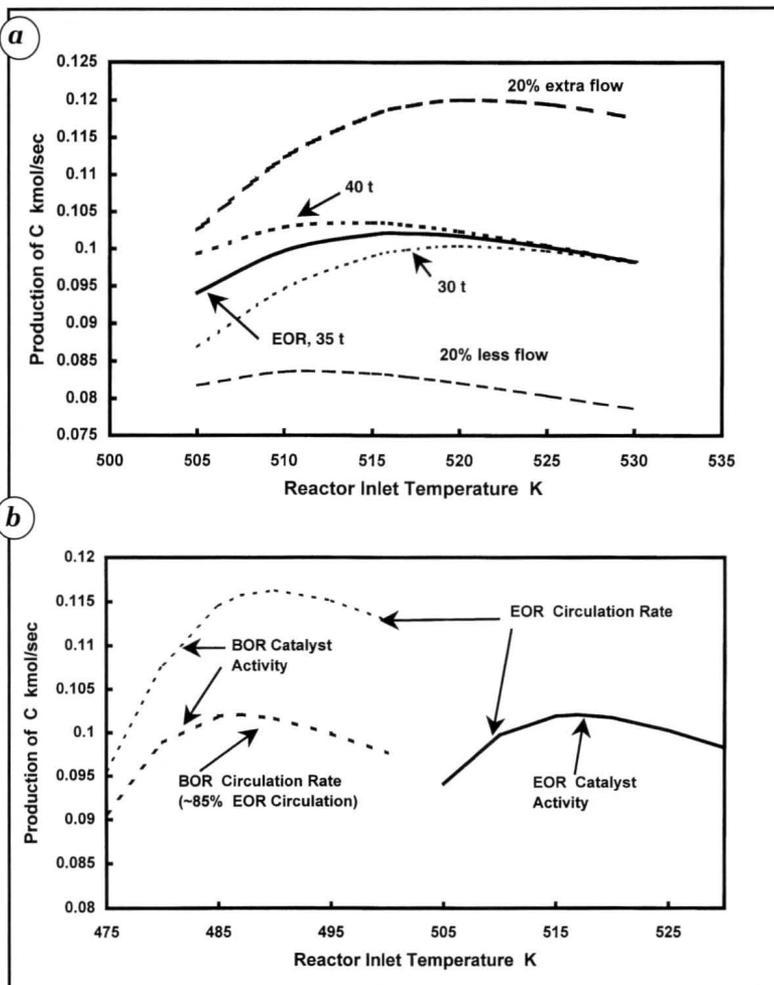


Figure 2.

**Parts 1 and 2 of this paper introduce flexibility by providing exercises that force the student to consider how the system will actually operate—this is an important first step for developing a robust design. Further, a wide-ranging knowledge of basic chemical engineering is required, making these exercises (particularly Part 2) ideal as the basis for project work.**

15% less than that for EOR; if the EOR circulation rate were implemented at BOR, overproduction would result.

Normal design practice would be to set the loop process parameters for EOR operation, but producing a design sufficiently flexible to operate at BOR is clearly very desirable. Loop circulation is normally produced using a variable speed centrifugal compressor, so compressor characteristics become important in meeting process flexibility.

Centrifugal compressor characteristics are represented by a head-capacity curve and, for recycle systems (where the loop pressure drop is 10% or less of the nominal operating pressure) the loop can be treated as one of constant density, and the compressor characteristics will have roughly the same shape as those obtained for centrifugal pumps.

Figure 3 shows the operating point to be defined where the system curve intersects the compressor characteristic; for a recycle loop the system curve is based solely on friction losses because the discharge returns to the suction.

Also shown in Figure 3 is the implementation of reduced circulation rate via compressor speed reduction. The affinity laws<sup>51</sup> can be applied to relate compressor performance at different speeds. Sometimes the speed reduction required is quite large, taking the compressor close to a critical speed, which induces synchronous whirling of the shaft; this condition must be avoided and hence places a lower bound on operation.

Typically, critical speeds are found in the range of 60 to 80% of normal running speed. Two other constraints that arise from compressor operation are

- Maintenance of sufficient volumetric flowrate through the machine to avoid surge; for a low-head compressor (as considered here) this constraint will lie well to the left on the head-capacity curve (around 50% of normal capacity) and hence will not be influential.
- Overspeed trip, typically set at 10 to 15% above the normal running speed; this constraint obviously “bites” for operating modes requiring higher circulation rates.

The constraints imposed by compressor operation lead to the third parameter that required further consideration—namely,

loop pressure. Varying loop pressure is helpful when matching compressor operation to process requirements because

- A reduction in loop pressure increases the circulating gas specific volume; hence, circulating the same quantity of gas would require a faster compressor speed to cope with the larger volumetric flowrate, i.e., moving operation away from the critical speed.
- If the reaction is one where there is volume reduction as the reaction proceeds, pressure reduction will give a lower, thermodynamic limited, conversion, and this will lead to a larger circulation rate and a move away from the critical speed.

The loop pressure cannot be set independently, however. In a simple example where the feed contains no inert component, the rate of reactant consumption (in the reactor) must balance the rate of make-up gas (MUG) flow into the loop in order for the pressure to remain steady. In other words, at steady-state, the reactor inlet temperature and circulation rate (combined with the pressure) must give a reaction rate that just balances the MUG rate. If the circulation rate, say, were smaller, the loop would equilibrate at a higher pressure with the extent of the pressure increase being limited by the relief valve setting on the loop.

Finally, we need to consider an inert component in the MUG. In many industrial examples, the MUG to the synthesis loop is not pure reactant, but contains 1 to 2% by volume of an inert component. Unless the inert is removed, it will accumulate in the loop and slow the rate of reaction. In a pressurized loop, some inert will dissolve in the product, but

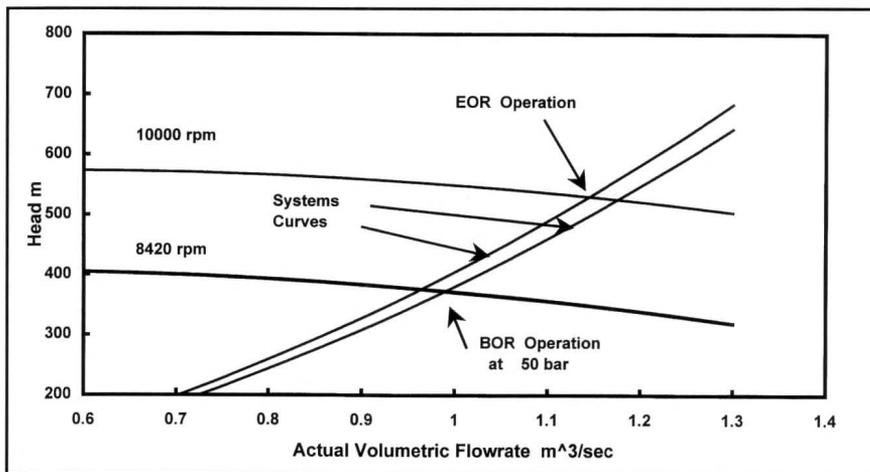


Figure 3.

most has to be purged from the loop (see Figure 1). A relatively high purge rate ensures the inert composition in the recycle loop is low and the rate of reaction high for the pressure because the inert has only a small diluting effect. A high purge rate, however, results in a large reactant loss and, in design mode, setting the purge rate is an economic optimization that adds the third dimension of MUG rate to the reactor size- separation load/circulation-rate balance already discussed.

From a flexibility viewpoint, recycle loops with purge can fully exploit the interacting trio of parameters (circulation rate, reactor inlet temperature, and pressure) because pressure can now be set independently via the purge rate rather than being a consequence, as previously noted.

To illustrate, if the loop is initially at steady state, reducing the purge rate causes the inert composition to increase, so the loop pressure must increase to restore the reactant partial pressures. There will be a compensating reduction in MUG demand. If the circulation rate is also increased, it will limit the change in pressure needed.

In view of the complexity added by considering an inert in the MUG, the main part of the exercise concentrates on pure MUG; handling an inert in the MUG is considered at the end of the exercise.

