



Eric M. Stuve

... of the University of Washington



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and ChE at . . . **Tulane University**

For the sake of argument— *If the conventional lecture is dead, why is it alive and thriving?*



Don Woods, CEE Publications Board

Straight lecturing is the least effective way to improve student learning. Students tend to remember 10 to 50% from “passive” involvement in the learning process (we remember about 10% of what we read; 20% of what we hear; 30% of what we see; and 50% of what we hear and see). Students remember 70 and 90%, however, if they are “actively” involved (we remember about 70% of what we say and 90% of what we say and do). Also, students in learning environments where lecturing dominates become more “rote learners”; students learning in problem-based or cooperative learning environments become more “deep learners.”

Recently, research was done on the effectiveness of updating courses for medical doctors. Those courses that were lectures produced no change in practice. Courses that included active learning components *did* produce a change in practice.

Since we usually want to help students remember and since we want graduates who are deep learners instead of rote learners, why do faculty still give 50-minute lectures of teacher talk? Why do universities build more lecture auditoriums—instead of flat-floor learning environments with movable chairs and tables that are more conducive to cooperative and active learning? Why do courses in teacher training focus on “how to lecture,” and “how to lecture to large classes,” instead of “how to use active learning, cooperative learning, or problem-based learning?” Why are faculty called “lecturers”?

Perhaps the answer is that lecturing is relatively easy, most of us “learned” from lectures (so what’s wrong with the lecture?), and each of us gets a sense of power and usefulness when we walk into a “lecture hall” and all eyes look at us and wait to write down our every

thoughts. Perhaps that’s the only way that we see that we can cover the material—but our role is to *uncover* material so that students learn. Perhaps we don’t want to stop lecturing even though we know there are other options available.

So if I currently use straight lectures, what might I do? One simple way to change from straight lecturing to more effective learning environments is to never have more than 20 minutes of teacher talk. Boredom sets in after 20 minutes. A suggestion is to use a timer set for 20 minutes to remind you to shift from “teacher talk” to some activity.

Examples of “active” activities include:

- *Ask individuals to write reflections (2 min.) then discuss with a neighbor (90 sec.)*
- *Have students turn to their neighbor and say:*
 - “Did you understand that?”*
 - “Do you believe that?”*
 - “The key point so far is”*
 - “A practical application of this stuff is”*
- *Ask students to compare or rework notes*
- *Use Talk Aloud Pairs Problem Solve, or TAPPS*

Other options include using “rounds” (where students sit in circles of about four or five and each comments for about 30 seconds on a topic you pose) or using cooperative learning groups.

The straight lecture with 50 minutes of teacher talk really doesn’t improve student learning. It’s time to change. □

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Eric M. Stuve

of the University of Washington

BRUCE A. FINLAYSON

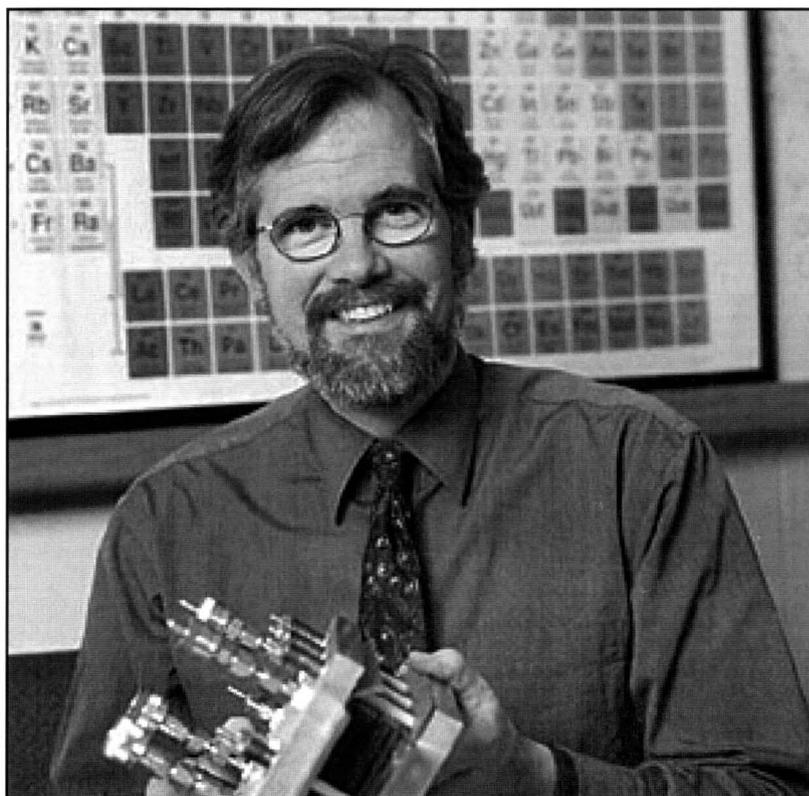
*University of Washington
Seattle, WA 98195-1750*

Eric is one of the few people I know who watches the Indianapolis 500 race. That's a legacy from growing up in Indiana.

He was born in Montana, but soon afterward his parents moved the family to the Midwest, living in Michigan, Wisconsin, and Indiana. It's typical of Eric that he retained his affection for that down-home pastime even as he embraced the intellectual challenges of studying the sciences and pursuing a professorial career. Eric has always been one to run his own race.

Since he was living in Milwaukee as a high-school senior, attending the University of Wisconsin, Milwaukee, was a natural choice. After one year, and upon the advice of Charles G. Hill, he transferred to the Madison campus, where he excelled. In preparing for graduate school, Eric was fortunate to receive good advice from the Wisconsin professors. Ed Lightfoot reviewed faculty at a number of schools and Hill, for whom Eric was doing an undergraduate research project, cautioned about getting involved in surface science as it was a lot of ultrahigh vacuum physics. It was good advice, but Eric had other plans.

Eric's research began at Stanford, where he worked with Bob Madix on surface reactions in ultrahigh vacuum on platinum and silver. He found the physics was fun. Following his Ph.D. (1984) he went to Berlin with an Alexander von Humboldt Fellowship in the Fritz-Haber-Institut der Max-Planck-Gesellschaft, and it was in Berlin that he met Monika, who was born and raised in East Germany. They wed in 1985, which was also the year Eric came to the University of Wash-

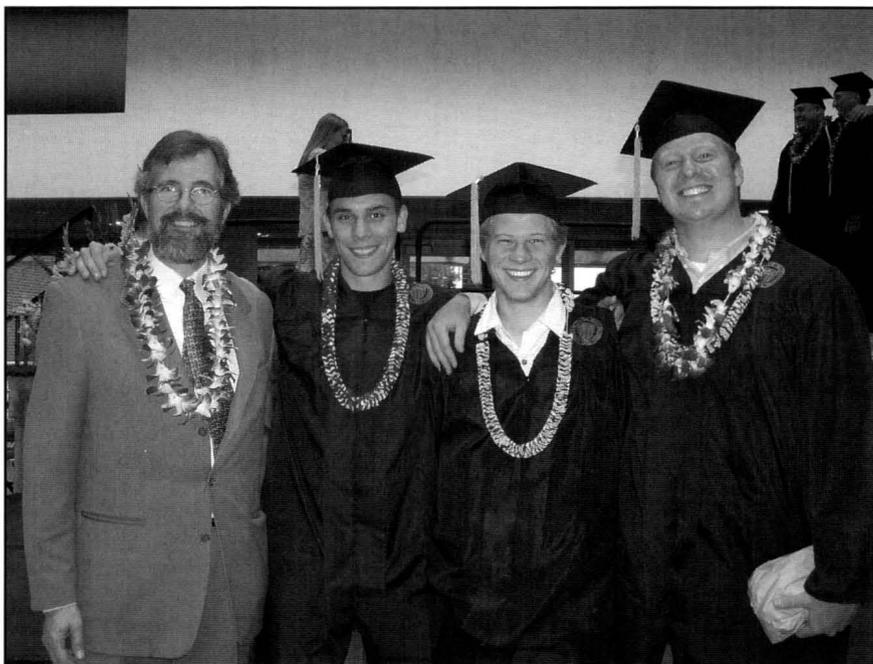


ington, where he is now chair of the Department of Chemical Engineering.

Eric is committed to involving students in innovative projects in both design and research, and he brings considerable enthusiasm, humor, and a fundamental understanding to all his interactions with the students.

TEACHING AND RESEARCH

With Eric, teaching and research are inseparable. Learning by teaching has served him well. He reports that, in his first year teaching the process design course, he learned to put



Eric and three very happy grads let loose with some leis following commencement ceremonies on campus.

into perspective what he did at the molecular level, helping him as an educator *and* researcher. Likewise, teaching his first course in graduate thermodynamics challenged him to make the homework problems relevant—and he suddenly saw how he could bring electrical engineering and chemical engineering to the course. Furthermore, he says, he had one of those eureka moments: “I could do this.”

Thus spawned his work on high electric fields, which ran for 10 years and provided important data no one else had: A field ion microscope was used to study field-induced surface chemistry at very high electric fields (100 MV/cm); adsorption and reaction of water on sharp (10-100 nm) field emitter tips elucidated the basic ionization of water to hydronium ions and hydroxide ions induced by the electric field and the structure of water at the interface. This information is useful for rational catalyst design for fuel cells, understanding ice chemistry in oceanic and atmospheric environments (ozone hole chemistry), and development of ultra-capacitors for high-energy/high-power electrical devices.

As he began his research at the University of Washington, Eric branched out into electrochemical problems as well, providing the underlying support for his later work on fuel cells. While in Berlin, he had learned how to apply electrochemical concepts to surface reactions on metal electrodes immersed in liquids. He then built equipment that enabled comparison of electrochemical and gas-solid surface phenomena under nearly identical conditions. This helped elucidate the importance of potential in reactions at the fluid-solid interface. The electrode surfaces could be analyzed using thermal desorption, low-energy electron diffraction, Auger and X-ray photoelectron spectroscopy, and secondary ion mass spectrometry.

For his work, Eric was chosen as an NSF Presidential Young
Spring 2006

Investigator. Since his work was mostly done under high vacuum, he joined the American Vacuum Society (AVS) and, over time, became a director, trustee, and chair of the Investment Advisory Committee. In his work with investments, he taught the other scientists the concept of net present value, which—fittingly for Eric—he had learned by teaching the undergraduate design course. He is currently a fellow of the AVS.

FUEL CELL LOCOMOTIVE

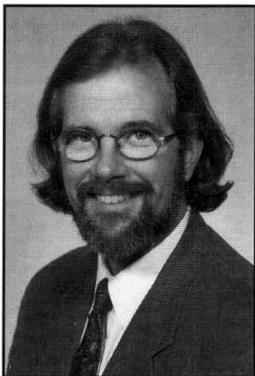
One day Eric and a professor from Aeronautics and Astronautics (Reiner Decher) came to see me in the chair’s office. They proposed making a fuel-cell driven locomotive, amusement park size.

Eric’s interest was in the fuel cell, and Reiner’s passion was with trains. They explained that combining the efficiency of a train for transporting goods with the efficiency of a fuel cell would make an ideal system. As we talked, the image of having a small train circle Frosh Pond during Engineering Open House came to mind as a great crowd pleaser. Except . . . the thought of inexperienced undergraduates handling hydrogen in a venue with thousands of middle school kids was a scary one, to say the least.

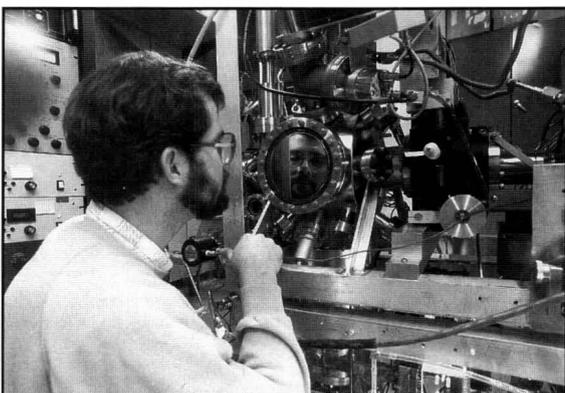
But Eric was undeterred, and had other ideas as well. Thus through his determination and vision was born one of the country’s best centers for fuel cell education, now encompassing several professors and several courses—undergraduate and graduate, one of which is delivered as televised distance learning.

The goal of the Fuel Cell Locomotive Project (which began in 1996) was to produce a fuel cell system, fully contained, that could provide 10 kW of power at 100 V to a proton exchange membrane system. The fuel cell would be the prime mover for an 18-inch-gauge locomotive (one-third size) that would pull two passenger coaches.

Eric’s plan to demonstrate the train setup at an Engineering Open House got the green light, and it became a combined project involving students and faculty from many dis-



Hey, long hair was in then, left. Eric and Monika on their wedding day in 1985, right. Eric's lab is a true reflection of his determination, below.



ciplines and two universities: the fuel cell chemistry interested chemical engineers; the special materials interested materials science students; the manufacturability interested mechanical engineers; and the applications interface interested electrical engineers. Through an NSF program, students at Penn State were also involved (in the 1997-98 school year). The students worked in groups, which required the development of communication skills and experience with teamwork. It marked probably the first time these students had been exposed to peer evaluation. It was also the first time most chemical engineering students came in close contact with students in other disciplines, at least at a high, working level. A key driving force that made the project fun was that it required the “hands-on” design of a complex system.

The chemical engineering and materials science students learned how to make and optimize a single cell, and then the chemical engineering students joined the mechanical engineering students to make a “stack,” or several single cells connected in electrical series. This task required designing the flow field plates and seals, and dealing with the ever-present safety concerns. Along the way students built several versions of fuel cell test stands, ranging from small to large scale.

Eric's role as project leader was to integrate all these disciplines and coordinate with faculty in other departments. It involved a degree of risk since the outcome wasn't certain at the beginning, but Eric kept a global view and ensured that students learned something at each stage. While the mechani-

cal engineers were way ahead in building the rolling stock for the train, the chemical engineers were learning that it is hard to build a fuel cell. The fuel cells worked, but they didn't provide enough power. Eric had the foresight to have students each quarter build on what was learned the previous quarter and improve it. In that way, progress was consistent and the students had a feeling of success in achieving their team goals.

As to my imagined fears at the outset, it turns out there was only one explosion (no injuries). And for good measure, the students were led through subsequent safety procedures to see that there was never another.

On top of his success in bringing the idea to fruition, Eric also learned how to guide such a project and avoid the end-of-quarter rush, which is very important to those schools still on a 10-week quarter system. In evaluating the experience, Eric says, “Students are over-confident and under-experienced.” He notes the biggest problems were communication (as in the real world) and time management (as in the real world), but he was surprised at what they could do. The course is definitely good preparation for work after school!

By 1999, under Eric's steady steering, the little train project had gone from “I think I can, I think I can,” to “I know I can, I know I can.”

FUEL CELL COURSES

The classroom program began to blossom when Eric asked to teach his new fuel cell course on TV. I had been encouraging faculty to present more of their specialty courses on TV so that they could be taken by engineers who couldn't come to campus. When Eric committed to giving it a try, we had to rearrange the teaching schedule, with some faculty doubling up to cover his previously assigned load, but we managed and the course was a great success. Engineers in fuel cell



As evidence of Eric's inner drive, he insists on maintaining his regimen of bicycling to work even in one of the rainiest months in Seattle's history. It takes more than a few raindrops and puddles to steer these wheels off course.

companies on both coasts took the course on TV, and approximately 160 University of Washington students and 85 distance-learning students have taken the course since 1998. It also has been offered as a professional short course at three national meetings of the Electrochemical Society.

With all this experience to bank on, Eric was able to partner with colleague Dan Schwartz and get funding from the Dreyfus Foundation to integrate fuel cells into the chemical engineering curriculum. They put a fuel cell in the unit operations laboratory and created new courses. Eric had already partnered with Chevron, Apple Computer, and Boeing to provide a high-vacuum device for the undergraduate unit operations laboratory, where the students investigated Knudsen flow in conditions pertinent to the electronics industry. But Eric isn't satisfied with having students make things without also understanding them.

Two classes were developed, one a course for juniors in science and engineering (and for fuel cell professionals) and the second a more rigorous course for seniors. As with all his courses, Eric makes good use of PowerPoint slides that are colorful and appeal to students for later viewing. They also make it possible for Eric's graduate students to teach the class as a distance-learning course (as part of a Huckabay Teaching Fellowship).