## PROBLEM STATEMENT

The reversible exothermic chemical reaction



takes place in the gas phase over a fixed catalyst bed in a reactor operated adiabatically. The reaction data are summarized in Table 1. The reactor forms part of a recycle loop (shown in Figure 1) where C is totally separated from the reactor effluent. For the first three parts of the exercise, you may assume the make-up gas contains only A and B in

**TABLE 1**  
**Reaction Data for the Exercise**

Heat of reaction = -14000 kJ per kmol of C formed

Rate of production of C by the forward reaction =  $k_F P_A P_B$

where

$$k_F = \text{BOR rate constant, kmol sec}^{-1} \text{ bar}^{-2} \text{ (kg of catalyst)}^{-1}$$

$$k_F = 100 \exp(-94000/8.314 T)$$

Rate of destruction of C by the reverse reaction =  $k_B P_C$

where

$$k_B = \text{BOR rate constant, kmol sec}^{-1} \text{ bar}^{-1} \text{ (kg of catalyst)}^{-1}$$

$$k_B = 525000 \exp(-108000/8.314 T)$$

$P_A, P_B, P_C$  = partial pressures of A, B, and C, bar

T = absolute temperature of the reacting mixture, K

Specific heat capacities:  $C_{PA}, C_{PB}, C_{PC} = 30, 40, 70 \text{ kJ kmol}^{-1} \text{ K}^{-1}$

stoichiometric proportions (mixture RMM=50); hence the recycle stream also contains only A and B, and the purge flowrate will be zero.

The recycle loop at end-of-run (EOR) is designed to operate at a nominal pressure of 50 bar, with a circulation rate through the reactor of  $2.2 \text{ kmol sec}^{-1}$ . The EOR loop pressure drop is 5 bar; this comprises 4 bar for all equipment excluding the reactor and 1 bar for the reactor. The EOR reactor pressure drop may be further decomposed:

- *Pressure drop (based on EOR circulation rate) for reactor if catalyst were in good mechanical condition: 0.7 bar*
- *Allowance (based on experience) for catalyst particle breakdown and loss of voidage: 0.3 bar*

Circulation through the reactor is provided by a single-stage centrifugal compressor whose head ( $H_C, \text{ m}$ ) - capacity ( $Q, \text{ m}^3 \text{ sec}^{-1}$ ) characteristic at 10,000 rpm is represented by

$$H_C = 530.5 + 149.52 Q - 130.585 Q^2$$

The exercises below examine the process flexibility requirements for the synthesis loop as the catalyst inventory of 35000 kg slowly deactivates. Catalyst deactivation is modeled by assuming EOR  $k_F$  and  $k_B$  values are only 30% of those applying at BOR (see Table 1).

You may assume the heat exchanger arrangements on the reactor feed have sufficient flexibility to produce a wide range of reactor feed temperatures and the compressor suction operates at  $40^\circ\text{C}$ . Also, assume the reactants A and B have negligible solubility in the product.

- 1) Determine the maximum production of C achievable at EOR conditions by varying the reactor inlet temperature.
- 2) You wish to achieve the same production rate of C as that calculated in (1), but using BOR catalyst.
  - a) Calculate the circulation rate required if the loop pressure remains at 50 bar.
  - b) If the circulation rate is maintained at  $2.2 \text{ kmol sec}^{-1}$ , at what pressure would the loop need to operate?
  - c) Use the insight you have gained from solving 2(a) and (b) to explain the interrelationship between loop pressure, circulation rate, and reactor inlet temperature. How might you exploit this flexibility to deal with variation of catalyst activity?
- 3)
  - a) Confirm the compressor speed of 10,000 rpm will satisfy EOR operating conditions.
  - b) Determine the compressor speed for 2(a).
  - c) Determine the compressor speed for 2(b).
  - d) Comment on your answer to 2(c) in light of the compressor speeds you have just calculated.

- 4) The MUG to the synthesis loop contains 2% of an inert compound, I, in addition to equal proportions of A and B. If the circulation rate is  $2.4 \text{ kmol sec}^{-1}$  and the purge rate is  $0.05091 \text{ kmol sec}^{-1}$ , determine the loop operating pressure to meet the production target from part 1. What would happen if the purge rate were reduced further, and how would you mitigate the consequences?

### SOLUTION

The solution of this problem requires a model for the chemical reactor, which is easily generated by integrating the differential mass and energy balances through the reactor:

$$\frac{dF_C}{dw} = q(k_F P_A P_B - k_B P_C)$$

$$\frac{dT}{dw} = \frac{q \cdot 14000 (k_F P_A P_B - k_B P_C)}{(F_A C_{PA} + F_B C_{PB} + F_C C_{PC})}$$

where  $w$  is the mass of catalyst and  $q$  is the multiplying factor to account for catalyst deactivation.

At the reactor inlet, the flowrates and temperatures are  $F_A = F_{A0}$ ,  $F_B = F_{B0}$ ,  $F_C = 0$ ,  $T = T_0$ , and at any subsequent point,  $F_A = F_{A0} - F_C$ ,  $F_B = F_{B0} - F_C$ . Ideal gas behavior is assumed to calculate the partial pressures, *e.g.*,  $P_A = P_T F_A / (F_A + F_B + F_C)$ , where  $P_T$  is the nominal loop pressure. Any one of a number of numerical integration packages can be used.

**1.** Setting  $F_{A0} = F_{B0} = 1.1 \text{ kmol sec}^{-1}$ ,  $q = 0.3$ , and  $P_T = 50 \text{ bar}$ , the model is run for a range of inlet temperatures  $T_0$ .  $F_C$  is noted after integration through 35 tons of catalyst and the results recorded as a plot of  $F_C$  against  $T_0$  (see the middle curve in Figure 2a). The peak indicates a maximum production of  $0.10206 \text{ kmol sec}^{-1}$  for C at an inlet temperature of 517K. (Note the sensitivity to circulation rate changes, but relative lack of sensitivity to catalyst inventory changes as indicated by the other curves in Figure 2a.)

**2(a).** For BOR catalyst  $q = 1.0$  and  $P_T = 50 \text{ bar}$ , the problem requires a trial-and-error solution to find  $F_{A0}$  and  $F_{B0}$  that give the required production of  $F_C$ . A solution is found for  $F_{A0} = F_{B0} = 0.951 \text{ kmol sec}^{-1}$  with a reactor inlet temperature of 487K (see Figure 2b). (Note: maintaining the EOR circulation rate gives a large overproduction.)

**2(b).** For BOR catalyst  $q = 1.0$  and  $F_{A0} = F_{B0} = 1.1 \text{ kmol sec}^{-1}$ , the problem requires a trial-and-error solution to find  $P_T$  that gives the required production of  $F_C$ . A solution is found for  $P_T = 43.64 \text{ bar}$  with a reactor inlet temperature of 495K.

**2(c).** By performing the calculations in 2(a) and 2(b), stu-

dents should be aware that there are three important variables. Reactor inlet temperature can and should be optimized for all situations, but circulation rate and loop pressure are related and cannot be set independently. The above exercises take the two extreme positions of maintaining loop pressure or maintaining circulation rate; the corresponding maximum reduction in circulation rate or loop pressure is then calculated. In practice, an operator would use a smaller change in circulation rate and allow the loop pressure to equilibrate with a reduction somewhat less than the maximum change previously calculated.

**3(a).** Plotting the head-capacity curve using the given equation produces the 10,000 rpm line in Figure 3. The EOR circulation rate is  $2.2 \text{ kmol sec}^{-1}$  or a compressor suction flowrate of  $[(2.2)(0.08314)(313)]/50 = 1.145 \text{ m}^3 \text{ sec}^{-1}$ , and as may be seen from the curve or equation, this implies that a  $H_C$  of 530.5m will be thrown up. If the loop pressure drop is 5 bar, this is equivalent to an  $H_S$  of  $(5)(10^5)/[(9.81)(96.07)] = 530.5\text{m}$ , *i.e.*,  $H_S = H_C$  and the compressor speed of 10,000 rpm will satisfy EOR operating conditions ( $96.07 \text{ kg m}^{-3}$  is the gas density at the compressor suction and is calculated from the ideal gas law).

**3(b).** In this case, the system head will be proportional to the (circulation rate)<sup>2</sup> because the loop pressure is maintained at 50 bar and thus the gas density can be assumed constant. We neglect the effect of minor composition and reactor exit temperature changes. Thus the system curve passes through the volumetric flowrate  $[(2)(0.951)(1.145)]/2.2 = 0.9899 \text{ m}^3 \text{ sec}^{-1}$  at a head of  $[(4.7)(530.5)(0.951\{2/2.2\})^2]/5 = 372.7\text{m}$ . Stable operation requires the compressor speed to be reduced such that the head-capacity curve also passes through this point. Let  $N$  be the new compressor speed and the stable operating point must map back onto the 10,000 rpm head-capacity curve. Thus

$$372.7 \left( \frac{10,000}{N} \right)^2 = 530.5 + \left( (149.52)(0.9899) \left( \frac{10,000}{N} \right) \right) - \left( (130.585)(0.9899^2) \left( \frac{10,000}{N} \right)^2 \right)$$

Solving the quadratic gives  $N = 8420 \text{ rpm}$ ; this is shown as the second compressor curve in Figure 3. (This is quite a large speed reduction and may bring the compressor quite close to the critical speed.)

**3(c).** In this case, the system head will be proportional to the

$$\left( \frac{\text{circulation rate}}{\text{loop pressure}} \right)^2$$

because dropping the loop pressure has a strong effect on gas density. The required point on the system curve is defined by  $[(1.145)(50)]/43.64=1.3119\text{m}^3\text{sec}^{-1}$  at a head of  $[(4.7)(530.5)((50/43.64)^2)]=654.6\text{m}$ . Using the same approach as that applied in 3(b), but this time anticipating a speed increase, we solve the quadratic to give  $N=11,160\text{rpm}$ . (This is quite a large speed increase and may bring the machine close to overspeed trip.)

**3(d).** Answer 2(c) advocates a middle path—some reduction in circulation rate and a corresponding loop pressure reduction. The answers to section 3(b) and (c) show that if loop pressure or circulation rate is maintained, the extremes of compressor speed are also approached, *i.e.*, 2(a) takes operation close the critical speed and 2(b) results in operation near overspeed trip. Hence, the middle path requires a steadier machine speed, closer to normal running speed.

**4.** The equations representing the reactor must be modified to include the presence of the inert. Two changes are needed:

1. Inclusion of the inert component flowrate,  $F_I$ , in the circulation rate ( $F_A+F_B+F_C+F_I$ ); this reduces the partial pressure of any reactant.
2. Inclusion of the inert component heat capacity,  $F_I C_{PI}$ , in the heat capacity ( $F_A C_{PA}+F_B C_{PB}+F_C C_{PC}+F_I C_{PI}$ ); this provides a greater heat sink and so reduces the temperature rise across the reactor.

Before the reactor simulation can be used, the effect of the inert component on the recycle loop material balance must be established. In particular we need the reactor feed composition. Figure 4 shows all the information easily derivable from the problem statements, but two important unknowns

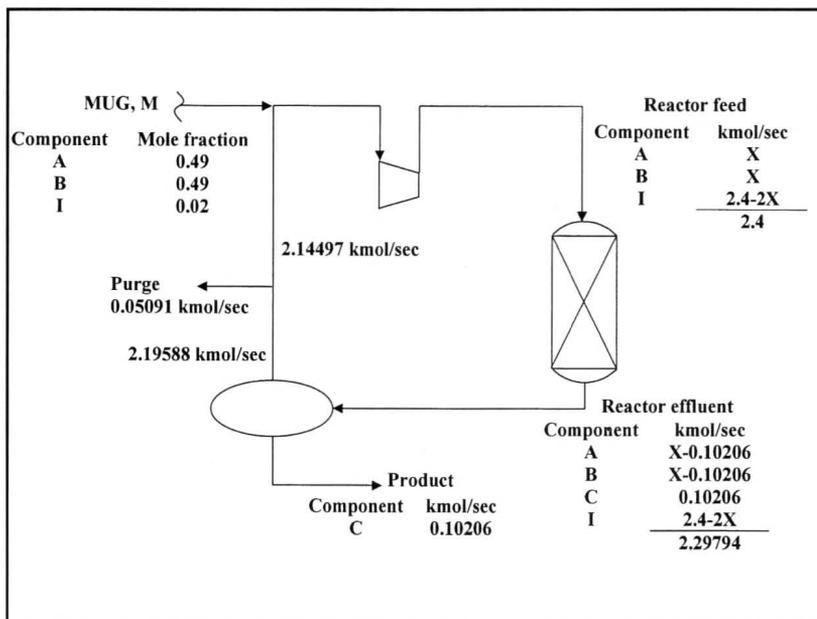


Figure 4.

remain; namely 1) flowrates of A or B in the reactor feed, X, and 2) MUG flowrate, M. Writing component mass balances for a reactant and the inert at the mixing point just before the compressor gives

$$X = 0.49M + (X - 0.10206) \left( \frac{2.14497}{2.19588} \right)$$

$$2.4 - 2X = 0.02M + (2.4 - 2X) \left( \frac{2.14497}{2.19588} \right)$$

Solving for X and M gives  $X=1.089976\text{ kmol sec}^{-1}$  and  $M=0.255028\text{ kmol sec}^{-1}$ , and hence the reactor feed for the simulation is A and B,  $1.089976\text{ kmol sec}^{-1}$  and I is  $0.220048\text{ kmol sec}^{-1}$ . Note particularly that the MUG rate has increased by 24.9%, compared to an inert free MUG, to account for the reactants lost in the purge. Solving for the loop pressure in this part of the exercise is also by trial and error. A loop operating pressure of 55.62 bar will ensure the target production is met if the reactor inlet temperature is optimized at 517K.

Reducing the purge will increase the inerts composition of the gas in the loop. At constant circulation rate, the change must cause the loop pressure to increase in order to restore the reactant partial pressures. For high-pressure systems, the relief valve is typically set at 10% above normal running pressure; hence the calculated loop pressure of 55.62 is probably unacceptable if 50 bar is viewed as normal operation. A further reduction in purge flow would certainly cause the relief valve to lift. To limit the pressure increase, the best tactic would be to increase the loop circulation rate.

## SUMMARY

Parts 1 and 2 of this paper introduce flexibility by providing exercises that force the student to consider how the system will actually operate—this is an important first step to developing a robust design. Further, a wide-ranging knowledge of basic chemical engineering is required, making these exercises (particularly Part 2) ideal as the basis for project work.

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# HUMAN SOCIETIES

## *A Curious Application of Thermodynamics*

ERICH A. MÜLLER

*Universidad Simón Bolívar • Caracas 1080, Venezuela*

There is a loose analogy between the intermolecular forces that govern the observable behavior of fluid systems and the social forces that drive human behavior. Based on this premise, at least in principle, we can use thermodynamics to describe social systems. This paper will put forth some ideas, basically similes, that will help understanding of some common social situations, such as divorce and racism, through thermodynamic reasoning.

The origins of classical equilibrium thermodynamics as we now know it rest on the early findings of Watt, Clausius, Carnot, Joule, and Gibbs, along with many others. The results obtained by these early thermodynamicists were based on careful and systematic study of idealized thermal systems. Curiously, none of these “founding fathers of thermodynamics” had an appreciable comprehension of the exact constitution of matter. As an extreme example, one can point out how Sadi Carnot established the second law of thermodynamics without knowing the law of conservation of energy or the molecular nature of matter. In fact, he had an erroneous idea of what heat was, even though that quantity was the basis of his analysis. The relations and results obtained in this early classical thermodynamic period are independent of the actual nature of the systems studied and are, indeed, very general. This happy occurrence is the reason we can extrapolate the fundamental concepts of thermodynamics to other modern disciplines (*e.g.*, geology,<sup>[1]</sup> information science,<sup>[2]</sup> and medicine<sup>[1]</sup>) if the analogies are carefully made.

Nowadays, we have elucidated many secrets of the nature of matter. Statistical thermodynamics faces the challenge of predicting macroscopic behavior of systems through knowledge of intermolecular interactions and appropriate averaging among the large number of molecules that constitute a system. It is fascinating to see how the statistical mechanical predictions line up perfectly with the earlier classical results. For example, for early scientists pressure was simply a property that described a system and could be related to work or energy. Today, we understand pressure as a result of forces between molecules in a fluid. In other words, today we can somehow understand the collective behavior of the system if

we comprehend the interactions on an individual level.

### THE INTERMOLECULAR POTENTIAL

In nature, molecules interact among themselves by means of forces that translate into the observable behavior of common substances. A few examples are the existence of a particular temperature at which liquid boils, the reason that two substances mix while others do not, and peculiar behavior such as ice floating on water—all of which can all be explained once we understand the molecular forces.