Students frequently take the courses because of their desire to contribute to improving society. They often report that after the course, they appreciate how hard it is to make a fuel cell system work, and they also are perceptive in seeing the potential of fuel cells and recognizing that the public doesn't understand where the hydrogen is coming from. Since Eric

attends conferences during the quarter, he comes back with real-life examples of fuel cells that demonstrate to the students that these are current topics and not just classroom lessons. As one student put it, "They are cool, very modern."

Lessons learned in the Fuel Cell Locomotive Project are applied in the fuel cell courses, too: design projects involve working with professors and other students, and developing a fuel cell system that incorporates constraints of size and functionality for real-life situations. As the courses proceed from year to year, the projects change to reflect what was learned previously. Since Eric is also now chair of the department, he shares the teaching load with Professors Dan Schwartz and Stuart Adler. The fuel cell curriculum has grown to include three faculty members and several courses. At the undergraduate level are Introduction to Fuel Cells, Fuel Cell Engineering, and Solid Oxide Fuel Cells. Courses at the graduate level are oriented to the scientific questions raised by fuel cells and other reactions on surfaces: Thin Film Science, Engineering, and Technology; Reactions at Solid Surfaces; and Electrons at Surfaces.

For Eric, the education program is a big part of his driving force. He says, "If we can't work with students, I don't see why we're here."

As a result of their experience in fuel cell projects, designs, and courses, many of our graduates have gone to work for fuel cell companies. Some were apprehensive about interviewing with such companies, saying, "But our fuel cell didn't work very well." In the course of their interviews, they found out that the companies' fuel cells didn't always work well either—and were hired!

REACHING OUT TO GRADUATE STUDENTS

Befitting his individualist nature, when graduate students start to work in Eric's lab, the first assignment he gives them is to watch the film *Dr. Strangelove*. It's his habit to advise his students on books to read, music to listen to, and movies to see.

After broadening the students' outlook on research, it's time to get down to work. New students quickly learn Eric's mantra for reading a technical paper is to read from left to right, stop at the end of each line, then see that you understand it before going on to the next one. He has new students read three to four papers, discuss them, and write a research proposal. This exercise sharpens their critical thinking skills and illustrates that the generation of new knowledge requires thought and hard work.

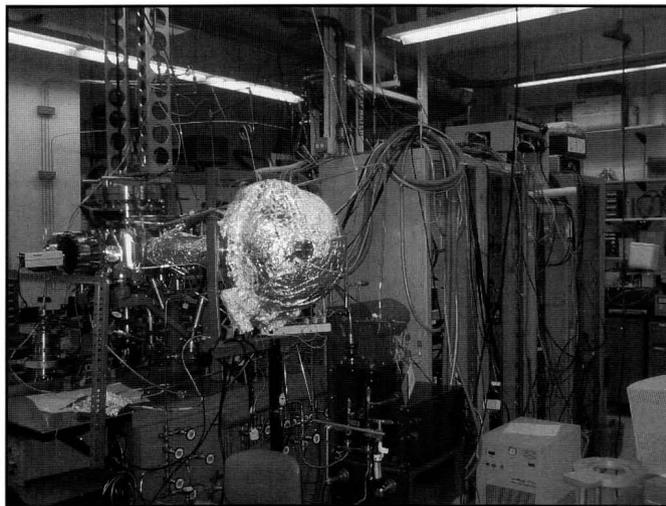
Students then begin working on a problem in his lab, possibly using the high-vacuum surface science equipment. As the work nears the point of publication, a draft is submitted, but it comes back covered in red ink. The laboratory holds a copy of Fowler's *Modern English Usage*, and students are expected to use it. Papers from Eric's laboratory don't have author lists as long as the abstract: you are expected to do the work yourself. As you might expect, some of his graduate students are getting a chemistry degree, and he teaches those students chemical engineering principles, too; he thinks everyone should know them! Eric believes in thorough preparation. His students are prepared for the future by writing and rewriting papers, and by presenting the work at conferences, always with a fundamental look at the problem. As you'd expect, Eric's Ph.D. students work predominately in companies dealing with fuel cells, electrochemistry, and surface science (see Table 1).

LAUNCHING A LAB

Sometimes a researcher will look around for a problem that can be solved with techniques and instruments he/she has available. Not Eric. He sees a problem and thinks how best to solve it, then proceeds. It was in this fashion that he built up his laboratory equipment to be the extensive lab that it is today (see Table 2). The philosophy does require creativity, though, since it often means learning a new area that one hasn't formally studied. Thus, the effects of high electric fields, ceramics (and solid oxide fuel cells), and linear density functional theory were things he learned in re-

sponse to particular problems.

One example of this philosophy in action is how Eric's group was able to resolve a scientific argument. The background involves a focus of current research: namely, to determine the reaction mechanisms that occur at surfaces. A major application is direct methanol fuel cells (DMFC) for portable power and low-power applications. Teasing out the



A look inside Eric's lab.

mechanism for the oxidation of methanol on platinum and platinum plus ruthenium requires careful work, often under high vacuum. Yet, the understanding is essential if DMFCs are to become widespread. Beginning with the Langmuir-Hinshelwood surface reactions, mechanisms are proposed and then experiments designed to determine the rate-controlling steps. Some researchers felt the reaction followed a parallel path, while others insisted it was a serial path. By elucidating four different controlling rates of reaction, Eric's group was able to determine that the previous findings in favor of the series path

were the result of reaction conditions and catalyst modifiers (e.g., ruthenium). Both sets of reactions are necessary, but local conditions determine which ones apply in any given situation.

Since fuel cells operate at temperatures above room temperature, Eric conducts studies at higher temperatures, too. More recently, work on solid-oxide-supported platinum catalysts supports the goal of fuel cells that run on diesel or other hydrocarbon fuels without having to reform the fuel to produce hydrogen. Copper-ceria electrocatalysts minimize carbon formation, thus avoiding the problems of nickel-based electrocatalysts. Solid oxide fuel cells have strong potential for use in transportation, defense, and industrial and residential applications.

The fundamentals of surface science have widespread application in other fields, too. The power of fundamentals was brought home to me one day when I was reading a paper about how polymers slip while being extruded, but the phenomena seemed to depend upon the type of surface. I asked Eric about that, and described some of the surfaces mentioned briefly in the paper. He proceeded to line them up for me, explaining which ones would allow slip at the lowest pressure drop, etc. Impressed, I called the author (at an industrial laboratory); the paper had not been completely forthcoming, but the author confirmed that the sequence Eric provided was exactly what was found in the laboratory.

ERIC AS CHAIR

Eric was appointed acting chair of chemical engineering in 1999 and soon became the permanent chair. One of the highlights of his chairmanship has been the preparation and execution of the department's Centennial, a celebration of the beginning of the department in 1904. It involved hundreds of people to organize, and Eric seems to have tapped into his student experience as an actor and techie to pull off the pageantry to the last detail. With Eric in the driver's seat, the event was carefully crafted to show off the department to alumni, the university, and ourselves. He reports he had the usual "opening night" jitters, but all the planning made for a memorable event. In the end, even his planning for contingencies got tested, as a thunderstorm erupted just as we were about to leave the luncheon to walk to the laboratories.

Eric enjoys hearing stories from retired alumni and values their friendships. In turn, alumni have been very generous to the department, and Eric loves the stories they tell about chemical engineering in the "early days." Chuck Matthaei (of Roman Meal Bread) has shown great interest in education and recently endowed a professorship. Neil Duffie (of Willamette Industries) knows what is important and challenges Eric to think strategically; Neil has been a longtime supporter of graduate fellowships.

PERSONAL CHARACTERISTICS

I have always valued Eric's creative side. If there is an idea to explore "outside the box," Eric is one of the people I want in the group. In addition to his comprehensive knowledge, his willingness to forge his own path means he has a knack of looking at problems in different, sometimes quirky, ways, and this spawns new ideas.

Eric is not all fuel cells and surface reactions, though. Well-known for his love of Gary Larson's *Far Side* cartoons, he has an endearing sense of humor that can defuse tense situations. His love of music is also well known: He and his wife Monika attend the opening night of Seattle Opera every year. Eric even drew upon his theatrical side at the departmental

holiday party in December 2005, when he serenaded the attendees by singing "O Tannenbaum."

Further evidence of his well-developed nonscientific side is his practiced penmanship: Eric's mother was artistic, and Eric learned calligraphy—so well, in fact, that his wife requires a card done in the elegant writing style for birthdays and special events. The artistic streak carries over to Monika, as well, who has achieved "teacher" status in Ikebana flower arranging. She quickly learned the Japanese art and has even displayed her accomplishments at a Seattle show along with a Japanese master and his entourage.

The Stuves also enjoy traveling, and one benefit of Eric's fuel cell research has been an increase in opportunities to do so. A repeat destination is Bangkok, Thailand, as part of an exchange program Eric participates in with Dow Chemical and the Chemical Technology Department of Chulalongkorn University. During their last visit, they encountered a situation we all hope to avoid. As the plane took off from Bangkok, a bird flew into an engine and the pilot aborted the takeoff. In the process, a wheel caught fire, and the plane was evacuated at the end of the runway. While the plane was quickly emptying, Eric was concerned about his wife and son Kurt, who were also onboard. As if sliding down the chute weren't enough excitement, it took some time for the family to reunite. Then, more problems appeared. Since everyone had left their carry-on baggage on the plane, no one had their passport. Thus, they could not enter Thailand again while waiting for another plane the next day! Eventually, sanity occurred among the authorities, and the passengers were taken to a nearby hotel to spend the night. The next day the plane took off without incident, and Eric and his family returned to Seattle safe and sound, and none the worse for wear. Leave it to Eric to take such an unplanned "pit stop" in stride.

CONCLUSION

With his commitment to keeping students on the right track and his fundamental approach to problems, you might say Eric is the kind of chemical engineering educator who helps set the pace for our profession. Not bad for an Indy fan. □

TABLE 1
Stuve's Ph.D. Graduates

Naushad Kizhakevariam - Varian in Portland Rod Borup - Los Alamos National Laboratories David Sauer - Intel Thomas Jarvi - UTC Fuel Cells Timothy Pinkerton - Intel Dawn Scovell - Intel Suresh Sriramulu - Tiax Consulting (formerly Arthur D. Little) Seng-Woon (David) Lim - UW Chemistry Dept. Thomas H. Madden - United Technologies Research Center Chris Rothfuss - U.S. Department of State Nallakkan Arvindan - Symyx Corp.
--

TABLE 2
Equipment in Stuve's Laboratory

Differential Electrochemical Mass Spectrometer Ultra-high vacuum (UHV) analysis chamber (4) Potential step chronoamperometry Linear and nonlinear electrochemical impedance spectroscopy (EIS and NLEIS) Field Ionization/Emission Microscopy (FIM/FEM) X-ray photoelectron spectroscopy (XPS or ESCA) Low energy electron diffraction (LEED) Thermal desorption spectroscopy (TDS) Time-of-flight mass spectrometer (TOF-MS) Auger electron spectroscopy (AES) Contact potential difference (CPD) Electron stimulated desorption ion angular distribution (ESDIAD)
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Some exhausted members of the Tulane University Uptown recovery team on Sept. 15, 2005—two weeks after Hurricane Katrina. Left to right: Greg Potter (chemistry, Washington Univ.), James Peel (Bruker Instruments), Russell Schmehl (chemistry), David Mullin (cell and molecular biology), Scott Grayson (chemistry), Qi Zhao (chemistry), Gary McPherson (chemistry), W Godbey (CBE), Brian Mitchell (CBE), Vijay John (CBE), and Bob Garry (microbiology).

From Survival to Renewal

*Katrina and its Aftermath
at Tulane's Chemical and Biomolecular Engineering Department*

BRIAN S. MITCHELL, JOHN A. PRINDLE, HENRY S. ASHBAUGH, AND VIJAY T. JOHN
Tulane University • New Orleans, LA 70118

The Chemical and Biomolecular Engineering Department at Tulane University has a rich tradition dating back to 1894, as the first established program in chemical engineering in the South and the third program in the country.⁽¹⁾ Tulane University faced a struggle for survival in the fall of 2005 when the city of New Orleans was devastated in the wake of the flooding from Hurricane Katrina. This article chronicles the experiences of the department and its efforts not just to maintain viability but also to look to the future with a renewed sense of purpose. In keeping with the

university's approach to describing the events of the period between Aug. 29, 2005, and the present, the article is divided into three sections: survival, recovery, and renewal.

As background, we give the reader an idea of the department. At the time of Katrina, there were nine full-time faculty (**Professors O'Connor, Papadopoulos, Law, Mitchell, Ashbaugh, Godbey, Lu, De Kee, and John**), two staff members (**Dr. Prindle** who serves as a senior instructor and laboratory supervisor, and **Ms. Lacoste**, the departmental administrative secretary), and **Professor Emeritus Gonzalez**, who

participates in teaching graduate courses and in collaborative research. The department had about 30 graduate students studying toward their Ph.D., and about five part-time M.S. students. Undergraduate enrollment was about 80 with graduating classes between 15 and 20 students. Undergraduate interest in the program, and enrollment numbers along with it, saw a steady increase as a result of the recent emphasis and inclusion of biomolecular engineering into the curriculum in 2003.

SURVIVAL

Residents in the New Orleans area are accustomed to threats from hurricanes, but there had been none to hit the city since Betsy in 1965. The horrendous traffic jams and inconveniences of evacuation that were experienced when Hurricanes Georges and Ivan came close but missed the city convinced many that evacuation was unnecessary. A sense of complacency had set in. But Katrina was no mere threat. By Aug. 25, it was clear the storm was zeroing in on the New Orleans area. Some 300 miles off shore, the hurricane strengthened to a Category 5 status, giving sufficient reason for the university to initiate evacuation plans for students. Ironically enough, the weekend of Aug. 27 was supposed to be the faculty's annual welcoming of the latest batch of freshmen, but hasty departures were being urged instead. **President Scott Cowen** called a meeting of all students and requested that they all return home or evacuate to Jackson on buses the university had arranged. Temporary housing had also been arranged for evacuating students at Jackson State University. Our faculty made individual plans for the storm while making sure their graduate students had concrete evacuation plans. Two of our faculty decided not to evacuate prior to Katrina, but the consequent flooding and the infrastructure and security issues in the city mandated they leave a few days after the hurricane. Most faculty and students first evacuated toward the Baton Rouge, Houston, and Jackson areas.

The events of Hurricane Katrina have been well documented. We all watched the disaster in real time with acute sadness, for we could clearly identify with all the locations in the images. The stress was heightened by the fact that phones were not working and we were unable to get in touch with our colleagues and students. Tulane's information technology services were disrupted and university e-mail addresses were useless. Communication was slowly established through text-messaging and the use of temporary e-mail addresses. It was at this time that Hank Ashbaugh got through

to colleagues in the chemical engineering community with his request for help in placing our students (see box on page 82 for his personal recollections). Vijay John followed up with a separate e-mail. The department will forever be grateful for the outpouring of help for our students and faculty. The major ChE departments geographically closest to Tulane—in Houston and in Baton Rouge (Rice, the University of Houston, and LSU) took in many of our students and offered our faculty laboratory and office space—we are so tremendously thankful.

Katrina wrought significant damage to Tulane. Two-thirds of our picturesque campus in the historic Uptown neighborhood of New Orleans had flooded. Winds from Katrina damaged the roofs of several buildings. The computer systems were down, with the university backup tapes located safely yet inaccessibly in high-rise buildings downtown near the Superdome, the site of so much trauma and sadness. The upper administration was operating from Tulane's Executive Business School campus in Houston—the saga of how they brought back function to operations and coordinated the recovery is an interesting story in itself (see <www.tulane.edu>). The breakdown in payroll systems was the first major crisis, since the university had no idea how to issue paychecks or even a way to identify those on its payroll. We were dealing with emergency financial personnel who had to be educated that a graduate stipend simply meant salary. With the help of the deans, department chairs, and faculty members, all employees and graduate students were identified and paychecks issued through direct deposit. Professor Dan De Kee, who also serves as the associate dean for graduate studies, was invaluable as he kept the pressure on payroll administration from his

It was particularly heartwarming to see the graduate students back and helping us clean the laboratories to resume research activities. Even though some had damaged apartments, they teamed up and those with livable apartments opened their doors and hearts to those without.

evacuation location of Gaithersburg, Md. In many instances, the university simply took the word of the deans that individuals belonged on the payroll and issued paychecks. It is to the credit of the university that all employees and graduate students were paid during the entirety of the period between Sept. 1 and Dec. 31, 2005, while the university remained closed.

Within a couple of weeks following Katrina, faculty members Brian Mitchell and Vijay John—who live to the north and to the west of the city—had returned to their homes, grateful to find minimal damage. John Prindle, who lives near Baton Rouge and had not evacuated, served as a communications conduit (see his personal account in box on page 83). Hank Ashbaugh slowly traveled from Jacksonville, Fla., up the eastern seaboard to Troy, N.Y. (Rensselaer) where he even-

Professor Hank Ashbaugh's recollections of connecting with his research group and the chemical engineering community

*After Hurricane Katrina hit on Aug. 29, 2005, a sense of helplessness grew in me as I watched the perpetual coverage of the flooding of New Orleans from my father's house in Jacksonville, Fla. The storm had knocked out the phone network for anyone with a New Orleans area code, so communications with the faculty in my department were spotty at best. Foremost on my mind was where my research group had scattered in the wake of Katrina. I quickly located one postdoc who still had a New York area code on his cell phone, and learned that he'd safely evacuated with Professor Yunfeng Lu's group to Shreveport, La. More worrisome were the two graduate students from India who had just arrived in the United States to join my group the week before the storm. How do you locate two newcomers to this country who had scattered in a panic? Then I remembered that I had recruited these two students from UICT with the help of **Professor V.G. Pangarkar**. I e-mailed him at 11 p.m. and by 2 a.m. my two students had contacted me to say they were safely on their way to Texas.*

My success in locating my far-flung group gave me the idea that we should try to reconstitute the department over the Internet. The first step was to locate the individual faculty members. The Internet servers for Tulane had been shut down before the storm, so using campus e-mail addresses was out. Instead, on Sept. 1, I wrote an open e-mail to the chemical engineering community—copying every department chair—to tell our story and request the whereabouts of any Tulane faculty. The response was phenomenal. Over the course of the next three days I responded to over 400 e-mails wishing us well, volunteering support, and, more importantly, giving me clues as to where our faculty had evacuated. Within a week and a half I managed to locate all our faculty, get alternate contact information for each, and begin to reassemble the department. Two weeks after the storm I sent a second e-mail to the ChE community providing news of our faculty's whereabouts. As faculty members were being located, we started to compile lists of graduate and undergraduate students to expand our "virtual" department. Using the contacts we had developed outside the department, we were able to connect students with departments and universities that had volunteered to host them during our semester in exile. To facilitate interdepartmental communications, we created a blog (spaces.msn.com/members/TulaneCBE/) to disseminate information on support for students, student registration, communications from our chair, and miscellaneous tidbits. Moreover, the blog provided a window for our friends outside the department to keep updated on our status. □

tually spent the rest of the semester. During his travels, he stopped in at universities along the way (North Carolina, Delaware, Princeton) where he had studied. Kyriakos Papadopoulos also evacuated to New York (Columbia) after a two-week stay in Lafayette, La. W Godbey ended up in Houston (Rice) by way of Huntington, W.Va., Dallas, Texas, Grapevine, Texas, and Fort Smith, Ark. Kim O'Connor went to Houston (Baylor Medical School); Yunfeng Lu to Albuquerque (University of New Mexico) by way of Houston; Richard Gonzalez to Jackson, Miss.; and Ms. Lacoste to relatives who live north of the city. Victor Law went to Angleton, Texas, and had to evacuate a *second* time due to Hurricane Rita. Our students were scattered all over the country and were welcomed in at all universities. We had survived the hurricane. The next step was to plan our recovery.

RECOVERY

The early days following the hurricane, when the campus and surrounding Uptown neighborhood were without electrical power, are detailed in Brian Mitchell's account of the recovery efforts (see box on page 85). The university hired Belfor, an international disaster-recovery corporation, and the campus was teeming with Belfor employees. Huge power generators and trailers were scattered across campus as Belfor set about draining water from building basements (note: basements in New Orleans = bad idea!), gutting damaged floors, and reinstalling utilities. By early to mid-October, electrical power had been restored to the neighborhood and most of the campus had power, with the notable exception of the science building where electrical transformers and other utilities placed in the basement had been destroyed. The university's senior administration had returned to the city and had started operations in the main administration building (Gibson Hall). From there they monitored the recovery and began the strategy for renewal.

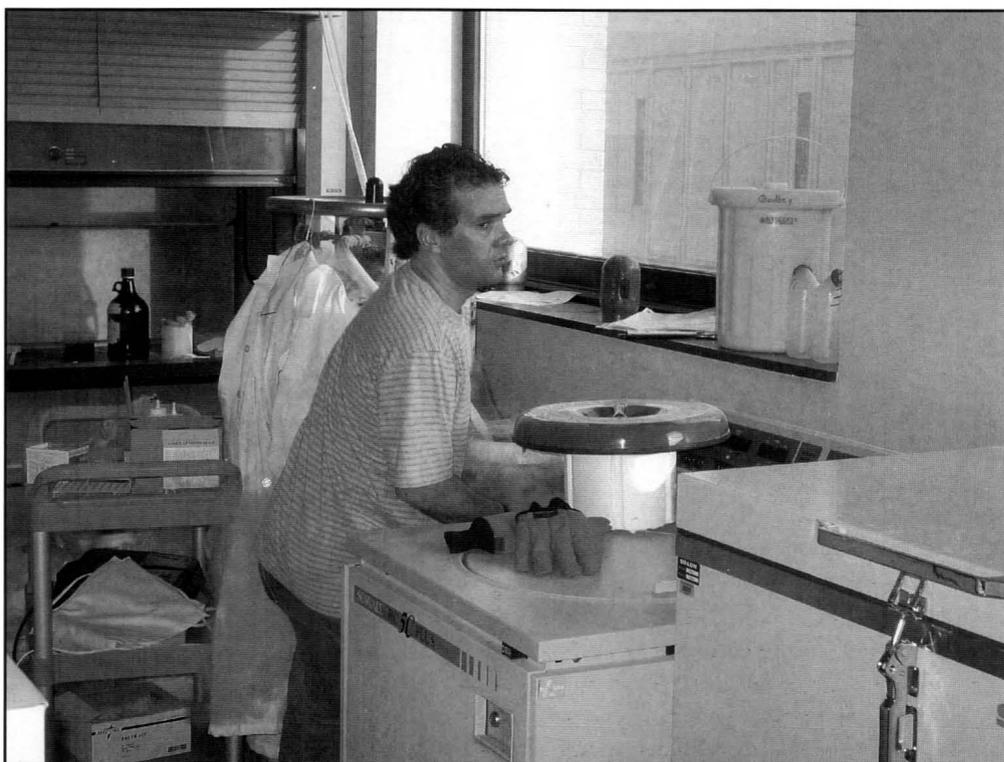
From the department's perspective, this was a time to take stock of our losses. Brian Mitchell, Vijay John, and John Prindle were among a handful of faculty and staff cleared for regular entry into the engineering building. All other employees had to get clearance to enter the building (usually by calling Brian or **Nick Altiero**, the dean) and were escorted into the engineering building by Brian to recover computer hard drives, etc. There were significant safety issues, as the building ventilation systems had not yet been decontaminated. During the months of October and November, the computer and communication systems at Tulane returned to normal operation and we slowly transitioned back to our university e-mail addresses. It was an interesting time, as Brian, John, and Vijay came in almost every day to man the phones, keeping in touch with our colleagues and our students. We had to balance these duties with our personal lives, in which Katrina had impacted school openings for our children, job conditions for our spouses, and much more. There was very little

time for intellectual work. It was a time in which we all realized the frailty of the human condition and learned to act with newfound compassion. Three of our colleagues had suffered such damage to their homes that they needed temporary housing. Overall at Tulane, 25-40 percent of the employees had homes significantly damaged by flooding. There was, and continues to be, a resounding spirit of helping one another.

We learned several lessons from our experiences in survival and recovery that are useful to pass on. When planning for disasters, science and engineering departments should always take into account the consequences of electrical power and communication failures for extended periods. It is wise to maintain extra supplies of liquid nitrogen to preserve biological samples. Personnel and graduate students should have alternative e-mails that can be accessed anywhere through the Internet. Inventories of chemicals, instruments, and general property must be maintained by the department. Access to buildings under repair should be tightly controlled even to employees—a faculty member paying a nostalgic visit to the medical school building before the power had been restored is said to have caused significant water damage by using the plumbing while the system was under repair. Even if thawed biologicals (e.g., tissue samples) have been removed, decontamination of the entire building must be performed

under professional supervision.

By early December, most buildings were functional and the campus was being spruced up for the return of the students. Faculty members throughout the university were excited about returning to work. President Cowen and the upper administration had done a wonderful job in maintaining student morale by presenting Tulane as a unique institution where rigorous education would be combined with exceptional opportunities to participate in public service to rebuild a great city. Early registration rates were high and the faculty was looking forward to the future. We knew that the univer-



W Godbey contemplates the whoosh of liquid nitrogen vapors that indicated his dewar full of biological samples was still cold—evidence that years of research were still safe.

Dr. John Prindle's recollections of maintaining connections with the undergraduates

Students are any chemical engineering department's lifeblood. They challenge the faculty to continually improve teaching skills. Their tuition pays for a portion of the department's expenses. And with each freshmen class comes a distinctive view of the world and how to improve it. In many ways, students are a department's primary legacy. So, it is not surprising that a strong personal connection forms between faculty members and each student they instruct.

In the aftermath of Hurricane Katrina, this personal connection was severely tested. For more than a month after the event, the university's network servers were down, rendering the familiar student e-mail addresses useless. Shortly after Tulane announced it was canceling the fall semester, students began calling faculty at home to discuss their options. Student concerns ranged from whether they should attend another university for the semester to whether they should register for chemical engineering coursework at that university. During these discussions, the faculty realized most students simply wanted to be reassured that we would assist them any way we could. With each call, students were

*See **Maintaining Connections with Undergraduates**,
continued on page 98*



Members of the faculty and instructional staff in less stressful times. From left, standing: W T. Godbey, Daniel De Kee, Vijay John, Yunfeng Lu, Kim O'Connor, Kyriakos Papadopoulos, Brian Mitchell, and John Prindle. Seated: Richard Gonzalez, Hank Ashbaugh, Victor Law.

sity, as with all employers in the New Orleans region, would be in a difficult financial situation. But there was a contagious spirit to get the students back, work hard, build up research, and try to recover. It was particularly heartwarming to see the graduate students back and helping us clean the laboratories to resume research activities. Even though some had damaged apartments, they teamed up and those with livable apartments opened their doors and hearts to those without. Yunfeng Lu, who lives a block from campus, feverishly worked to repair his damaged home so his sizable group of graduate students could have a place to stay if they were unable to find appropriate accommodations.

RENEWAL

On Dec. 8, the Board of Administrators at Tulane University announced a renewal plan as a consequence of the financial exigency. The plan has turned out to be the largest restructuring of an American institution of higher education on record. Under the plan, some 230 faculty members were terminated, including 35 members of the School of Engineering. The Departments of Civil and Environmental Engineering, Mechanical Engineering, Electrical Engineering, and Computer Science have been slated for elimination by the fall of 2007. The university has been reorganized with the formation of a School of Liberal Arts and a School of Science and Engineering, in addition to the professional schools, to fully constitute a comprehensive university. Chemical and

Biomolecular Engineering is one of only two surviving engineering departments; Biomedical Engineering is the other. Both were merged into the School of Science and Engineering, which has been further divided into academic divisions. Biomedical Engineering is now part of the Division of Biological Sciences and Engineering. Chemical and Biomolecular Engineering and the Department of Chemistry form the Division of Chemical Science and Engineering. The entire renewal plan makes for fascinating reading for those interested in academic organization, strategy, and administration. It can be found at <http://renewal.tulane.edu/>. Long-term goals of the plan as stated by the Board of Administrators are: (1) diligence in retaining our institutional quality and working to heighten that quality; (2) dedication to providing an unparalleled, holistic undergraduate experience for our students; (3) continued strengthening of core research areas and graduate programs that build on our strengths and can achieve world-class excellence; and (4) an absolute commitment to using the lessons learned from Katrina to help rebuild the city of New Orleans and to then extend those lessons to other communities.

We mourn the breakup of the School of Engineering, an institution that existed for over a century. We also mourn the departure of our colleagues who have worked tirelessly to improve the school. It is sufficient to say that we will continue to work hard toward enhancing the reputation of the department. The current dean of the engineering school, Nick

Altiero, has been appointed the new dean of the School of Science and Engineering. We believe his appointment indicates the university's recognition that engineering is still a significant and continuing component of Tulane, and we look forward to working with him to renew, reconstitute, and expand engineering as opportunities present themselves. He has been clearly told that the Board of Administrators will be receptive to new ideas for engineering at Tulane upon return to financial stability.

What is the future of the department? The university is expected to return to financial stability within a couple of years, with the bond market expressing confidence in the strong management team at Tulane.^[2] Our student body has returned and we are back to high intensity in both research and education. Our informal merger with chemistry is a seamless fit. Over the years, the two departments have formed strong bonds, with research collaborations and an environment of mutual support. The atmosphere of cooperation has led to the establishment of superb instrumentation facilities in advanced spectroscopy, electron microscopy, and organic and inorganic analysis. We are especially proud of our high-resolution electron microscopy and confocal microscopy facilities wherein we are instituting a full range of cryoimaging techniques for biological imaging. Collaborations with the Medical School have been set up and we are considered a vital player in Tulane's objective to become world-class in health sciences research. Such collaborations are in stem-cell culture, gene delivery to cancer cells, and vaccine development and delivery technologies. The department has significant strengths in the areas of computational chemistry, self-assembly, nanostructured materials, colloid science, and polymer and ceramics processing. The university has clearly stated its intent to bring every Ph.D.-granting department up to national prominence, and we expect significant investments to our department as the university returns to financial viability.

The next couple of years will be difficult. In addition to their intellectual lives, faculty and students will worry about

rebuilding their personal lives, which must come first. Kindness and compassion will be the order of the day in the department in dealing with such issues. It will also be terribly exciting to witness and participate in the rebuilding of the city. It is incredibly heartening to see students mobilizing on all kinds of public service projects, from involvement in public school education, to gutting destroyed houses so that residents can return to rebuild and establish communities, to providing meals to the thousands of laborers who are working to rebuild the city.

We are determined to persevere. Please wish us well . . . and come visit.

ACKNOWLEDGMENTS

W T. Godbey made very helpful suggestions to the article. The faculty, staff, and students of the Department of Chemical and Biomolecular Engineering express our deepest gratitude to our colleagues in the chemical engineering community for their many gestures of kindness in the wake of Hurricane Katrina, and for their numerous forms of support in helping us to re-attain our prestorm level of excellence.

Department chair's note: I am privileged to work with my faculty and staff colleagues who showed so much courage and dedication to restoring the department to viability. The three coauthors of this article (Prindle, Ashbaugh, and Mitchell) were especially helpful with their efforts to contact every undergraduate and graduate student and their efforts to restore the research infrastructure. They were always available to help, and Professor Mitchell coordinated the entire recovery aspects of the engineering school. To rebuild the department with such colleagues is the best job I could hope for.

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Professor Brian Mitchell's narrative on the recovery of our physical facilities

Two weeks after Hurricane Katrina, the department's personnel situation was still critical, but much more stable. All faculty and staff had been located and were in communication, most undergraduates had been advised which courses to take at their host institutions, and graduate students were in contact with their advisors. While many continued to struggle with personal issues related to assessment of their home damage, FEMA, the Red Cross, insurance, accommodations, and informing friends and family of their whereabouts, it became clear that it was time to give some attention to the status of departmental facilities, especially those related to research. The concern for research facilities was uniform throughout Tulane's research community, but the urgency in engineering was associated primarily with biological samples that had now been in unreplenished liquid nitrogen (LN₂)-cooled dewars for two weeks in the sweltering New Orleans summer heat.

*Laura Levy, senior vice president for research, authorized a convoy for Sept. 15 to the Tulane campuses to assess damage. The convoy, led by **John Clements**, professor and chair of microbiology and immunology, departed early that Thursday morning from the Tulane University Regional Primate Center in Covington, which is located on the Northshore*

*See **Recovery of Physical Facilities***

continued on page 86

Recovery of Physical Facilities

Continued from page 85

of Lake Pontchartrain and had not received any significant damage from the storm. The eight-vehicle convoy consisted of researchers from both Uptown (Engineering and Science) and Downtown (Medical School) campuses, and traversed the 24-mile Lake Pontchartrain Causeway bridge in record-setting time with the assistance of a police escort. Its entrance into the city marked for many of the recovery-team members their first views of Metairie and New Orleans since the hurricane. The sights, sounds, and smells did not bode well for finding facilities intact.