Even the most insignificant molecule of the simplest compound interacts with its neighbors by means of specific forces. The underlying cause for the presence of these forces is the physical separation of positive and negative charges in the atoms. The fundamental electrostatics and quantum mechanics needed to fully explain the nature and form of intermolecular forces are beyond the scope of this discussion. It will suffice to understand that if two atoms attempt to come too close to each other there will be an electrostatic repulsion between them. A macroscopic manifestation of this is the fact that matter cannot occupy the same space; in a simpler fashion, we witness this repulsion when two billiard balls collide. On the other hand, in atoms and molecules the electrons are not fixed in their orbits but rather move around in average locations. These fluctuations in position lead to fluctuating molecular dipoles, and they account for a weak type of attraction among molecules (sometimes called dispersion, or van der Waals forces). It is this attraction that accounts for the existence of condensed phases in which



**Erich A. Müller** is Professor at Simón Bolívar University (USB). He received his engineering and MSc degree at USM and his PhD at Cornell University. His research programs include molecular simulation of complex fluids and the production of software for chemical engineering applications. He is author of the text *Termodinámica Básica* (editorial Equinoccio, 1991).

molecules are closely packed. These attraction forces are of rather short range and are basically imperceptible if the centers of the molecules are separated by more than three or four molecular diameters. At larger distances, the majority of molecules do not interact directly.\* (See Figure 1.)

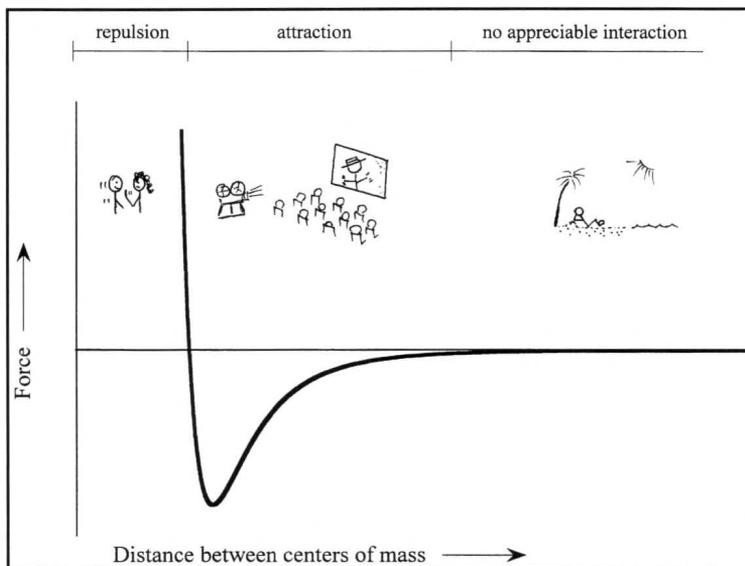
Instead of speaking of forces, thermodynamicists prefer to talk about potentials, whose variation with respect to distance represents the force. Potentials have the advantage of having units of energy; thus a discussion of some concepts is simplified. A typical potential function has basically three zones. At short distances, the potential is positive and becomes larger in magnitude as molecules come closer together (indicating an increasing repulsion). At intermediate distances there is an attraction. The potential is negative and, in fact, presents a minimum corresponding to a distance at which the molecules find a balance between attractive and repulsive forces. Lastly, at large distances, molecules do not interact directly and the potential is effectively zero.

## THE INTERHUMAN POTENTIAL

The central point of this essay is that with a little bit of imagination, one can see that the social behavior of humans may be governed by an "interhuman potential" similar to that of insignificant molecules. To explain, let us assume we are studying people at a large fancy party. As guests enter the ballroom, the first thing they do (after serving themselves a drink) is to mingle, wandering without direction. They place themselves at judicious distances, not too close but not too far away, from others—a distance corresponding to the minimum of the interhuman potential. If we attempt to get too close to an individual, there will be an inherent repulsion. It is the typical discomfort we feel when we are approached by a "close-talker" and are compelled to take a small step back, thus regaining the

appropriate distance. It is clear that two people cannot occupy the same space; thus repulsion becomes infinite at extremely short distances. On the other hand, one will rarely be isolated at a large party and somehow will be attracted to some of the clusters. Humans are social beings, attracted to their fellows. Lastly, the presence of persons at a large distance away will not affect us. We do not know, and usually do not care, who is at the other end of the ballroom.

An interesting point of this logic is that both at a human and a molecular level, even when the individual interactions may be somehow different and the fluctuations around the mean significant, the ensemble will have seemingly homogeneous properties if the number of individuals studied is extremely large.



**Figure 1.** The solid line shows in a qualitative way the intermolecular force for two simple molecules as a function of the distance between their centers. A positive value indicates repulsion among molecules, and a negative value, attraction. The relation to human interactions is evident. An isolated individual (the sunbather) is at peace without interactions from other humans. Nevertheless, he may come relatively close to other individuals for certain occasions (like going to the movies). Too close an encounter, however, usually leads to repulsion.

## FLUIDS AND SOCIETIES

If we start from the premise that molecules and humans are governed by roughly similar potentials, thermodynamics (which serves to study and comprehend the former) may well describe the latter. Moreover, the thermodynamic laws applicable to fluids may possibly describe some aspects of human society.

In a multicomponent fluid, each type of molecule will have its own peculiar interaction. Even though the qualitative shape will usually be similar, there are differences among species (e.g., if there are two types of molecules, say type A and type

B, the potential minimum might be deeper between self-self A-A and B-B interactions than with unlike A-B interactions). Additionally, other types of specific interactions may also be present due to multipolar forces (dipoles, quadrupoles, etc.), association forces (hydrogen bonds, for example), and others. In a complex fluid there might also be symbiotic relations—two molecules may bond for mutual benefit (as exemplified by electron-transfer bonds), or there may be a strong repulsion due to dissimilar cross-interaction forces. Similarly, in human society, our own individuality will draw us to some other people while we strongly dislike others.

**Racism** • Segregation (or intermolecular racism) is common in fluid systems. A classical example is an oil droplet in water. An oil molecule, being so different with respect to its

\* An exception to this comment are the forces among ionic fluids (salts dissolved in water, for example) and polar fluids where long-range forces, due to strongly anisotropic charge distributions, are present.

immediate surroundings, will tend to migrate to a border, avoiding unfavorable interaction with the homogeneous water majority. If other oil molecules are present, they will attempt to aggregate, thus achieving a more stable system and forming a "molecular ghetto." If oil molecules are present in significant numbers, a phase separation will occur, creating a region where all interactions will be favorable (since all of the members of the phase are compatible). The border with the aqueous phase will not be free from a high interfacial tension. The analogy with a homogeneous society, where a small racial, cultural, and/or religious group appears is obvious. World history is plagued with examples such as the persecution of our native inhabitants during the colonization of the Americas, the separation of Pakistan and India, the Arab-Israeli conflict, and the disintegration of the Balkan states.

A very heterogeneous fluid may mix under one of two conditions: 1) by constantly adding a high influx of energy, or by 2) modifying the interactions between the molecules. Following the above example, we can vigorously shake a water/oil mixture, forming a homogeneous system during the process (much in the way one mixes a salad dressing). But the result is not the most stable equilibrium state, and as soon as the energy flux is suspended, the system will spontaneously phase separate, independent of the previous effort to keep it homogeneous. The old Soviet block comes to mind; it disintegrated into its "natural" communities once the stronghold of a central government ceased to exist. All the homogenizing efforts through the decades were futile since they did not alter the basic relations between the republics.

The second method to obtain homogeneity is to modify interactions between molecules by adding amphiphilic molecules (molecules that present one type of behavior on one side of the molecules and a different behavior on the other side). Common examples are soaps and detergents. These molecules, when added to oil/water systems, may convert the system to a stable emulsion. This suggests a rather fool-proof way to eliminate racism and intolerance among divided societies. It is essential to maximize the number of people that can be accepted by both conflicting groups, thus minimizing the formation of distinct "phases." In South American societies, existing races have crossbred since colonial times and the majority of inhabitants have some amount of racial mixture in them. In these societies, racism as such is unheard of since this mixed group does not differentiate by race and "accepts by equal." In a similar fashion, the existence of a large middle class in a country is the only sensible thermodynamic path to obtain social stability.

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\* *Strictly speaking, only a small amount of surfactant is needed to emulsify oil and water. Therefore, only a small "middle" class would be needed to get some mixing of society as stated. A large amount of surfactant is needed to form a microemulsion where the mixing is at a fine level, thus obtaining a stable society.*

**Love** • Other important interactions among molecules are those of association. They are characterized by being specific, discriminatory, and producing a much stronger attraction than van der Waals forces. A typical example is the formation of hydrogen bonds. At a molecular level, two molecules forming a hydrogen bond will maintain themselves at a much closer distance than that expected for normal molecules and will be bonded for a longer time than two non-associating molecules. Again, the analogy between this behavior and that of humans is apparent. There are certain humans who form tightly bonded pairs or clusters for relatively long times. Buddies or lovers, certain humans form bonds among themselves that have the same characteristics as hydrogen bonds.