Upon arriving at the Uptown campus, the Downtown team continued on to the more heavily damaged Medical School campus, while the representatives from Science and Engineering set to work. The team from the Chemical and Biomolecular Engineering Department consisted of Professor and Chair Vijay T. John, Assistant Professor W T. Godbey, and Professor Brian S. Mitchell. Flashlights in hand, the team entered the Lindy Claiborne Boggs Center for Energy and Biotechnology around 9 a.m., and trudged up the back stairs to the third and fourth floors that comprise the bulk of the department's research facilities.

An initial scan of the department showed it to be in relatively good condition: no blown-out windows, no water damage, and no indications of unauthorized entry, save for one broken interior window in the department's Electronic Classroom. A keypad on the door and no missing equipment in the classroom soon led to the conclusion that security personnel had broken the glass simply to gain entry and evaluate damage. As doors were opened and each lab inspected, hope grew that the department had evaded major damage. Lab benches looked as if students had simply left for lunch. Only one lab had minor damage, the result of a window being left partially open and the hurricane-force winds toppling some glassware.

The team then concentrated its efforts on two general areas: securing biological samples and recovering research data. W Godbey was elated to find that his LN_2 dewar full of biological samples—including rare cells and tissue specimens that were collected over years of research—was still cold. (One can equate his joy at seeing the cold, white cloud rise from his liquid nitrogen storage freezer with the emotions exhibited by JPL engineers when a probe successfully lands on Mars.) He quickly replenished the dewar with LN_2 from a pre-Katrina storage tank in his lab, and did the same with

Professor Kim O'Connor's samples in an adjacent laboratory. The team then collected biological samples from dewars in the Biomedical Engineering Department, consolidated the samples into one 25 l dewar with wheels, and placed the dewar by a service elevator to facilitate future refilling operations. Some thought was given to carrying the portable dewar down the stairs and placing it on the first floor since there was no power in the building, but there were indications that power to the elevators could be restored on a temporary basis, if necessary. Unfortunately, biological samples that had been frozen in a refrigerator freezer were no longer cold and had begun to decompose. DNA samples that had been placed in a freezer to slow decomposition could withstand room temperatures for moderate time periods, so they were still salvageable and were therefore retrieved.

As doors were opened and each lab inspected, hope grew that the department had evaded major damage. Lab benches looked as if students had simply left for lunch.

Similar operations related to the collection and consolidation of biological samples were conducted in the chemistry and biochemistry departments, as well as at the Downtown campus. For example, a recent Public Broadcasting NOVA segment documents the heroic efforts of Tulane researcher **Tyler Curiel** to save irreplaceable sinonasal undifferentiated carcinoma (SNUC) samples from his laboratory (<<http://www.pbs.org/wgbh/nova/sciencenow/3302/08.html>>). LN_2 is also critical to the operation of some advanced analytical tools, such as Nuclear Magnetic Resonance Spectrometers (NMRs). **Gary McPherson** and **Russell Schmehl**, our colleagues from chemistry, diligently worked to ensure that the NMR magnets

in both the Department of Chemistry and Tulane's Coordinated Instrumentation Facility (CIF) did not quench. Eventually, these units also required that their liquid helium reservoirs be recharged, a task which involved several other dedicated individuals from both chemistry and CIF.

The recovery of research data consisted primarily of retrieving laboratory notebooks and computers from investigators' offices and labs. It was unknown at that point how long the university would remain closed, and some investigators had not decided whether to relocate to other universities for the semester. Many opted to leave their computers for the time being. As it turned out, Tulane would be closed for the entire semester, and many faculty members did indeed relocate to continue their research, if only out of their homes. As a result, many computers and hard drives were retrieved during subsequent recovery trips. The retrieval and shipping of computers for faculty, staff, and graduate students proved to be problematic. Some requested only hard drives, which required opening computers, and some requested not only computers, but monitors and other peripherals as well. Shipment of large pieces of equipment required travel to neigh-

TABLE 1
Some Lessons Learned

Biological Materials	For brief power interruptions, a chest freezer is preferable to an upright freezer for storage of biologicals at -80 ° because it will remain cold for longer periods of time.
	If space and funds permit, store biological samples in LN ₂ rather than a freezer, because <ul style="list-style-type: none"> • a full LN₂ dewar will stay cold for months, even in 100 °F heat, if unopened; however . . . • the storage of tissue samples with bacterial samples creates a potential contamination issue, so . . . • transform bacteria and lyophilize the modified culture broths with bacteria in them, for storage at room temperature for indefinite periods of time.
	Keep an adequate supply of LN ₂ on hand.
	Consolidate LN ₂ samples into one container whenever amenable, even if that means sharing one between laboratories, subject to the constraints described above.
Research Data	Back up your electronic data on a regular basis to an easily retrievable location.
	Consider replacing your desktop computer with a laptop and docking station so data is easily portable in an emergency.
	Have students store research notes, laboratory notebooks, and samples in a predefined location so critical nonelectronic data can be easily located in their absence.
	Store flammable research notebooks in a fireproof and waterproof container.
Electrical Equipment	Place all electrical devices on appropriately sized battery backups with surge protection to guard against short-term power interruptions.
	For longer power interruptions, if time permits, shut down all electrical devices and turn off electrical breakers to prevent damage due to power surges upon being re-energized.

boring communities where postal facilities were open (and packed with people trying to get their mail). In some cases, computers and supplies were driven to their final destinations by faculty or staff members. Much of this effort could have been avoided with proper data storage practices. Though there are certainly security and accessibility issues with off-site data storage, in a case like this, in which faculty is forced to scatter to various locations without sufficient warning to retrieve or back up data, the ability to retrieve important information from a neutral site would be invaluable. One such resource currently under development is the Louisiana Optical Network Initiative (LONI)—<<http://mycenit.latech.edu/LONI2005/>>—which will provide a high-speed optical network for researchers at a number of Louisiana universities, including Tulane. But until such networks are in place and easily accessible to the research community, individual investigators must accept the responsibility for ensuring that their research data are secure and readily retrievable. A list of other “Lessons Learned” is shown in Table 1. An area for further research is listed in Table 2.

By Sept. 26, residents were being allowed back into Orleans Parish on a limited basis, so police escorts and convoys were no longer necessary. Recovery trips to the campus continued, and it was during the ensuing six- to eight-week period that the majority of computers and research equipment were removed to allow investigators to continue their research at external sites. In most instances, the investigators, or their representatives, were escorted onto the Uptown campus by either the dean of engineering or his designee. All

TABLE 2
More Information Needed

There is an issue with vapor phase vs. liquid phase storage of biologicals: There is a high probability that fungal spores will be floating in LN₂, and if the storage tubes are submerged in the liquid then there is a chance of sample contamination. On the other hand, a full dewar, if left unopened, can keep samples cold for months. Some kind of study would help clarify whether liquid phase storage is indeed safe for biologicals.

visitors to campus had to be cleared with the Office of Public Safety prior to their visits, and random identification checks from armed security officers were the norm. A system was established for recording institutional identification numbers for all equipment removed from the campus. Investigators were allowed to remove equipment for research purposes, but were informed that doing so could have insurance implications; i.e., if there was hurricane-related damage, they may not be able to prove it since insurance adjustors had not yet arrived on campus. A few investigators moved their labs—equipment, graduate students, and all—to host universities for the semester. Some chose to remain at Tulane and carry out their research with graduate students who had either remained behind or returned. By mid-November, escorted visits had virtually ceased, cleanup operations were well under way, and the Department of Chemical and Biomolecular Engineering was gearing up for the spring term. Tulane University officially opened to faculty and staff on Dec. 19, 2005, and the spring 2006 term began Jan. 16, 2006, right on schedule. □

DESIGN PROJECTS OF THE FUTURE

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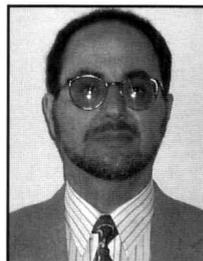
It is generally accepted that the chemical engineering profession is in a state of change. Fewer graduates from U.S. chemical engineering departments are entering the petroleum, petrochemical, and chemical industries, since most expansion in these industries is not in the United States. More graduates from U.S. chemical engineering departments are entering product-based industries (e.g., pharmaceutical, food, new materials) rather than the traditional commodity-chemical-based industries (ethylene oxide, benzene, sulfuric acid).^[1, 2] Therefore, changes in the undergraduate chemical engineering curriculum—which has been static for about 40 years (not counting advances in computing)—are imminent, if not already in progress.

Three significant changes in the chemical engineering curriculum are under way.^[3] First of all, biology is now considered to be an “enabling” science, along with chemistry and physics. Some education in the life sciences will soon be required for accreditation.^[4] Secondly, chemical engineers need to be taught about product design, either instead of or in addition to process design. It will become more important to teach batch operations, since the manufacture of new chemical products will certainly involve batch rather than continuous operations. Finally, over the past generation, advances in chemical engineering research have involved the ability to understand and to manipulate phenomena at the colloidal, nano, molecular, and atomic scales. A key issue is the effect on macroscopic properties of colloidal-, nano-, molecular-, and atomic-scale phenomena, *i.e.*, structure-property relations. It is time these advances became part of the undergraduate curriculum.

Radical changes to the traditional chemical engineering curriculum have been proposed.^[3] Changes are on the horizon, although the speed and degree of implementation of these changes is not yet obvious. It could also be argued, however, that traditional chemical process engineering must still be taught, because the soon-to-retire baby boom generation must

be replaced by newcomers equally capable of operating, maintaining, and updating existing chemical plants.

Given the importance of the capstone experience in the undergraduate education process, a question that arises when considering curriculum changes is: *What will the capstone chemical engineering design project of the future look like?* It is virtually certain that the capstone chemical engineering project of the future will not involve sulfuric acid or ethylene oxide production. Instead, it may have a life science basis. It may involve design of a product. It may involve multiscale phenomena, *i.e.*, the effect of nano- or molecular-scale interactions on the performance of the product. It is more likely to involve batch processing than continuous processing. And, it is also possible that manufacture of items and unit packaging—two concepts far removed from traditional chemical engineering—will be included.



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Richard Turton received his B.S. degree from the University of Nottingham and his M.S. and Ph.D. degrees from Oregon State University. His research interests are in fluidization and particle technology and their application to particle coating for pharmaceutical applications. Dick is a co-author of the text *Analysis, Synthesis, and Design of Chemical Processes (2nd Ed.)*, published by Prentice Hall in 2003.



In an effort to initiate a new capstone-design paradigm, the yearlong capstone design project at West Virginia University for 2003-04 and 2004-05 involved biologically oriented, multiscale product designs. These two projects are described in this paper. More details are available elsewhere^[5] and from the authors.

CLASS ORGANIZATION

In the senior year of chemical engineering at West Virginia University, the entire class works on a large project for two semesters under the direction of a student chief engineer. More details are presented elsewhere.^[6] Briefly, faculty members play roles: one is the client, for whom the students are “hired” to complete a design project; another is the “vice president” of the students’ company, who helps the students with technical matters. The student chief engineer divides the class into groups, each headed by a group leader. The role of the chief engineer is to represent the entire team to the client and to provide leadership from the “big picture” perspective. The group leaders receive assignments from the chief engineer and are responsible for completing the work within their groups. Assignments are deliberately vague and open ended. One goal is to force students to define their own work statement, with input from faculty members. Another is to learn material not normally taught in class. The exact topics students must learn are a function of the project. A further goal

is to make students realize that they will have to continue learning new material throughout their careers, and that they have the ability to do so.

In the fall semester, the project involves researching alternatives and a feasibility study. For example, in ice cream production, the assignment was to identify, screen, and recommend food products for production, with attention focused on products that have low-fat and/or low-carbohydrate alternatives. Students set their own direction with a minimum of input from the instructors. The client chooses one alternative for design in the spring semester. This is really the only opportunity for the instructors to influence the direction of the project; however, the client’s choice is always one of the top two student recommendations.

ICE CREAM PRODUCTION

This project was completed by 26 students over the course of the entire 2004-05 academic year. It started with a very open-ended assignment: to investigate opportunities in food processing, particularly those involving low-fat and low-carbohydrate alternatives. The market for these foods was to be analyzed, and the issues associated with producing the low-fat and low-carbohydrate alternatives were to be identified. A summary of the colloidal- and molecular-scale issues identified by students is shown Table 1. Production of any of these

Product	Processing Challenge
Ice Cream	Ice crystal formation must be kept to a minimum. Otherwise, the ice cream has a grainy texture. Nut and fruit size must be controlled to control the rheology. Processing conditions must be controlled to prevent nuts and fruit additives from becoming soggy. One method for making low-fat ice cream have the same mouth feel as regular ice cream is slow churning, a proprietary process of Edy/Dreyers. ^[5] By churning the ice cream at higher pressures and lower temperatures, smaller, more dispersed fat globules are formed that have similar mouth feel to regular ice cream.
Cookies	Almond flour is often substituted for wheat flour in low-carbohydrate cookies. Since almond flour contains more fat, the result is a chewier cookie. Granulated sugar is required in cookie manufacture so that the sugar will spread throughout the cookie during baking. Coarse sugar results in cracking. This has implications as to which sugar substitute can be used in low-carbohydrate cookies. Reduced-fat cookies require longer baking times to allow the existing fat to coat the flour and sugar particles. For sandwich cookies to stick together, the surface energy of the solid must be higher than that of the filling. One way to accomplish this is to raise the temperature of the filling and add more fat to the filling, both of which reduce its surface energy. (This is also true for ice cream sandwiches.)
Bread	Protein and fiber are often substituted for wheat flour in low-carbohydrate bread. Binding agents are required to hold these ingredients together. Dough conditioners are added for strength.
Cereal Bars	Binders are added to hold the cereal pieces together. They crosslink to form a flow-resistant structure. There are two common binders. One involves dipolar interactions between OH groups on glucose molecules in the binder and the cereal pieces. The other involves COO ⁻ groups bonding covalently with the cereal pieces.

products would make a good design project. Each involves batch processing of a product as well as manipulation at the molecular or colloidal levels to obtain desired macroscopic properties. Another feature involved, but traditionally unfamiliar to chemical engineers, is packaging.

Students used product screening methods to rank the alternatives.^[7] Ultimately, ice cream production to capture 1% of the domestic market was chosen for a complete design. Production of 1.75-quart containers plus some novelties (pops and bars, in this case) were included in the design. Ice cream production involves traditional chemical engineering, product design, and multiscale analysis. It involves application of principles of chemical engineering at scales from the molecular level to the process level.

Ice Cream Science. There are three categories of ingredients in the ice cream mix: dairy, sweeteners, and additives. Milk, cream, and nonfat milk solids make up the dairy portion of ice cream. Sucrose or Splenda® is used to sweeten the mix, and stabilizers and emulsifiers are added to give the ice cream the desired body and mouth feel. Significant quantities of air are also present in finished ice cream. Standard ice cream contains an equal volume of mix and air, or an “overrun” of 100%. Premium ice cream, however, has an overrun of only 80% to give it a richer, more-creamy, mouth feel.

Milk is a colloidal suspension of water, fat, and milk solids. Fat particles in the suspension range in size from 0.8 to 20 μm. The sugar—lactose—is also present in milk, at a concentration of about 4.9%. In “lactose-free” ice creams, the milk is treated with the enzyme lactase, which breaks lactose down into the simpler sugars glucose and galactose.

In this design, regular table sugar, or sucrose, is used as a sweetener in all the ice cream mixes except the low-carbohydrate ice cream. Sucralose is used to sweeten the low-carbohydrate ice cream because it is indigestible but still sweetens the mix.

Stabilizers and emulsifiers are essential in the production of ice cream products. Both components help to give ice cream a smooth body and texture and help to improve the overall mouth feel of the ice cream. Stabilizers work by reducing the amount of free water in the ice cream mixture. This retards ice-crystal growth during storage and also provides resistance to melting. Stabilization is accomplished through two mechanisms, depending on the type of stabilizer used, and both mechanisms may be involved depending on the structure of the gum used. Charged gums, such as carageenan, help to reduce the amount of free water because the charged groups interact with water to restrict the movement of water molecules within the mixture. Branched gums, such as guar gum, also reduce free water within the system. This is accomplished because the branched side chains contain hydroxyl groups that hydrogen-bond with water, a reaction that also reduces the amount of free water. Similarly, emulsifiers help to reduce fat-globule coalescence by stabilizing the fat globules within the ice cream matrix. Mono- and diglycerides are the most commonly used emulsifying agents. The addition of stabilizers and emulsifiers is particularly important for ice cream base mixes that are lower in fat content, because whole milk already contains natural stabilizing and emulsifying materials.