Hydrogen bonds are not chemical, but physical, in nature and thus may be fragile. Usually, the collision with a third molecule produces a perturbation large enough for the bond to break. To keep the energy at a minimum (the thermodynamic equilibrium condition), it is possible that one of the molecules of the broken pair bonds with the third one (molecular infidelity and divorce). There are also metastable and short-lived bonds (molecular one-night stands).

Macroscopically, an associating fluid is denser and will persist as a condensed phase at higher temperatures than its' non-associating counterpart. In a similar fashion, societies where the concept of family is deeply rooted tend to be more solid and stable. Models of collective societies like the classic Spartan or the modern Israeli kibbutz are based on the thermodynamically inconsistent idea that they are solid due to their number and collective behavior. The solidness of a society depends on the strength of the particular bonds among their members. Here, for example, is the understandable force of the Mafia. There is no human force greater than love, and therefore it must be the base of a stable society. Hate, on the other hand, is a clearly repulsive force, and it tends to disintegrate societies the way a high temperature disperses a liquid into a gas by boiling.

**Resistance to Change** • Another aspect of society that can be considered from the viewpoint of thermodynamics and statistical mechanics is the ability to relate the capacity for change to transport coefficients. It takes a while for society to move from one state to another. The laws of irreversible thermodynamics indicate that the rate of change depends basically on two parameters: the driving force and the transport coefficient,\* which is a property of the substance. In a society, the driving force is the real need for change. The transport coefficient depends on the overall cultural level of the members, their education, and their willingness to undergo change. Large changes may be due to large values of the driving force, of the transport coefficient, or both. Political revolutions are characterized by large driving

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\* *For example, the flow of a liquid will depend on the pressure gradient (driving force) and its viscosity (transport coefficient).*

forces; on the other hand, the so-called German and Japanese miracles following WW II can be explained by high transport coefficients.

The heterogeneity seen in all societies has clear resemblance to fluid transport, say through a pipe where molecules move at very different relative velocities, even when the flow seems uniform. We notice that molecules near the wall do not move while those at the center move with the highest speeds. In society, we have individuals who cling to the walls of the “status quo” while other, more progressive types, usually lead the way.

## THE LAWS OF LIFE (AND THERMODYNAMICS)

Among the first things a student of thermodynamics learns are the statements of the laws of thermodynamics, postulates written in stone that indicate the way in which energy is transferred. The first law guarantees that we cannot create energy—a lesson all humans have experienced. Things are not done by themselves; someone has to do them. The second law is more difficult to put into human terms and is therefore frequently ignored, with tragic results for society. It places restrictions on the flow of energy, giving it a preferred direction. This is done by defining a mathematical quantity called entropy, which upon being measured during a spontaneous change in an isolated system must increase (almost in the same fashion as that thing we call time). A common, albeit undesirable, analogy of entropy is as a measure of disorder in a system.

The second law tells us there is no reasonable expectation that an isolated system may order itself spontaneously. The janitor of our school knows this quite well since every day he places chairs in a perfect Cartesian ordering, only to find them in total disorder at the end of the day. The only way to order either molecules or humans is through a transfer of energy between the system and its surroundings. Societies, being a collective of human beings, cannot escape the consequences of the second law. To obtain an ordered society (low entropy), one has to balance the entropy generation by inputting large quantities of work into the system via a strong government. The Marxist experiment has lasted for over eighty years, but was thermodynamically inconsistent and doomed to failure from the start. Dialectic materialists believed that societies would eventually tend to become ordered and organized systems in which the government would eventually disappear. The second law states quite the opposite—a society without government tends to total disorder and anarchy. Curiously enough, Marxist societies evolved according to thermodynamic postulates, evolving into strong dictatorships. It seems that large empires (complex systems with lots of order and very low entropy) may not survive without disordering the environment and will eventually collapse when the energy transfer through its boundaries is stopped.

**Civilization** • Human society has evolved from a rather chaotic ensemble of cavemen to organized civilizations with a large number of specialized individuals. Energetically speaking, the more complex a society becomes, the higher its energy dissipation rate. This seems to contradict the second law in the sense that isolated systems seek chaos and a homogeneous energy condition. But human societies are open systems, with significant interactions with their surroundings. They can only be maintained by an abnormally large amount of energy. One can easily imagine the catastrophic consequences of a city left without electricity. The fact that some societies tend to decrease their entropy while increasing their energy consumption implies that there must be some parts of the biosphere that suffer the consequences, increasing their entropy in a corresponding way. In fact, the appearance of civilization is regarded as a mechanism to hasten the thermal death of our universe.<sup>[3]</sup> Individuals themselves<sup>[4]</sup> and other animal societies, such as ants,<sup>[5]</sup> can be studied in the same way.

## TO OTHER FRONTIERS

The obsession of a thermodynamicist to explain the world in which he lives in terms of his basic laws is an old, long, and endless one. Many of us attempt to explain economy, understand computers, analyze art and poetry, or prove the existence of God through our skewed optic. The article by Kyle<sup>[6]</sup> does a nice job reviewing some of these attempts.

In spite of this, and without wanting to appear ostentatious, it may be suggested that sociological studies must recognize the existence of two points of view: a global, or collective, one and an individual one. Generalities or laws can be applied on the larger scale since they conform to ensemble averages of individuals' behavior. In this sense, human communities parallel simple fluid systems, which we believe are better understood.

## ACKNOWLEDGMENTS

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# A SEMINAR COURSE ON PROFESSIONAL DEVELOPMENT

EDMOND I. KO\*

Carnegie Mellon University • Pittsburgh, PA 15213-3890

Practicing engineers have long known that it takes more than just technical competence to succeed and advance in a career. This fact was most recently acknowledged by the Accreditation Board for Engineering and Technology (ABET) in its Engineering Criteria 2000. Besides reaffirming the importance of mathematics, science, engineering, and design in an engineering curriculum, ABET explicitly lists other educational objectives such as the ability to function on multidisciplinary teams, an understanding of professional and ethical responsibilities, the ability to communicate effectively, a knowledge of contemporary issues, and the acquisition of a broad enough education to enable the student to understand the impact of engineering solutions in a global/societal context.

One of the challenges that engineering educators face is how to achieve these desired outcomes within the constraints of a four-year curriculum. One possible solution is to break the problem into two parts: first, we must make our students aware of the importance of non-technical skills, and second, we need to help them develop these skills through meaningful exercises that are integrated into their technical courses.

In order to raise the students' awareness of professional skills and to provide them with some context of an engineering education, in 1997 we introduced a 2-unit (equivalent to

1-credit) course that juniors are required to take in the fall semester. In this article, I will share my experiences in teaching this course for the first time.

## ORGANIZATION OF THE COURSE

### Course Objectives

The class meets once a week for fifty minutes. Through a series of 11 discussions, I expect my students to

- *Articulate what they would like to get out of a college education and what kinds of careers they would like to pursue*
- *Identify their strengths and weaknesses*
- *Develop skills that will make them better students in the near term and better workers in the long term*
- *Become more confident in finding their first jobs*
- *Be in a better position to make the transition from the college to the next phase in their lives*

Simply put, the course is about professionalism and about the skills that are essential to having a productive career.

### Textbook

I adopted *The Career Tool Kit: Skills for Success*<sup>[1]</sup> as the textbook for the course. As stated on its back cover, the book "develops the practical and interpersonal skills essential in modern business settings." The course schedule (see below) roughly follows the flow of the ten chapters in the book. We only had time to cover selected sections of each chapter in class, but I asked the students to read through the entire book. I also told the students about several other books that cover similar topics.<sup>[2-5]</sup>

### Schedule

We spent each week discussing a particular topic. The key word here is *discussing*. In each class meeting I gave the students a handout listing several items for discussion. After



*Edmond I. Ko is Professor of Chemical Engineering at Carnegie Mellon University, where he has been since 1980. He received his BS from the University of Wisconsin-Madison and his MS and PhD from Stanford University, all in chemical engineering. His research interests are in the sol-gel preparation and characterization of catalytic materials.*

\* Current Address: City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong

*I must admit that I approached the teaching of this course with some trepidation. . . [but] the fear turned out to be unfounded. Students reacted very positively to the discussion of issues that are relevant to their study, their lives, and their careers.*

providing some background for the chosen topic, I became more like a moderator than a lecturer, encouraging the students to express their viewpoints and sometimes even encouraging them to argue with each other. The topics and selected discussion items are shown in Table 1.

The order of these topics follows the chapters in the book, but there is some flexibility in moving the topics around. Certain topics follow each other naturally; for example, time management and money management fall into the grouping of “resource management.” In the two weeks that I was out of town, I arranged for two guest lecturers to speak with the students. One was a writing consultant who talked about writing as an intellectual exercise, and the other was a career consultant who did a workshop on internships.

Because of time constraints, I chose not to repeat certain topics that students had already been exposed to elsewhere in our curriculum. For example, professional ethics and resume writing, two topics that would normally belong to a course on professionalism, are covered in our first-year introductory course and our sophomore seminar course, respectively. Together, these three courses provide a firm foundation for the professional development of our students early in their college careers.

**Grading Criteria**

I designed the grading system in such a way that students don’t have to compete with each other. Instead, everyone was given 100 points at the beginning of the course and lost points only when they displayed “unprofessional behavior,” defined as

- *Missing a class (minus 5 points)*
- *Showing up late for a class*

<b>TABLE 1</b> <b>Items for Discussion</b>
<p><b>Universal Work Skills</b></p> <ul style="list-style-type: none"> <li>• Skills needed by the American work force</li> <li>• ABET Engineering Criteria 2000</li> <li>• Life-long learning</li> </ul>
<p><b>Self-Image and Motivation</b></p> <ul style="list-style-type: none"> <li>• Self-esteem</li> <li>• Self-confidence</li> <li>• Commitment</li> <li>• Integrity</li> </ul>
<p><b>Diversity in the Workplace</b></p> <ul style="list-style-type: none"> <li>• Being adaptable</li> <li>• Being tolerant</li> <li>• Being thoughtful</li> <li>• Being unprejudiced</li> <li>• Being empathetic</li> </ul>
<p><b>Setting Priorities and Managing Time</b></p> <ul style="list-style-type: none"> <li>• Setting goals</li> <li>• Taking inventory</li> <li>• Identifying time wasters</li> </ul>
<p><b>Budgeting and Investing</b></p> <ul style="list-style-type: none"> <li>• Gross vs. net income</li> <li>• Fixed vs. discretionary expenses</li> <li>• Savings vs. investment</li> </ul>
<p><b>Concentration and Memory</b></p> <ul style="list-style-type: none"> <li>• Staying focused</li> <li>• Avoiding distractions</li> <li>• Making associations</li> <li>• Using mnemonic devices</li> </ul>
<p><b>Communication</b></p> <ul style="list-style-type: none"> <li>• Communication in building and maintaining relationships</li> <li>• Nonverbal communication</li> <li>• Getting along with people</li> </ul>
<p><b>Staying Focused and Managing Stress</b></p> <ul style="list-style-type: none"> <li>• Keeping promises</li> <li>• Avoiding procrastination</li> <li>• Taking care of yourself</li> </ul>
<p><b>Networking and Tracking Down Career Leads</b></p> <ul style="list-style-type: none"> <li>• Establishing contacts</li> <li>• Finding mentors</li> <li>• Talking with people</li> <li>• Job searches</li> </ul>
<p><b>Interviews</b></p> <ul style="list-style-type: none"> <li>• Things to do before, during, and after an interview</li> </ul>
<p><b>Making the Transition to and Moving Up in the Workplace</b></p> <ul style="list-style-type: none"> <li>• Striving for excellence</li> <li>• Taking the initiative</li> <li>• Being adaptable</li> <li>• Continuing to grow</li> <li>• Looking at the big picture</li> </ul>

(minus 3 points)

- *Turning in homework late (minus 3 points)*
- *Turning in homework that is unsatisfactory or missing one (minus 5 points).*

The penalty was not imposed if the student provided me with a valid excuse (e.g., medical reason) in writing.

I told the students that I would hold myself to the same professional standard, i.e., that they each would get 5 points if I missed a class without prior notice or a valid excuse, showed up late for class, or did not return their homework in the following class meeting.

At the end of the semester, a student who lost less than 11 points received an A; less than 21 points, a B; 31 points, a C.

**Homework**

Students were required to submit an essay after each class meeting. The essays were graded satisfactory/unsatisfactory; the guidelines for a satisfactory essay were

- *It should be no more than one page long*
- *It should be professionally formatted and presented*
- *It should be well written (at least free of typographical and grammatical errors).*

Other than giving students ample opportunity to write, the essay assignments were intended to encourage them to be reflective, a point that is best demonstrated by the following examples:

- ▶ “Describe two accomplishments that you are most proud of and explain briefly why. These accomplishments can be things you did at home, at school, in a job, or in a hobby.”
- ▶ “State two of your short-term and two of your long-term goals. Describe the extent to which these goals have been influenced by others (your family, friends, or teachers).”
- ▶ “Identify two items in our discussion on savings and investment from which you gained the most. For each of them, indicate how you plan to use this information to shape your behavior when you start your career.”
- ▶ “Think of an instance in your life when miscommunication has cost you time, money, or peace of mind. Analyze the situation and describe the cause for miscommunication and how it could have been avoided.”
- ▶ “Identify an idea that meant the most to you from our discussion in class. Give an example of how you will use that idea in order to achieve success in your career. Indicate specific changes you plan to make as well as how you will continue, or reinforce, existing behavior.”

### **Time Commitment**

Students spent, on average, less than two hours a week outside of class on the reading and writing assignments. For myself, the time spent on developing the course was comparable to that needed for a typical technical course on a per-credit basis, but it actually took less time to teach the course than it does a technical course because there were no problem sets or exams.

## **EVALUATION OF THE COURSE**

### **Essays**

Reading the students’ essays each week was one of the most enjoyable grading experiences I have had as a teacher. First of all, it was clear from the essays that most of the students paid attention and followed the discussion in class. More importantly, students were uniformly open and honest in expressing their views and sharing their life experiences. In fact, I came to know many students in the class very well by reading their reflective essays—quite an accomplishment in a course where I met with the fifty-two students only one contact hour a week. Throughout and after the course, many students asked me to write letters of recommendation for them—another indication that the format of the course promoted student-faculty interaction.

### **Grades**

At the end of the course, 47 out of the 52 students received A’s. Although a student could miss one class and one assignment and still get an A, 21 of them did not lose a single point! I found this to be encouraging because it showed that

students could and would meet high expectations that were clearly articulated to them.

### **Students’ Comments**

I conducted a mid-semester evaluation and found that at seven weeks into the semester, most of the students felt that they understood the goals of the course and what was expected of them. They also found continuity among the lectures, the reading assignments, and the homework. At the formal end-of-semester course evaluation, the students gave an overall course rating of 4.5 out of 5 (for comparison, the department average is 4.0 and the university average is 4.1). Perhaps more telling are the students’ (voluntary) comments, some of which are reproduced below.

*“The course really prepared me for the professional life. I really believe the material from the course is worth keeping for life.”*

*“I felt that this course has helped me grow as a person and has significantly aided me in learning how to be successful in my job search and in my career.”*

*“This course must definitely stay since it really helped in getting to know what the real world is like.”*

*“I liked this course because we discussed things that we never learn in other classes. I definitely think I benefited from this class.”*

*“I thought this class was a really good use of our time. This has been my most beneficial class so far in college.”*

Students also made specific recommendations for areas that they felt needed improvement. For example, many of them found the textbook not to be very useful. In retrospect, I could have chosen a book intended for an audience closer to chemical engineering juniors at Carnegie Mellon (for example, reference 4). And despite my conscious attempt not to lecture in class, many students felt that there should be more time spent on discussion, especially among the students themselves. I later realized that most of the discussion did take place between students and myself.

### **Pre-Test and Post-Test**

The critical question, of course, is whether the course helped students to learn. For that purpose, I conducted a pre-test and post-test by asking the students to answer the following questions both at the beginning and at the end of the semester.

- *What are the essential skills necessary for a successful career in engineering?*
- *What personal qualities can enhance or detract one’s success?*
- *How do you set goals and prioritize?*
- *What time management strategies do you use, if any?*
- *What communication strategies can enhance relation-*

ships? Hinder relationships?

- What is networking (in the human sense) and how can you best accomplish it?
- What should you do before, during, and after an interview?

Note that these questions were designed to test only for increased student awareness of the important skills (which, after all, was the course's main goal) and not for actual mastery of these skills. Furthermore, these questions do not provide a direct correlation to all the course objectives stated earlier. Despite these caveats, an analysis of students' answers (done by an independent, objective assessor<sup>[6]</sup>) showed that the course was most effective in increasing student awareness of issues related to the interview process, goal setting and prioritization, and effective communication; it was less effective in helping students to identify the skills and qualities that would most help them to be successful in their careers, and in teaching them networking skills; and it was least effective in conveying information regarding time management strategies.