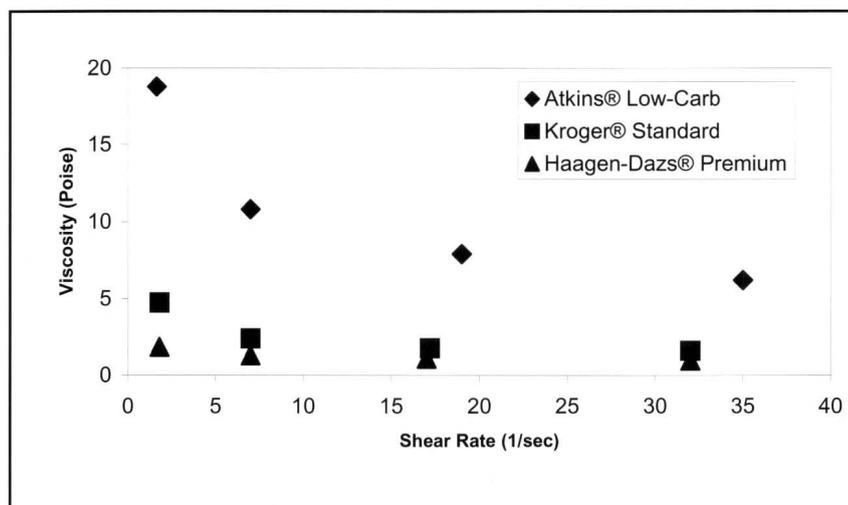
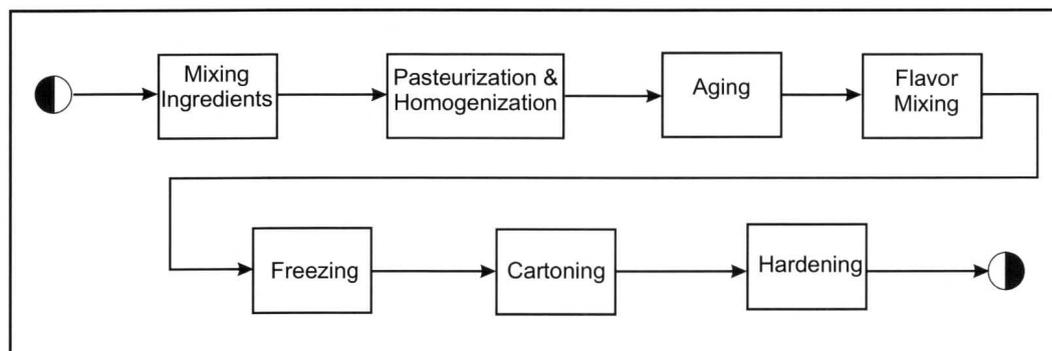


Figure 1. Viscosity of different ice cream products.

Figure 2. Block flow diagram for ice cream production.



The viscosity of ice cream varies with the type. During a class tour of a local ice cream production facility, the host remarked that production of low-carbohydrate ice cream was “difficult on the equipment,” which had been placed into operation before low-carbohydrate ice cream was developed. Further investigation revealed that many ice creams, particularly the low-carbohydrate vanillas, contain TiO_2 pigments to make the ice cream look whiter. It is possible that the TiO_2 colloidal particles cause erosion of process equipment. Students also wondered whether there was a variation between viscosities of different ice cream types. One student, who was doing research in the polymer research laboratory of our colleague Rakesh Gupta, measured the viscosity of three types of ice cream. The results are shown in Figure 1. Low-carbohydrate ice cream is clearly more viscous than standard ice cream.

Facility Design. A facility to manufacture, store, and ship ice cream was designed. Production volumes were 52 million 1.75-quart ice cream containers (varying flavors), 2.3 million six-packs of sandwiches, and 4.3 million six-packs of pops (ice cream bars with sticks). The manufacturing process of the ice cream facility is broken down into seven steps, as illustrated in Figure 2. A 5400-m² warehouse for ice cream storage was also designed. It was designed to hold three months of production. Because of the need to refrigerate the warehouse, the construction requires special insulation, and the capital investment for this part of the process (>80%) dominates the overall fixed capital investment (almost \$100 million)—a result that was not anticipated.

Refrigeration Cycle. Refrigeration (600 tons) is required three places: in the warehouse, in the hardening step in ice cream production, and for cooling the milk at the front end of the process. An ammonia refrigeration-cycle design, used for the warehouse, is displayed in Figure 3. The refrigeration cycle is a traditional chemical engineering component of this design. Using the number of interstage coolers on the compressors and the type of cooling medium used in E-101 through E-104 as decision variables, students optimized the refrigeration process.

Steam Generation. In the facility, low-pressure steam is used for pasteurization, for jacketed heating of the mixing equipment, and for heating water for equipment cleaning. These steps are necessary to ensure that there is no product contamination by bacteria, which is part of “good manufacturing processes” in food production. Therefore, a typical steam-production facility was designed.

Wastewater. A system was designed to process wastewater from the ice cream manufacturing facility. There were two reasons for this. First, it was assumed that the ice cream plant would produce too much additional wastewater for an existing municipal wastewater facility. Second, based on information from the local water authority, having a water treatment facility in-house appeared to be the less-expensive option. Wastewater treatment is needed because the equipment must be cleaned daily, generating significant amounts of wastewater. The operation plan involves production on two

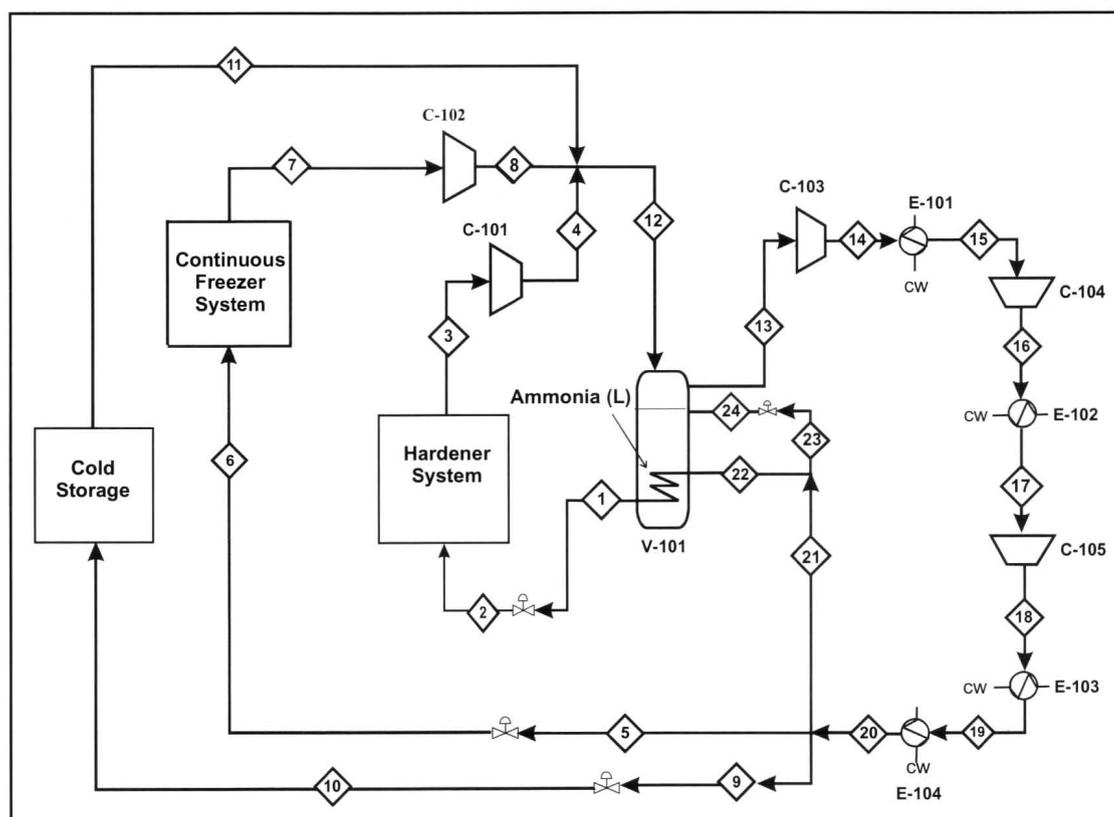
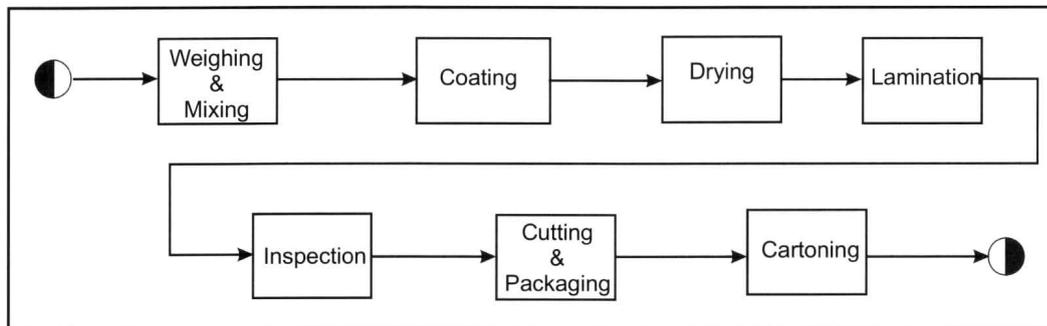


Figure 3. PFD for the optimized ammonia refrigeration system unit 1.

Figure 4.
Block flow diagram
for transdermal
drug delivery patch
manufacture.



shifts per day followed by a cleaning shift. Most of the cleaning is done using hot water.

Economics. It costs approximately \$0.56 to produce a 1.75-quart container of ice cream, including the initial capital investment. Even with the markup associated with the food distribution chain, the process is very profitable. The net present value (NPV) was found to be \$97 million, assuming a 10-year plant lifetime and a 15% before-tax rate of return. A Monte Carlo analysis showed that there is only an 8% chance of losing money, *i.e.*, an NPV less than zero. Remarks from an ice cream expert at the final student presentation indicated that prices for milk products could vary over a wide range, leading to significantly greater variation in the NPV. These factors were not considered in the students' analysis but could easily be incorporated.

DESIGN OF A TRANSDERMAL DRUG DELIVERY SYSTEM

This project was completed by 11 students over the course of the entire 2003-04 academic year. It also started with a very open-ended assignment: to investigate alternative forms of drug delivery, and to suggest a product to be manufactured. Within the transdermal patch category, students learned the properties that make a drug suitable for use in a transdermal patch, which are: (1) low molecular weight, (2) high potency, so low dosage required, (3) resistance to enzymes in skin layers, and (4) desire to have constant dosage in body over time. Item number 4 means that a transdermal patch would not be used to treat a simple headache, because, for a headache, rapid entry of the drug into the blood is desired. Students used product-screening methods to choose between alternative drugs.^[7] Ultimately, production of a contraceptive transdermal patch for females was chosen for a complete design.

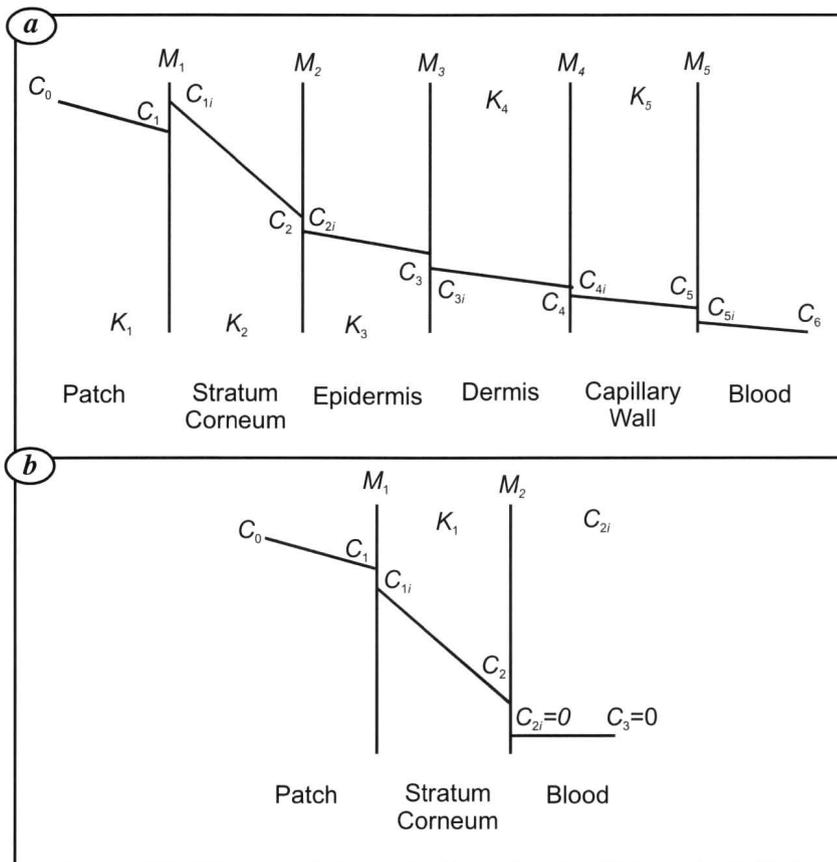


Figure 5. Model for diffusion through skin layers.

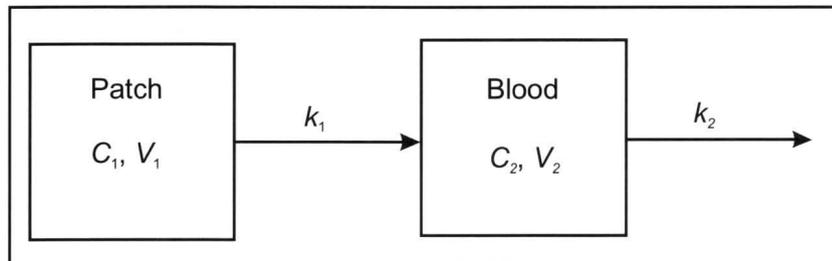


Figure 6. Two-compartment pharmacokinetic model.

Patch Design. The patch contains norelgestromin and ethinyl estradiol. The proposed size of the patch is 10 cm², manufactured as a single-layer, matrix system.

Pressure-sensitive adhesives are the common form of adhesive used in transdermal systems. They are permanently tacky at room temperature, they are easily applied with light pressure, and they do not require solvents for activation. Polyisobutylene was chosen because it provides excellent adhesion in high-moisture environments and because of its low cost. Polyisobutylene has a surface tension of 30-32 dyne/cm, which is lower than the critical surface tension of skin of 38-56 dyne/cm, depending on humidity and temperature. Therefore, the adhesive will wet the skin—a requirement for adhesion. This is an example of colloid-scale considerations in the transdermal patch design.

Skin penetration enhancers increase the mass flux of a drug across the desired surface area. The driving force for the drug is the concentration gradient between the patch and the skin. The enhancer used in this patch is crospovidone, which draws water to the surface of the skin. This in turn causes swelling, which provides more surface area for diffusion.

Excipients are ingredients within a drug product that are considered inactive, from a pharmacological perspective. In this case, there is one excipient used, propylene glycol monolaurate, which acts as an emollient.

Manufacturing. The block flow diagram for manufacture of the transdermal patch is shown in Figure 4. It is a batch operation. First, the ingredients must be weighed and mixed. The drugs are mixed with the adhesive. The appropriate mixing time and impeller arrangement are estimated using typical chemical engineering principles.^[8] Then, the mixture is coated on the backing. Hexane is used as a solvent to help lower the viscosity of the solution and to ensure a well-mixed product. After coating, the hexane is evaporated and is subsequently incinerated, because it was determined that there was not enough hexane present to justify a recovery system. Next, the release liner is added to sandwich the drug/adhesive mixture. After inspection (as required by law) large sheets are cut into 10 cm² patches, packaged individually, and then packaged again, three per carton. Finally, cartons of the three-packs are packaged for distribution.

Part of the design involved identifying “good manufacturing practices” in the pharmaceutical industry, which ensure that the product is pure and free of contamination.

Economics. Students determined that the cost of manufacturing one patch is between \$0.28 and \$0.30, depending on employee salaries and the plant location. The U.S. pharmacy price for a similar, brand-name product is approximately \$15 per patch. Since this product is to be a generic version, it was assumed that its price would be about half of the brand-name product. The markup at the pharmacy is assumed to be twice the price for which it was purchased. Therefore, the estimated manufacturer’s patch price is \$3.75. Selling the patches for \$3.75 per patch yields a net present value of \$684 million assuming a 10-year plant lifetime and a 15% before-tax rate

A . . . goal is to make students realize that they will have to continue learning new material throughout their careers, and that they have the ability to do so.

of return. No information was available from industry sources to verify these assumptions or the resulting NPV estimate.

Mathematical Modeling. In the design of a transdermal patch, the dose is a key factor to consider. The drug is delivered from the patch to the body by diffusion through the multiple layers of skin, so students were required to model diffusion through multiple, immiscible layers. The flux of a given drug from a transdermal system into the body can be modeled as shown in Figure 5a. The result is

$$j = \frac{C_0 - \frac{C_n}{\prod_{j=1}^n M_j}}{\frac{1}{K_0} + \sum_{j=1}^n \frac{1}{K_j \left(\prod_{j=1}^n M_j \right)}} \quad (1)$$

where C_0 is the concentration of the drug in the patch, K_j is the inverse of the resistance to diffusion of the drug provided by each skin layer, and M_j is the partition coefficient of the drug between a layer and the subsequent layer ($M_j = C_{ji}/C_j$). It was found that the rate-limiting step is diffusion through the stratum corneum layer. So, if it is assumed that the concentration in the blood is zero ($C_n = 0$), the model reduces to Figure 5b, and Equation (1) becomes

$$j = C_0 K_1 M_1 \quad (2)$$

A pharmacokinetic model was also developed, which can be used to predict the concentration of the active ingredients in the blood. The model is illustrated in Figure 6, and the equations are

$$\frac{dC_1}{dt} = \frac{-k_1 C_1}{V_1} \quad (3)$$

$$\frac{dC_2}{dt} = \frac{k_1 C_1 - k_2 C_2}{V_2} \quad (4)$$

where C_1 is the concentration of an active ingredient in the patch, k_1 is the elimination rate constant from the patch, V_1 is the volume of the patch, C_2 is the concentration of the active ingredient in the blood, k_2 is the elimination rate constant from the blood, and V_2 represents the volume of blood in which the drug is distributed. Students fit this model to published data to determine the values of k_1 and k_2 .^[9, 10]

Multiscale Design. In terms of multiscale analysis, design of a transdermal drug delivery system requires design from the molecular scale through the macroscopic scale. These

items are summarized in Table 2. At the molecular scale, the drug itself is designed. This is beyond the scope of this project. At either the molecular or nano scales, one finds the presence of excipients and/or enhancers in the patch. The adhesive to hold the transdermal patch to the skin could involve design at multiple scales. Since the drug is mixed with the adhesive, if there were a molecular interaction between the drug and adhesive, it would have to be understood. For an adhesive to stick, it must wet the skin, so an understanding of colloid-scale wetting phenomena is required. The patch must be removed without significant discomfort, yet not become detached in the shower or during physical activity that causes sweating—both macro-scale phenomena. At the microscopic scale, the mechanism of transport of the drug through the skin must be understood. Modeling drug transport through the skin layers is standard transport phenomena. Similarly, there is system modeling, in which the pharmacokinetics of the drug in the body can be modeled. Finally, at the macroscopic scale, the components must be combined appropriately, manufactured into the desired product, and packaged for sale.

ASSESSMENT

Two assessment measures were used. In one, the two instructors use a rubric to evaluate, separately, all aspects of the final design report and oral presentation submitted by the students each semester. This rubric was developed in the context of more traditional chemical engineering design problems. For example, since biology is not (yet) required in our curriculum, it is not listed as a science that students are expected to demonstrate an ability to apply. The ability to learn and to apply biological concepts as needed is evaluated under the ability to learn new material not taught in class. The complete rubric is available on the Web.^[11] Table 3 shows the results, averaged for the two instructors, for both projects. The score of three indicates *meets expectations*, and the score of four indicates *exceeds expectations*. Clearly, our assessment of the students suggests that they exhibited superior performance in the ability to teach themselves new material.

In our student evaluation of instruction, it is possible for the instructor to add an individually defined question. Table 4 shows several such questions and the student responses. The responses are on a 5-point Likert Scale, thus indicating student responses were all between “agree” and “strongly agree.” Therefore, we conclude that the students involved in these projects believed them to be beneficial.

DISCUSSION

One of the advantages of a project such as ice cream production is that it has traditional chemical engineering components (*e.g.*, refrigeration cycle, wastewater treatment, steam production) along with multiscale considerations, product design and manufacture, and packaging. Design of a transdermal drug patch has a stronger life science component and involves more transport phenomena-oriented mathematical modeling (*i.e.*, systems analysis) than a traditional chemical process design.

While the multiscale aspects of these projects have been identified, the molecular-scale phenomena have not yet been incorporated into the design. For example, we do not believe that we are in a position to design a new drug or to manipulate the microstructure of ice cream. If, however, a product design assignment were based on a faculty member’s research, it might be possible to include molecular-, nano-, or colloidal-scale design aspects, especially if students were in a position to perform experiments.

A reasonable question is what other design projects of this type are envisioned. The list of potential life science-related projects is long and could include innovative drug-delivery devices (*e.g.*, drugs on a chip) or tissue growth. Our class of 2003 designed a facility for the batch production of amino acids.^[5] Design of a microprocessor production facility would involve multiscale phenomena and could also involve traditional chemical engineering in the production of ultra-pure water and in wastewater treatment. Design of an advanced material based on its micro- or nano-structure is also possible. The importance of multiscale phenomena in paper manufacture was recently presented,^[12] so manufacture of fine paper products is a possibility.

More detailed synopses of these projects are available on our design project Web site.^[5] The final reports are also available to faculty members by contacting the authors.

CONCLUSIONS

As the profession of chemical engineering moves toward product development and design and away from process development and design, a new paradigm for chemical engineering education is evolving, requiring a new generation of capstone design projects. Two examples have been presented here. In ice cream manufacture, multiscale considerations are important, yet there are traditional chemical engineering components included. Production of other food products involves

nano scale	the action of enhancers and excipients at a molecular level on the skin surface
colloid scale	mechanism of adhesion
micro scale	transdermal transport phenomena
	pharmacokinetics
macro scale	product manufacture

many of the same considerations. In design of a transdermal drug delivery patch, life science considerations, multiscale factors, and systems modeling are required. Both involve aspects of product design. They also require manufacture and packaging of unit items—topics traditionally foreign to chemical engineering education. As the chemical engineering curriculum changes in response to the changes in our profession, similar design projects will find their way into capstone experiences.

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TABLE 3
Assessment Results for Design Projects

Assessment	Patch	Ice Cream
Design of equipment, understand interrelationship between equipment in process	3.0	3.0
Apply chemistry, math, physics, engineering science	3.5	3.5
Resolve complex problem into components	3.0	3.5
Apply economic, physical constraints, and optimization methods to obtain solution	3.0	3.0
Use of computer-based and other information systems	3.0	3.0
Demonstrate ability to learn new material not taught in class	4.0	4.0
Demonstrate ability to function in assigned role	3.0	3.0
Demonstration of ethical behavior	3.0	3.0
Demonstrate understanding of societal impact and need for assigned design	3.0	3.0

TABLE 4
Student Evaluation of Instruction Results

Result	Group Asked	Out of 5.0
Tackling the nontraditional problem posed in the large-group project enhanced my confidence in solving new problems.	Patch	4.90
I feel that my experience with the group design taught me the importance of and the need for continuously learning new material.	Patch	4.17
In my career, I will be required to solve problems appearing to be outside the mainstream of chemical engineering, such as food processing.	Ice cream	4.17
I feel confident that I can apply my chemical engineering knowledge to any application.	Ice cream	4.40
The teamwork experience in this class will be valuable in my future career.	Ice cream	4.57

Random Thoughts . . .

A WHOLE NEW MIND FOR A FLAT WORLD

RICHARD M. FELDER

North Carolina State University

Interviewer: “Good morning, Mr. Allen. I’m Angela Macher—project engineering and human services at Consolidated Industries.”

Senior: “Good morning, Ms. Macher—nice to meet you.”

I: “So, I understand you’re getting ready to graduate in May and you’re looking for a position with Consolidated . . . and I also see you’ve got a 3.75 GPA coming into this semester—very impressive. What kind of position did you have in mind?”

S: “Well, I liked most of my engineering courses but especially the ones with lots of math and computer applications—I’ve gotten pretty good at Excel and Matlab and I also know some Visual Basic. I was thinking about control systems or design.”

I: “I see. To be honest, we have very few openings in those areas—we’ve moved most of our manufacturing and design work to China and Romania and most of our programming to India. Got any foreign languages?”

S: “Um, a couple of years of Spanish in high school but I couldn’t take any more in college—no room in the curriculum.”

I: “How would you feel about taking an intensive language course for a few months and moving to one of our overseas facilities? If you do well you could be on a fast track to management.”

S: “Uh...I was really hoping I could stay in the States. Aren’t

any positions left over here?”

I: “Sure, but not like 10 years ago, and you need different skills to get them. Let me ask you a couple of questions to see if we can find a fit. First, what do you think your strengths are outside of math and computers?”

S: “Well, I’ve always been good in physics.”

I: “How about social sciences and humanities?”

S: “I did all right in those courses—mostly A’s—but I can’t honestly say I enjoy that stuff.”

I: “Right. And would you describe yourself as a people person?”

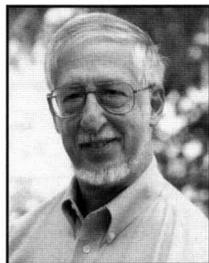
S: “Um...I get along with most people, but I guess I’m kind of introverted.”

I: “I see” (Stands up.) OK, Mr. Allen—thanks. I’ll forward your application to our central headquarters, and if we find any slots that might work we’ll be in touch. Have a nice day.”

* * *

This hypothetical interview is not all that hypothetical. The American job market is changing, and to get and keep jobs future graduates will need skills beyond those that used to be sufficient. This message is brought home by two recent books—Thomas Friedman’s *The World is Flat*¹ and Daniel Pink’s *A Whole New Mind*²—that I believe should be required reading for every engineering professor and administrator. The books come from different perspectives—the first economic, the second cognitive—but make almost identical points about current global trends that have profound implications for education.

An implication for engineering education is that we’re teaching the wrong stuff. Since the 1960s, we have concentrated almost exclusively on equipping students with analyti-



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¹ T.A. Friedman, *The World is Flat*, New York, Farrar, Straus, & Giroux, 2005.

² D.H. Pink, *A Whole New Mind*, New York, Riverhead Books, 2005.

cal (left-brain) problem-solving skills. Both Friedman and Pink argue convincingly that most jobs calling for those skills can now be done better and/or cheaper by either computers or skilled foreign workers—and if they can be, they will be.³ They also predict that American workers with certain different (right-brain) skills will continue to find jobs in the new economy:

- *creative researchers, developers, and entrepreneurs who can help their companies stay ahead of the technology development curve;*
- *designers capable of creating products that are attractive as well as functional;*
- *holistic, multidisciplinary thinkers who can recognize complex patterns and opportunities in the global economy and formulate strategies to capitalize on them;*
- *people with strong interpersonal skills that equip them to establish and maintain good relationships with current and potential customers and commercial partners;*
- *people with the language skills and cultural awareness needed to build bridges between companies and workers in developing nations (where many manufacturing facilities and jobs are migrating) and developed nations (where many customers and consumers will continue to be located);*
- *self-directed learners, who can keep acquiring the new knowledge and skills they need to stay abreast of rapidly changing technological and economic conditions.*

Those are the attributes our students will need to be employable in the coming American engineering job market. The question is, are we helping them to develop those attributes? With isolated exceptions, the answer is no. We still spend most of our time and effort teaching them to “Derive an equation relating A to B” and “Calculate Z from specified values of X and Y.” We also offer them one or two lab courses that call on them to apply well-defined procedures to well-designed experiments, and we give them a capstone design course that may require a little creativity but mostly calls for the same calculations that occupy the rest of the curriculum. Nowhere in most engineering curricula do we provide systematic training in the abilities that most graduates will need to get jobs—the skills to think innovatively and holistically and entrepreneurially, design for aesthetics as well as function, communicate persuasively, bridge cultural gaps, and periodically re-engineer themselves to adjust to changing market conditions.

Why don't we? It's because people as a rule don't want to leave their comfort zones, and engineering professors are as subject to that rule as anyone else. We are all comfortable deriving and solving equations for well-structured single-discipline systems, but most of us are not so sure about our ability to handle ill-defined open-ended multidisciplinary problems or to teach creative thinking or entrepreneurship. So, despite a crescendo of headlines and best-sellers about the growing exodus of traditional skilled jobs to developing countries (including high-level research and development jobs, which are increasingly moving to India and China⁴), many engineering faculty members vigorously resist suggestions to make room in the curriculum for multidisciplinary courses and projects or anything that might be labeled “soft.” Even though most of our alumni in industry—95%? 99%?—assure us (as they have done for decades) that they haven't seen a derivative or integral since they graduated, the traditionalists still insist that we can only produce competent engineers by devoting almost every course in the curriculum to deriving and solving equations, analytically and with Matlab. The same professors are no less resistant to efforts to move them away from the traditional “I talk, you listen” pedagogy toward the active, cooperative, problem-based approaches that have been repeatedly shown to equip students with the skills Friedman and Pink are talking about. (See bibliography on p. 113.)

So far we've gotten away with it, although sharply declining engineering enrollments in recent years should be a red flag. We can't count on getting away with it much longer, however. The relentless movement of industry to computer-based design and operation and offshoring of skilled functions and entire manufacturing operations is not about to go away. On the contrary, as computer chips get faster and developing countries acquire greater expertise and better infrastructure, the movement will inevitably accelerate. The American engineering schools that respond by shifting toward more multidisciplinary problem- and project-based instruction—the way Olin, Rowan, Rose-Hulman, the Colorado School of Mines, and a number of others have already started to do—will survive. The schools that try to stick with business as usual may not. □

³ If you don't think this is already happening in engineering, check out a 2005 NAE Report called “Offshoring and the Future of U.S. Engineering: An Overview,” <www.nae.edu/NAE/bridgecom.nsf/weblinks/MKEZ-6G6R4D?OpenDocument>.

⁴ S. Lohr, “Outsourcing is Climbing Skills Ladder,” *New York Times*, Feb. 16, 2006. This article reports that of 200 multinational corporations surveyed, 38% said they planned to “change substantially” the worldwide distribution of their R&D work in the next three years . . . and this particular trend is still in its infancy.

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

Maintaining Connections with Undergraduates

Continued from page 83

requested to provide contact information for classmates (e-mail addresses, cell phone numbers, etc.). If they were uncomfortable doing this, they were asked to contact classmates themselves and encourage them to contact one of the faculty. This approach, along with posting a request on the department's blog (see Professor Ashbaugh's account), still only allowed direct contact information to be gathered for about 50 percent of our students. The junior and senior classes, however, had set up their own Yahoo groups prior to the storm, which meant departmental e-mails ultimately reached more students. In one instance, a student posted faculty messages to a Web site the student had built specifically for sharing department information with classmates. In retrospect, gathering alternate contact information prior to Katrina as a regular part of getting acquainted with students would have allowed department outreach efforts to be more effective after the hurricane.

Student feedback from phone conversations led to the realization that our core course curriculum was aligned with only a fraction of other chemical engineering programs. Our unique Practice School program during the senior year⁽³⁾ requires that most core courses be offered a semester earlier than other programs. As a result, students found it challenging to find the chemical engineering courses they needed. Of particular concern were the seniors and their need to complete a capstone design course before graduation. Within a day of recognizing this issue, the consensus from the faculty was that our process design course would be offered during the spring semester. This information was quickly communicated to the seniors. The speed with which decisions of this type were made and communicated ultimately affected the options our students had during fall registration. Since Katrina made landfall the weekend before the semester started, however, even the best efforts meant students began attending classes at other universities two to three weeks late.