In most cases there is a correlation between a course's effectiveness and students' prior knowledge (as shown in the pre-test). In other words, if students have good prior knowledge about a particular topic (such as time management), then the course was less likely to enhance their knowledge in that area. This finding may be simple common sense, but it highlights the importance of assessing prior knowledge in the planning stage of such a course. Overall, the course did add some value, even though many of the students had at least *some* good prior knowledge on every pre-/post-test question.

## SUMMARY

I must admit that I approached the teaching of this course with some trepidation, not knowing how well chemical engineering students would react to a "non-technical" course offered by their home department, let alone a course that involved numerous writing assignments. The fear turned out to be unfounded. Students reacted very positively to the discussion of issues that are relevant to their study, their lives, and their careers. They participated actively in class discussion, wrote openly about their aspirations and fears, and were delighted to have the opportunity to place their education in context. I encourage other departments to consider offering such a course to their students. My course syllabus can be found at

<http://www.andrew.cmu.edu/course/06-208>

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## BOOK REVIEW: *Thermodynamics*

*Continued from page 223*

and Bridgman relations are very concisely and logically developed in Chapter 7, together with an excellent discussion of the Clapeyron equation. Chapter 8 uses the derivations of the previous chapter to develop relations for properties of real fluids using each of the PVT relations of Chapter 3 to derive departure functions for both gases and liquids. Graphical and equation representations are given. Property tables and diagrams are briefly discussed.

Chapters 9 through 13 deal with phase equilibria. The first chapter defines and calculates partial molar properties, chemical potentials, and fugacity coefficients, the latter by applying the definition to the various equations of state. Mixing rules and calculations of both thermal and equilibrium properties for real fluid mixtures follow. Chapter 10 discusses stability of equilibrium systems as well as pure fluid phase transitions, vapor pressure, and the phase rule.

Properties of solutions from ideal to very nonideal, simple phase equilibria predictions, and the full Gibbs-Duhem equation and its use, including derivation of excess free energy models for activity coefficient correlation, are given in Chapter 11, together with activity coefficient prediction methods.

Chapter 12 discusses vapor-liquid equilibrium in a methodical and logical way and is a high point of the book. Basic relations used to equate fugacity for both low-pressure and high-pressure systems are detailed with many examples. Tests for VLE thermodynamic consistency are discussed. Qualitative discussions of both vapor-liquid and vapor-liquid-liquid equilibria are discussed and illustrated. A short treatment of dilute solution laws and liquid-vapor-solid solubilities is contained in Chapter 13.

Chemical reaction equilibrium is the subject of Chapter 14, which discusses basic free energy-equilibrium constant reactions, homogeneous gas reactions and the effects of variables, adiabatic reactions, and phase-rule analysis of and calculation of equilibrium for simultaneous equilibrium reactions. A short discussion of simple liquid phase and heterogeneous reactions concludes the chapter. This chapter could be improved by including more material on solid-gas reactions and a discussion of solution of simultaneous reaction equilibria by free-energy minimization.

Appendices include pure component data properties from various sources as well as thermodynamic data for steam and common refrigerants. The pure component data section should be updated to the data now accepted as the most accurate.

In summary, the book is a credit to the author and to his profession. In my opinion, it is definitely competitive with the leading first textbooks in chemical engineering thermodynamics. Faculty, students, and practitioners will all find material of value. The only negative is that the book is softbound and poorly glued; my copy split after very little use. □

# QUANTIFYING THE “CURVE”

JUDE T. SOMMERFELD

Georgia Institute of Technology • Atlanta, GA 30332

Perhaps one of the most agonizing tasks associated with an educator's work is that of assigning grades to students. The task is somewhat complicated by the traditional need to convert numerical scores into letter grades. Ironically, letter grades are then typically combined in some fashion and converted back to a numerical score (such as a grade-point average, or “GPA”). Throughout this paper, the latter quantity is understood to mean the conventional GPA computed on the basis of an “A” letter grade being worth four points, a “B” grade worth three points, etc.

While most experienced engineers (educators and practitioners alike) would probably agree that a person's GPA in college is quite irrelevant to the progress of one's career only a few years down the road, the fact remains that the GPA is often the single most important factor in evaluating a student's performance. Both companies and graduate schools weigh this quantity heavily in their respective selection processes. And for the student still in school, the GPA is about the only thing that can be pointed to for measurement of scholastic performance (at least in most students' minds).

So, it behooves faculty members to at least appreciate this all-consuming importance of grades, rightly or wrongly, in the student perception of education. Until a better system comes along, we must make the best of what is probably a suboptimal grading methodology. Anything that tends to minimize this distraction from real learning should be a welcome tool to any educator. It is within this framework that the following suggestions are offered.

**Jude T. Sommerfeld** is Professor in the School of Chemical Engineering at Georgia Tech. He received his BChE from the University of Detroit and his MSE and PhD degrees, also in chemical engineering, from the University of Michigan. His industrial and academic experience has been primarily in the area of computer-aided design, and he has published over 100 articles in this and other areas.



## BACKGROUND

Most professors have probably had the experience of being asked one or more of the following questions after returning a quiz or examination to the students, graded on the basis of 0 to 100 points (or some other numerical scale).

- Do you curve your grades?
- How do you curve your grades?
- What letter grade do I now have in the course?
- Do you do negative curving of your grades?

Using the term “curve” seems quite ubiquitous for most students, even though professors often have difficulty in responding to the above questions. The first two questions are likely to be asked after a particularly difficult exam (one with an average of around 50, for example), while the last question often arises after a relatively easy exam with an average student score of 80 or more.

The questions also seem to be asked more frequently in sophomore-level or lower-division courses where letter grades are not as high as they are in upper-division courses (junior- and senior-level). But it is not unusual to see a good student at any level drop a course (even a required one) after getting a score of 60-70 on an exam with a class average of 50 or less, for fear of “ruining” his or her GPA.

## GUIDELINES

This instructor has found it useful to distribute some guidelines to students immediately after returning their first examinations. The guidelines are based on the mean (or average) and standard deviation of the actual distribution for a given examination. The latter two quantities are also reported to the students (in addition to the median and range). My experience has been that questions regarding “curving” of the numerical grades to letter grades are virtually eliminated after distribution of the guidelines. Unfortunately, some good students still feel compelled to drop the course (par-

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**TABLE 1**

**Guidelines for Converting Numerical Quiz Scores to Letter Grades in Sophomore ChE Courses**

[M=class average (or mean);  $\sigma$ =standard deviation]

Letter Grade	Quiz Score	Normal Distribution %	Quality Points
A(4.0)	Greater than $(M + 1.0 \sigma)$	15.9	0.636
B(3.0)	Between $(M + 0.2 \sigma)$ and $(M + 1.0 \sigma)$	26.2	0.786
C(2.0)	Between $(M - 1.0 \sigma)$ and $(M + 0.2 \sigma)$	42.0	0.840
D(1.0)	Between $(M - 2.0 \sigma)$ and $(M - 1.0 \sigma)$	13.6	0.136
F(0.0)	Less than $(M - 2.0 \sigma)$	2.3	0.000
<b>Class GPA</b>			<b>2.398</b>

**TABLE 2**

**Guidelines for Converting Numerical Quiz Scores to Letter Grades in Junior ChE Courses**

[M=class average (or mean);  $\sigma$ =standard deviation]

Letter Grade	Quiz Score	Normal Distribution %	Quality Points
A(4.0)	Greater than $(M + 0.6 \sigma)$	27.4	1.096
B(3.0)	Between $(M - 0.2 \sigma)$ and $(M + 0.6 \sigma)$	30.5	0.915
C(2.0)	Between $(M - 1.5 \sigma)$ and $(M - 0.2 \sigma)$	35.4	0.708
D(1.0)	Between $(M - 2.25 \sigma)$ and $(M - 1.5 \sigma)$	5.5	0.055
F(0.0)	Less than $(M - 2.25 \sigma)$	1.2	0.000
<b>Class GPA</b>			<b>2.774</b>

**TABLE 3**

**Guidelines for Converting Numerical Quiz Scores to Letter Grades in Senior ChE Courses**

[M=class average (or mean);  $\sigma$ -standard deviation]

Letter Grade	Quiz Score	Normal Distribution %	Quality Points
A(4.0)	Greater than $(M + 0.5 \sigma)$	30.8	1.232
B(3.0)	Between $(M - 0.4 \sigma)$ and $(M + 0.5 \sigma)$	34.7	1.041
C(2.0)	Between $(M - 2.0 \sigma)$ and $(M - 0.4 \sigma)$	32.2	0.644
D(1.0)	Between $(M - 2.5 \sigma)$ and $(M - 2.0 \sigma)$	1.7	0.017
F(0.0)	Less than $(M - 2.5 \sigma)$	0.6	0.000
<b>Class GPA</b>			<b>2.934</b>

ticularly if they know it is being offered again in the following quarter).