Many students evacuated New Orleans without their textbooks or notes. Because of the broad scope of most capstone design courses, the most affected group was those seniors who managed to enroll in this course. As a result, the faculty member who would have taught this course within our department during the fall semester offered to provide supporting information from books that the students owned but left in New Orleans.

Those students who attended other universities in the fall were requested to send us the name of the university and the courses for which they were registered. This provided a means of double checking what the student thought was an equivalent core course. If the course was not adequately equivalent, the student was quickly notified. Under the difficult circumstances, many students pragmatically chose to take their remaining non-ChE courses during the fall.

Near the end of September, the faculty began discussing the course schedule for the spring and Lagniappe semesters. From the fall registration information provided by our students, it became evident that offering all core courses during these two semesters would be a requirement in order to keep the students on track. By mid-October, a course schedule for both semesters had been established which met this objective.

Registration for the spring semester at Tulane began in early November. Two weeks prior to registration, all students were sent an e-mail requesting they update their fall course-enrollment information. In this e-mail, students were also informed that they would be able to contact three departmental advisors (Drs. Mitchell, John, and Prindle) by phone for advising assistance over the five-day period just prior to the beginning of registration. This call center setup provided the students with assistance in addressing their registration questions. Since the university Internet and e-mail servers were restored in mid-October, there was no problem contacting all of our students using their university e-mail addresses. The response to this request was substantially higher.

Several challenges had to be overcome in manning the call center. Since the campus was closed and security was tight, department offices could not be entered without special permission. In addition, service to department phones was not activated until the second day. Despite obstacles, the call center was ultimately successful in providing students with assistance in addressing their concerns prior to registration.

All of these efforts in establishing and maintaining the faculty-student connection were difficult under the challenging conditions. We believe, however, that they have forged even stronger ties between both groups. As a result of these experiences, some students feel more comfortable discussing problems with faculty. Faculty interest in our students and their well-being has increased as well. While both groups looked forward to the start of the spring semester and a return to a sense of normalcy, that normal state will be distinctly different. And, in many ways, better. □

INTRODUCTION

TO A SPECIAL SECTION ON THE

Patten Centennial Scientific Workshop:

THE NEXT MILLENNIUM IN CHEMICAL ENGINEERING

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Over the past several years, a number of chemical engineering programs around the country have been honoring the 100-year anniversaries of their origins. The 2004-05 academic year marked a similar time at the University of Colorado. In 1904-05, coursework for a B.S. in chemical engineering included Slide Rule, Surveying, Oil and Fuel Laboratory, and Heat Treatment of Steel, whereas today's curriculum includes courses such as Engineering Computing, Environmental Separations, Polymer Science, Particle Technology, Tissue Engineering, and Pharmaceutical Biotechnology. Similar—if not greater—changes to the chemical engineering discipline are expected during the next century.

To commemorate the centennial year, a scientific workshop dedicated to discussions on the future of the discipline was hosted by the Department of Chemical and Biological Engineering at the University of Colorado on Feb. 3 and 4, 2005. The participants included Professors Kristi Anseth (Univ. Colorado), Bob

Armstrong (MIT), Arup Chakraborty (UC Berkeley), Ed Cussler (Univ. Minnesota), Mike Doherty (UC Santa Barbara), Richard Felder (NC State), and Jerry Schultz (UC Riverside)—see Figure 1, next page. The workshop consisted of two parts, namely oral presentations and panel discussions. This feature section is intended to share these exchanges with the greater ChE community.

In the first portion of the workshop, each of the seven participants was asked to give an oral presentation on a topic of his or her choice, with a theme that is both broad in scope and forward thinking. An ordered list-

ing of the talks is given in Table 1, next page. Corresponding written perspectives were requested of each participant; these perspectives are contained in the accompanying group of articles. The manuscripts cover pedagogical issues (Professors Armstrong and Felder), a view on the current chemical industry (Professor Cussler), and outlooks on emerging areas (Professors Doherty and Schultz).



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H. Scott Fogler. After receiving his Ph.D. from the University of Colorado, he joined the University of Michigan where he is currently the Ame and Catherine Vennema Distinguished Professor of Chemical Engineering. He is author of the text Elements of Chemical Reaction Engineering. His current research interests are in the areas of colloids, wax gelation kinetics, dissolution kinetics of zeolites, and the pharmacokinetics of acute toxicology. He has graduated 36 Ph.D. students in these and related areas.



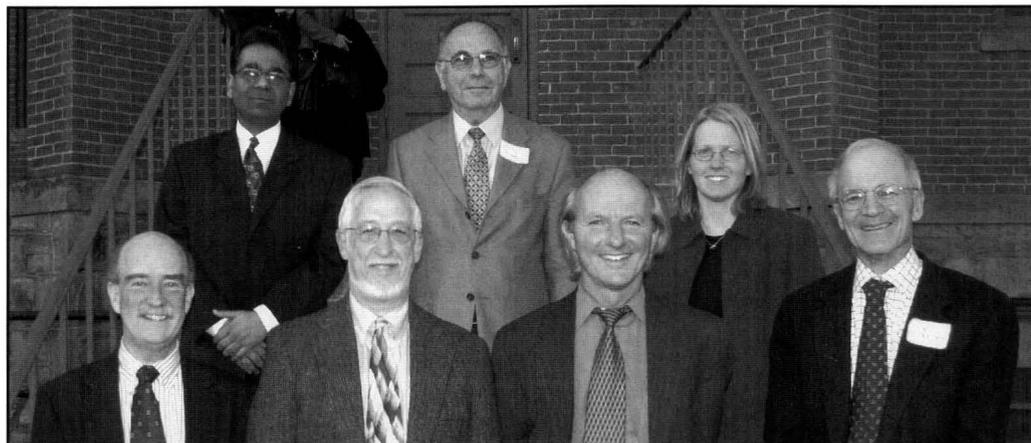


Figure 1.
 Participants in the Patten Centennial Scientific Workshop—University of Colorado, February 2005.
 Top row:
 Arup Chakraborty,
 Jerry Schultz,
 Kristi Anseth.
 Bottom Row:
 Bob Armstrong,
 Richard Felder,
 Mike Doherty,
 Ed Cussler.

Q AND A

The second portion of the workshop comprised two panel discussions, both of which were driven by questions from the attending faculty and graduate students. A paraphrased overview of this exchange, grouped according to topic, is given below. The respondents are indicated according to their initials (see Table 1). Since these discussions took place after individual presentations, the reader may choose to read this portion after the ensuing manuscripts to keep the chronology of the interactions intact.

Curriculum

Question (to BA): How do you envision the curriculum change you have proposed occurring (see related perspective by Bob Armstrong)?

BA: I think we should start with a clean slate and start by adding back in the most important areas and then stop adding when four years are full. I think the approach should not include adding more classes than we currently have, as that will lead to an overcrowding of schedules and then the students would have no time to think about what they are learning.

We have not changed the curriculum in the last 40 years due to the large research engine created after World War II. Faculty were too busy with research to improve significantly the content in the classroom. Faculty have to take time from research, for example to write textbooks or Web modules. We need to do this together as a community of universities. You have got to reward faculty for implementing change.

EC: There is no way that we could possibly do what Bob is saying. Also, committee books are really bad usually. I think modifications need to be done one course at a time. Let me liken it to the past when periodic tables were put on the classroom walls. At that time, boiling points were the only important properties we

TABLE 1
Presentation Listing

Participant	Title
Prof. Richard Felder (RF)	Teaching Engineering in the 21st Century with a 12th-Century Teaching Model: How Bright is That?
Prof. Bob Armstrong (BA)	A Vision of the Chemical Engineering Curriculum of the Future
Prof. Arup Chakraborty (AC)	Quantitative Cellular and Molecular Immunology: A New Opportunity for Chemical Engineering
Prof. Jerry Schultz (JS)	In Vivo BioImaging: Advances and Challenges
Prof. Ed Cussler (EC)	A Different Chemical Industry
Prof. Mike Doherty (MD)	Crystal Engineering: From Molecules to Products
Prof. Kristi Anseth (KA)	Chemical Engineering in 2020: Return of the J.E.D.I.?

needed to know because everything was petrochemicals. Now, chemical engineers are using the information on the periodic table.

Question: With all the changes and additions that have been suggested, do you think there will need to be a five-year undergraduate degree? Or is it time that we separate the curriculum into new majors (*e.g.*, tissue engineering, metabolic engineering)?

RF: We cannot put in all the content, since the content is always changing. We have to emphasize how to learn, skills, flexibility.

BA: You need to learn a good way of thinking—the courses are just vehicles. I think it is a mistake to fractionate into subareas at the undergraduate level. As a career evolves you are always introduced to new areas, so you learn to augment knowledge. Incidentally, the renaming of many departments that has occurred recently—to include “bio” in their name—is very different than the splitting into subareas we are talking about. The inclusion of “bio” in a department name reflects the change in our underlying molecular core science from chemistry alone to a combination of chemistry and biology.

EC: If you put in new material, you have to chop out fluff. We can do that by compressing courses (*e.g.*, transport phenomena). But we also need to adapt to what is relevant. For example, I think it is a tragedy that at Minnesota we teach thermodynamics without covering the topic of ionic solutions, which has tremendous biological relevance.

KA: It is important to consider which industries we want to serve when implementing changes into our curriculum.

Textbooks

Question: A number of the items discussed thus far have been about modifying courses and teaching new courses. One problem set I foresee is: Where are the textbooks, when will they come, and how will authors be rewarded?

MD: Scholars are responsible for writing research papers, books, patents, and grants. There is a need to de-emphasize papers and make a global contribution like writing texts. It’s so hard to write a book. Role models are key—if role models write books then others will be written; if they don’t, then there will be no books. A large problem is that there is insufficient reward for writing texts. Nevertheless, academics should do it as part of their job.

RF: It is hard to write books—hard and time consuming. Don’t write a book before you have tenure. Rewards? Don’t do it for rewards. A book only counts as a publication and the effort it takes is the same as for 25-50 publications. Write it because you want to write it—it will be a better book if it’s a labor of love.

BA: People need to step forward and do it—or at least convince others to do it. One reward is that the reputation of the school gets better when books are written by faculty. The rewards are not well-translated to individual rewards. One answer may be to get teams of faculty to write books. The books become much more interesting and have broader perspective if they are done as truly collaborative efforts, and there’s less work per person.

Role of Biology

Question (to JS): What do you see as the future for division of labor between materials science and bioengineering?

JS: We will have some aspects of materials science tailored to bioengineering. Why should a name be changed to Biochemical Engineering? There was no change to Plastic Chemical Engineering when plastics were the popular topic in chemical engineering. To be successful, engineering programs must collaborate with true biology programs. Also, engineers design new products based on physics, chemistry, and biology. Now that we can manipulate biology, biology is becoming more quantitative.

Question (to AC): Did basic biology prepare you for the biological research you are undertaking?

AC: The curriculum Bob talked about is exactly what is required. Learn the general idea and work from the molecular up to the macroscopic.

The Next Millennium in ChE

Teaching Methods

Question (to RF): Do you believe distance learning is better? I'm asking about isolationism vs. learning in the presence of other students?

RF: Compared with an active-learning class, distance learning is not better. There are some things technology can never replace. I don't believe software will ever be able to motivate students. That's not to say we can't supplement an active-learning classroom with technology.

Question: How should industry perspectives be incorporated into the undergrad classroom?

RF: Take industry problems and bring them into the classroom. Use a problem-solving method and let students take the lead in making decisions.

JS: Bring in industry representatives to be a part of the design team and problem-solving effort. Use real corporate resources and financial support to solve real, relevant, industrial problems.

MD: From real-world consulting experience with DuPont, I understand that engineers typically have very short windows in which to make decisions with limited information. It is important to develop skills to quickly and hierarchically make these decisions. Each result should yield a "yes" or "no" response for continuing or changing paths.

EC: Define complex problems and have some process for judging if a commercial product is likely to work. Expose students to situations where they have to make decisions with limited data.

Enrollments / Future of the Discipline

Question: What is happening with ChE enrollments?

EC: Although we are seeing decreasing enrollments, we should look at the bigger picture. There has been an increase of 50% in ChE programs and a decrease in enrollment—that makes sense. On my way here, I was doing a little research and did you know that there are 11 Ph.D. programs in the state of Ohio—that's silly! I think it is time to start killing programs for undergraduates and graduates.

BA: Undergraduate enrollment is on the increase again. In 2000, there were 6,000 undergraduates enrolling per year. Enrollment since 1973 can be fit with a sine wave and seems to follow job growth. Times change. It is up to educators to know what industries are growing/shrinking and make students aware of it. My concern is not so much at the B.S. level as it is to where are all the Ph.D.s are going to go for jobs?

AC: Ph.D. enrollment is flat during the same time.

JS: In ChE, enrollment varies up to about 10% a year. The amount of high school graduates going into the field of engineering, however, is about the same. It's all dependent on jobs.

Question: Say I am a high school senior who is really good at math and science. How would you convince me to be a chemical engineer?

JS: Out of all engineering, chemical engineering has the widest range of basic science. Chemical engineering offers students a good systems base for the next 30-50 years.

BA: Chemical engineering is preparation for a diverse range of career types.

MD: Our primary asset is that we can provide quantitative solutions. This differentiates us from chemists, biologists, etc. With a ChE B.S., one can go out into the real world with a good-paying job. Chemists and biologists tend to have a more difficult time finding more challenging, higher-paying jobs at the B.S. level.

RF: This is the only discipline that can put together so many sciences. Chemical engineers can be found in many, if not most, technical fields in industry. Also, most students don't know what they are interested in, so it keeps doors open (*e.g.*, environmental, health care).

Global Competition

Question: With the battle for global economy and our standard of living in jeopardy, what are your thoughts on lower-cost plants and research moving to other countries? How do we innovate and bring new products/technologies to market quickly to win? What can faculty do?

BA: We need to teach our students marketing, how to identify real needs, and how to solve problems to meet those needs. We can only succeed if we innovate—*not* by becoming a service-based country. One minus for the United States is that our culture is not one that tends to save money. There are concerns that we will not have money required for investment in R&D.

MD: There is a natural progression in history that the same main group of countries innovates, and the new technologies/products become more commodity and move to other places, *e.g.*, steel. In the 1880s, the 20 richest places in the world included North America, Europe, and Australia. In the 1980s the list had not changed much, with few exceptions, including the addition of Japan to the list. It is fairly hard to screw things up! Well-established systems and stable governments lead me to believe things will remain the same.

Energy and Water Research

Question: In the next 50 years, what will be the biggest problem of the world and what role will chemical engineers play in solving it?

EC: Energy and water. I do not think ChEs will dominate health care or food. Regarding water, ultrafiltration to remove viruses is needed. Regarding energy, gas will cost \$6 a gallon in 10 years. Because of that there will be a renaissance to energy research. A hydrogen economy is controversial and nonsensical. Fuel cells will need a major breakthrough, and one which is more applied in nature than universities are used to. Thus, universities won't dominate fuel-cell research.

MD: Energy is a huge problem—a national strategic problem. The developing world, including India and China, will increase the demand for energy. Two million cars were sold in China last year. In 10 years, there will be more cars in China than in the United States. India will be much the same as China. Bombay today is wall-to-wall cars. There will be a massive demand for energy, and not all will come from fossil fuels due to CO₂ problems. An H₂ economy does not change that because H₂ is also from fossil fuels. The best prospect is nuclear energy. Also, methane is a big area that needs research funding. Currently, nothing can be done with methane unless it is compressed to LNG (liquefied natural gas). Right now, 4 billion cubic feet of methane is flared per year. That amount of energy is equivalent to 300 million barrels of oil. If it were liquefied and consumed by offshore units, the energy produced would be very useful. Methane can also be changed to other forms for transport but it is not a priority to the government so success is slow coming. National governments need to make priorities, balancing CO₂ generation, global warming, and the risks of nuclear energy. A succession of U.S. governments have had their heads in the sand, which is a strategic mistake for this country.

BA: Hydrogen is only a carrier—the energy must come from some primary source such as nuclear. There is a huge need for energy carriers for automobiles. Other areas of energy research include biomass and carbon sequestration so that CO₂ problems can be alleviated. There are, of course, many alternative energy sources including solar (most expensive now), wind (farms are unpleasing aesthetically, but most economically sound right now), and biomass (two times the cost of wind). We need a government willing to admit that energy is a problem and then federal research money will be available. One really good way to get revenue for research is to tax gasoline at something on the order of 10 to 50 cents per gallon.