Separate guidelines have been developed for sophomore-, junior-, and senior-level courses in chemical engineering. They are presented in Tables 1, 2, and 3, respectively. The normal, or Gaussian, distribution was not specifically assumed in the development of these guidelines. The distribution percentages given in the tables were obtained from tabulating integrated values for the standard normal distribution; that is, one with a mean value of zero and standard deviation of unity. The class averages presented in the tables are then derived from the distribution percentages. Such tabulations can be readily found in many mathematical handbooks<sup>[1]</sup> and textbooks on statistical methods.<sup>[2]</sup> Thus, for example, in Table 1 the probability of or percentage of sampled values greater than one standard deviation above the mean (corresponding to a grade of "A" in a sophomore-level class) would be equal to 15.9%.

The guidelines for sophomore-level courses yield a class GPA of about 2.4 (on the 4.0 basis mentioned earlier), as indicated in Table 1. This class GPA compares with values of 2.77 and 2.93 for junior- and senior-level courses (Tables 2 and 3, respectively). The lower value for sophomore-level courses reflects the fact that many students in these courses are still maturing and fleshing out their career options and thus may not be that suited for (or interested in) chemical engineering. Typically, such courses would include material balances, energy balances, numerical methods, and fluid mechanics.

The actual relationship between these guidelines for the three class levels and the normal distribution is depicted in Figure 1. The curve plotted therein is for the standard normal distribution with a mean value of zero and a standard deviation of unity.

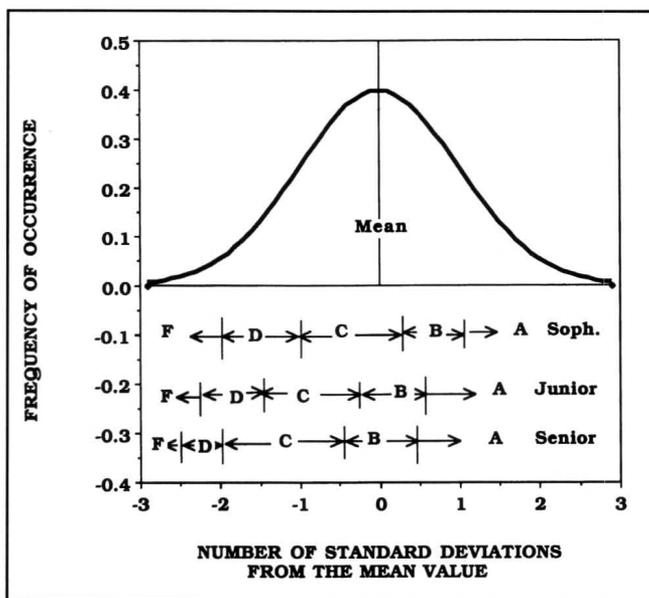


Figure 1.

tion of unity. One can clearly see the reduction in the cutoff point (number of standard deviations above the mean) between "A" and "B" grades in the progression from sophomore to senior level and, consequently, the increase in their frequency of occurrence (insofar as they lie to the right of the mean). Similarly, in this progression the frequency of occurrence of "D" and "F" grades, being to the left of the mean, is seen to decrease.

The class averages computed for upper-division courses in Tables 2 and 3 are somewhat closer to each other in addition to being higher than those for sophomore courses in Table 1. In all three cases, however, the computed class GPAs are probably slightly lower than the actual grade distribution resulting in most courses. In a sense, this is good news for an instructor insofar as dashing of students' expectations is minimized (better this situation than the reverse). By way of comparison, the median GPA of all junior chemical engineering students at Georgia Tech (173 total) enrolled in the fall quarter of 1997 was 3.05, versus a computed junior course GPA of 2.77 from Table 2. It should also be kept in mind, of course, that with the greater range below this median than above it, the mean class GPA would be somewhat lower than the median.

## EXPERIENCE

There has been no attempt to optimize the numerical coefficients in Tables 1 through 3 in order to achieve a particular shape of distribution. My primary purpose in presenting this information to students is to answer legitimate questions and to allay unnecessary fears. Clearly, if one wished, much effort could be devoted to adjusting these parameters, perhaps to match historical or even projected data—but that is not the focus of this paper.

Nonetheless, one detailed comparison of these guidelines with experience may be interesting to the reader. Table 4 presents grade results from a dozen different offerings of a senior-level computer-aided process design course offered at Georgia Tech. These data span the 7-year period from 1991 through 1997 and pertain to a total of 349 students. The

class size in these various sections varied from a low of 11 to a maximum of 53, with an average of 29 students.

The data in Table 4 indicate course GPAs ranging from 2.88 to 3.21. The average GPA for all students in all of the sections is 2.99, compared to the value of 2.93 suggested by the Table 3 guidelines. Also, the percentages of "A" and "C" grades from the 7-year history given in Table 4 are both slightly less than those resulting from the Table 3 guidelines, while the percentage of "B" grades actually given is somewhat higher. There have been no "F" grades given in this course during the 7-year period, and the small percentage of "D" grades (1.7%) is exactly in conformance with Table 3.

One clear benefit of these guidelines cannot be overemphasized. In assigning letter grades at the end of a term, most faculty probably spend some time agonizing over the cutoff points between "A" and "B" grades and between "B" and "C" grades. It is not uncommon to hear from the highest "B" or highest "C" student at the beginning of the next term, with a view to possible grade negotiation. I have found these guidelines useful both in the initial assignment of letter grades and in any subsequent grade-negotiation discussions.

One last benefit to the entire educational enterprise should be noted. Assuming that distribution and discussion of the guidelines with the students is performed early in a term (about the time, say, of the first quiz), it serves as a pep talk or morale booster for

the students. This is particularly true with sophomore students who are still accustomed to more standardized tests, such as found in college freshman courses or high school SAT examinations. Rampant dropping of courses, particularly required ones, is an expensive exercise for students (and parents?), not to mention the drain on institutional resources. My experience with publicizing the guidelines has been reduced student withdrawal rates from required chemical engineering courses.

## REFERENCES

1. Spiegel, M.R., *Mathematical Handbook of Formulas and Tables*, McGraw-Hill, New York, NY (1968)
2. McNeese, W.H., and R.A. Klein, *Statistical Methods for the Process Industries*, ASQC Quality Press, Milwaukee, WI (1991) □

**TABLE 4**  
Distribution of Letter Grades in a Senior-Level Computer-Aided Design Course

Year	Quarter	Letter Grades (number thereof)					Total Students	Class GPA
		A	B	C	D	F		
1991	Fall	2	7	1	1	0	11	2.91
1992	Spring	6	9	8	0	0	23	2.91
1993	Winter	10	25	14	1	0	50	2.88
1993	Fall	2	8	1	0	0	11	3.09
1994	Spring	13	20	13	0	0	46	3.00
1995	Winter	14	24	13	2	0	53	2.94
1995	Fall	7	9	7	0	0	23	3.00
1996	Winter	8	15	7	0	0	30	3.03
1996	Spring	8	10	8	1	0	27	2.93
1997	Winter (A)	15	11	8	0	0	34	3.21
1997	Winter (B)	6	10	6	1	0	23	2.91
1997	Fall	8	5	5	0	0	18	3.17
<b>Totals</b>		<b>99</b>	<b>153</b>	<b>91</b>	<b>6</b>	<b>0</b>	<b>349</b>	<b>2.99</b>
<b>Percentages</b>		<b>28.37</b>	<b>43.84</b>	<b>26.07</b>	<b>1.72</b>	<b>0.00</b>	<b>100</b>	

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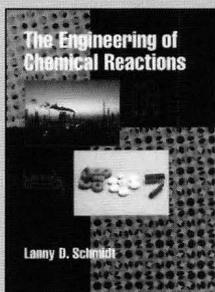
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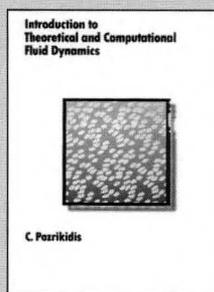
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