ACKNOWLEDGMENTS

We are grateful to the numerous graduate students at the Department of Chemical and Biological Engineering at the University of Colorado who volunteered their time and helped make this workshop possible. □

A Vision of **THE CURRICULUM OF THE FUTURE**

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Over the past 40 years, the discipline of chemical engineering has undergone dramatic changes. We are no longer a discipline largely coupled to a single industry, namely the petrochemical industry. Rather our graduates go to a wide variety of industries including chemicals, fuels, electronics, food and consumer products, materials, and biotechnology and pharmaceuticals.^[1]

Moreover, the character of the chemical industry has changed significantly, particularly in recent years:

- *the chemical industry is today very much a global enterprise;*
- *companies have been reshaped by a series of mergers, acquisitions, and spin-offs;*
- *some major chemical companies have become life science companies and spun off their chemical units;*
- *and the time-to-market for new products has been significantly shortened.*

Similarly, the research enterprise in chemical engineering has exploded over the past 40 years both in dollar volume and in breadth. The exciting research opportunities that we explore today as a discipline were well illustrated in the “Future of Chemical Engineering Research” sessions at the 2004 Annual Meeting of AIChE. Particularly notable shifts in research over this period include much more biologically related research and a much stronger molecular perspective in the research.

Over this same 40-year period the undergraduate curriculum in chemical engineering has remained nearly unchanged. The stagnation in the curriculum is well illustrated by Figure 1, which is taken from a paper by Olaf Hougen.^[2] The flow chart in the figure shows the evolution of the curriculum decade by decade from 1905 to 1965. In each decade, new con-

tent entering the curriculum is shown as well as material that was removed in order to “conserve mass.” The center of each box defines a core theme(s) for the decade.

I would like to make two observations about this figure. First, over the 60 years shown, the curriculum was very dynamic with significant changes in each decade. Second, by 1965 we had developed a curriculum for undergraduate education that is very nearly the same as today’s. Why is this? It is possible that after 60 years of hard work on the curriculum the discipline arrived at a more or less timeless implementation. But this seems hard to believe in the face of all of the change that has taken place over the past 40 years outside of the curriculum. On the other hand, it is possible that we have simply not paid the attention we should to curriculum development over this period. This is what I believe has happened. This same period has seen an enormous growth in federal research funding in universities, and this growth is reflected in the large number of doctoral research programs in chemical engineering around the country. This research has created valuable intellectual growth in our community, but it consumes an enormous fraction of the time of our faculty members just to keep the research engine running, with grant pro-

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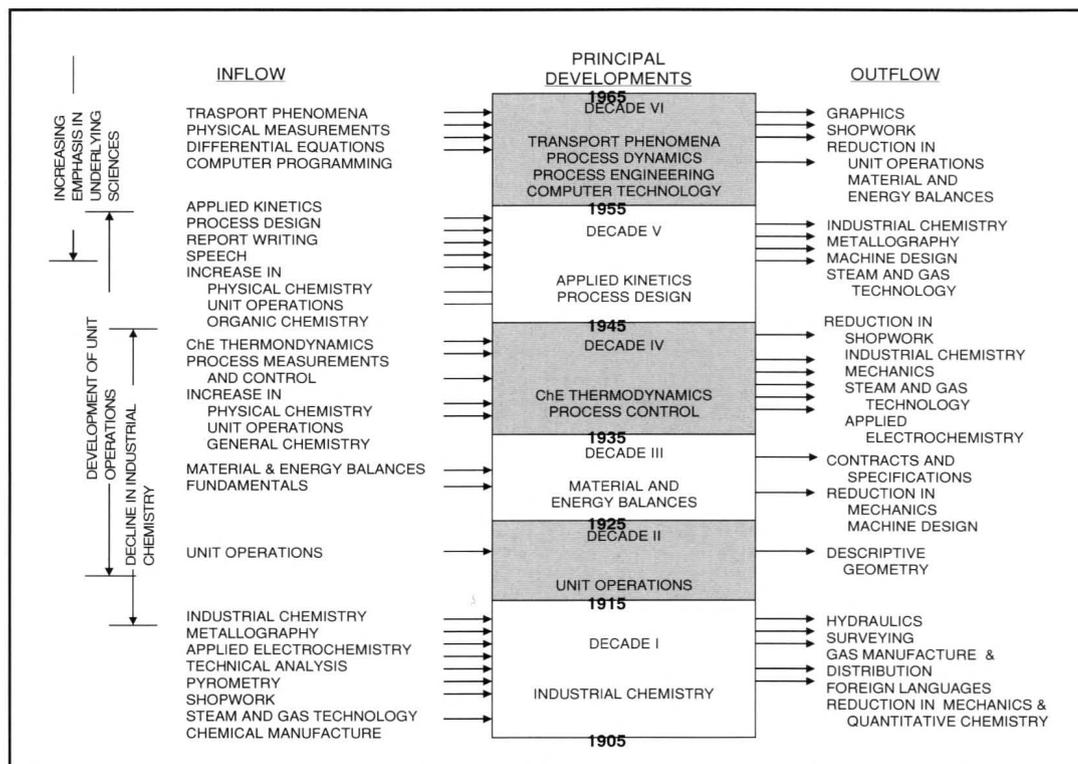


Figure 1. Changes in a typical undergraduate chemical engineering curriculum during 60 years. The initial curriculum in 1905 consisted of separate courses in chemistry and conventional engineering.^[3]

posals, contractors' meetings, review panels, annual reports, etc. The price has been neglect of the curricular content in chemical engineering and a widening gap between the research done in modern chemical engineering and the content taught in our undergraduate programs.

The opportunities for chemical engineering today are great (see Figure 2). We are uniquely positioned at the interface between molecular sciences and engineering, and this affords us many opportunities in a broad range of technologies that lie at the interface between chemical engineering and other science and engineering fields. This image of chemical engineering creates a number of tensions in our curriculum. There is a strong outward pull on our curriculum toward the many disciplines with which we interact at the interfaces in Figure 2. The opportunity to teach our students more about these particular areas of technology is exciting educationally, but it does tend to have a fragmenting effect on the discipline. Opposing the strong outward pull is an equally compelling need to look inward at the core of chemical engineering. Some departments have dealt with this tension by developing curriculum tracks in specialized areas. Students begin by taking a common core in chemical engineering and then specialize in a number of technology areas, e.g., biotechnology, materials. An alternative approach,

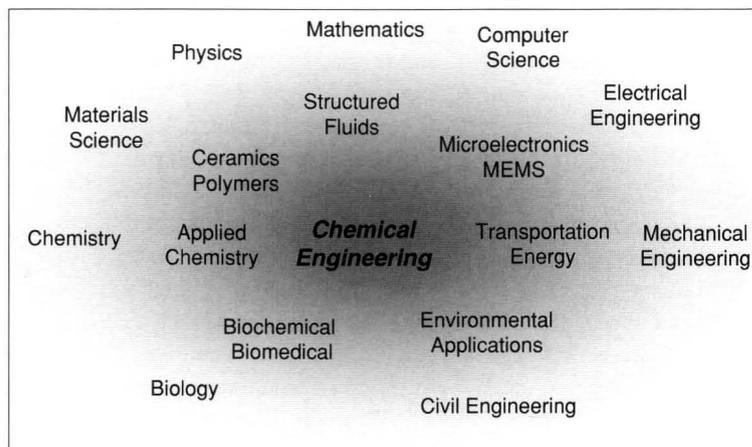


Figure 2. Chemical engineering has a special position between the molecular sciences and engineering.

proposed here, is to refocus on the core content of chemical engineering. Thinking clearly about what constitutes the core of chemical engineering that will make our future graduates key contributors in interdisciplinary problems is essential. It is important to remember that the current core we teach was developed when chemical engineering was described by the horizontal axis in Figure 2. That is, chemical engineering was dominated by the intersection of chemistry and mechanical engineering. We need to reexamine whether that core is the

The Next Millennium in ChE

appropriate core for the two-dimensional image in Figure 2. The broad range of applications of chemical engineering can be included in the curriculum by way of examples, problems,

It is possible that after 60 years of hard work on the curriculum the discipline arrived at a more or less timeless implementation. But this seems hard to believe in the face of all of the change that has taken place over the past 40 years outside of the curriculum.

case studies, and laboratories. In this way we maintain a common education for all chemical engineers that demonstrates the versatility of the degree to all of our students.

CCR/NSF FRONTIERS IN CHEMICAL ENGINEERING EDUCATION WORKSHOPS

The opportunities for reform in chemical engineering curricula are so compelling and broad that an appropriate response requires wide-ranging participation across the entire discipline. This is important for a number of reasons. First, the opportunities/frontiers are too broad for any one department or several departments to address effectively. Second, the costs—time and money—of developing new educational materials are too high for any of us to absorb alone. Finally, the coherence resulting from a joint effort will serve the discipline well in maintaining a clear identity to the world (potential students, industry, and government), ensuring good manpower supply to industry and to our graduate programs, and ensuring that curriculum developments are used.

Nearly 100 faculty members from 53 universities along with industrial representatives from five different companies met in a series of three workshops sponsored by the Council for Chemical Research and the National Science Foundation to discuss curricular opportunities and to map out a path forward. Below I will highlight some of the key findings of the workshops. I encourage you to look at the detailed work product and proceedings from these workshops, which can be found at <http://mit.edu/checurriculum/>.^[3]

Before I begin with the summary of the workshop results, I would like to relate an interesting observation made by many of us at the workshops: if we think about the curriculum in the large blocks we usually use—thermodynamics, transport

phenomena, kinetics, etc.—then change will be difficult or impossible. The reason is very simple. The current curriculum is full (or overflowing); if we take these large units to be givens in a new curriculum, then there is simply no room for new content. Hence we felt it worthwhile and important to put everything on the table and to start with a clean slate in thinking about the future. We asked ourselves, what should a “Decade XI” box covering the years 2005 to 2015 look like if we were to extend the Hougen analysis?

Principles

The first valuable lesson to emerge from the workshops was a set of principles that captured well the consensus of the group. These included:

- ☑ *Changes in science and the marketplace call for extensive changes to the chemical engineering curriculum*
- ☑ *The enabling sciences are: biology, chemistry, physics, mathematics*
- ☑ *There is a core set of organizing chemical engineering principles*
 - *Molecular transformations, multiscale analysis, systems*
 - ▶ *Molecular-level design is a new core organizing principle*
- ☑ *Chemical engineering contains both product and process design*
- ☑ *There is agreement on the general attributes of a chemical engineer*

Two of these elements need elaboration: the core organizing principles and the attributes of a chemical engineer.

Organizing principles

In order to arrive at a picture of the curriculum we began by enumerating the content—rather than the labels—that chemical engineering graduates should understand and be able to use. By then looking at the linkages and interconnections among these content elements, **three organizing principles** for the chemical engineering curriculum emerged. These are molecular transformations, multiscale analysis, and systems analysis and synthesis.

At the heart of chemical engineering is the manipulation of molecules to produce desired processes and products. This is encompassed by the organizing principle of **molecular transformations**. Our students must recognize by both qualitative reasoning and quantitative computation that properties can be changed by changing structure. Molecular changes can be architectural, for example by forming or breaking covalent bonds or by secondary or tertiary interactions to form super-

structures. Or molecular changes can be conformational, for example in the orientation and stretching of polymer molecules to change mechanical properties or in the folding of proteins. Chemical engineers need to understand the equilibrium properties of these molecular systems and the rates of reaction or structural changes. Finally our graduates should be equally comfortable with the manipulation of biological molecules as with the small organic and large synthetic polymer molecules that have been the traditional domain of chemical engineering.

It is not sufficient for chemical engineers to manipulate matter at the molecular level. In addition we must be able to connect behavior at the small scale with that at the large scale.

For example, we need to be able to take the molecular-level understanding of the kinetics of a chemical reaction and use this to design an appropriate reactor for commercial use. Or we need to be able to exploit the understanding of polymer conformation on properties in order to design a commercial spinning process to make high-strength fibers.

The organizing principle of **multiscale analysis** addresses the application of chemical engineering principles over many scales of length and time. It is not the goal of multiscale analysis to have students work from the atomic or molecular level up to the macroscopic level in every problem. Rather, it is important that students develop the ability to recognize, in any given problem, what the important length and time scales are for analysis and design.

Ultimately chemical engineers cannot be successful unless we can take the knowledge of molecular processes and the ability to manipulate these across appropriate scales and integrate these into functional systems. The organizing principle of **systems analysis and synthesis** deals with the tools for synthesis, analysis, and design of processes, units, and combinations of these. The systems of importance to chemical engineers cover a range of scales. They could be single cells in which we manipulate and control metabolic pathways to produce desired chemical products, or they could be the

entire globe or large regions of the globe in which we desire to regulate sources of emissions in order to control concentrations of undesirable chemical species.

In summary, chemical engineers leverage knowledge of molecular processes across multiple-length scales in order to synthesize and manipulate complex systems comprising processes and the products they produce. These new principles are summarized in Figure 3.

Attributes

Engineers are fundamentally problem solvers, seeking to achieve some objective of design or performance among technical, social, economic, regulatory, and environmental constraints.

Chemical engineers bring particular insights to problems in which the molecular nature of matter is important. As educators we cannot teach students everything that might be encountered; instead we aim to equip graduates with a confident grasp of fundamentals and engineering tools, enabling them to specialize or diversify as opportunity and initiative allow.

We seek in our curriculum to develop critical thinking and problem solving skills, especially for open-ended problems and those with noisy data or uncertain parameters; to cultivate professional attributes including oral and written communications skills; to broaden the technical base of the students by including examples from a variety of industries; and to cultivate an instinct for lifelong learning and an awareness of the social impacts of engineering and technology. The need for agile, inquisitive, and fearless engineers is strongly reinforced in the *Molecular Frontier* report on chemical sciences and engineering,^[4] which points out that the cutting-edge knowledge of chemical engineering practice across industries is changing constantly, as are global networks of technology development.

In working to create a curriculum for the future, it is our challenge to set a national vision for chemical engineering graduate practice beyond the norm, at the level described by several national commissions on engineering

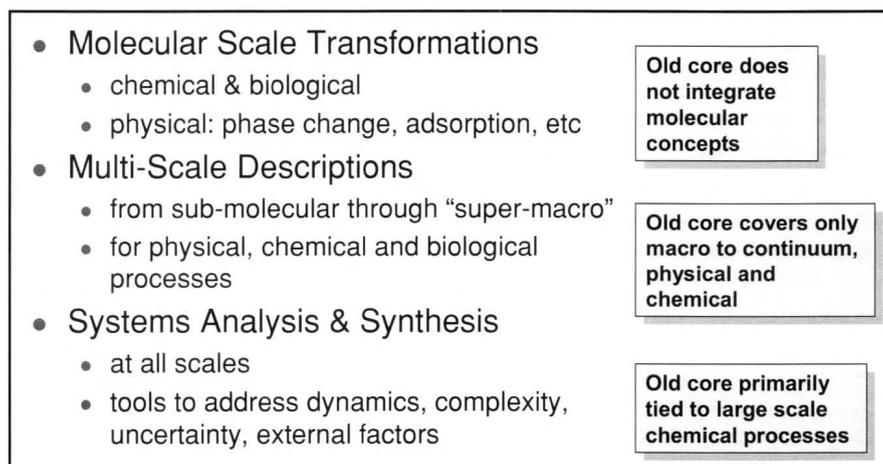


Figure 3. New organizing core principles for use in integrating the curriculum.

The Next Millennium in ChE

education that envision engineering graduates who are able to use fundamental knowledge of science and engineering in a flexible and creative manner. The *Molecular Frontier* report^[4] envisioned future graduates who can meet the following challenges:

- *Understand the basic chemistry of traditional chemical processes, living systems, advanced materials, and environmental control.*
- *Synthesize and manufacture any new substance that can have scientific or practical interest, using compact synthetic schemes and processes with high selectivity for the desired product, and with low energy consumption and benign environmental effects.*
- *Revolutionize design of chemical processes to make them safe, compact, flexible, energy efficient, environmentally benign, and conducive to the rapid commercialization of new products.*
- *Understand and control, to the limits of current knowledge and tools, how molecules react over all time scales and the full range of molecular size.*
- *Develop unlimited and inexpensive energy, with new ways of energy generation, storage, and transportation to pave the way to a truly sustainable future.*
- *Communicate effectively to the general public the contributions that chemical engineering makes to society.*
- *Be able to work in an interdisciplinary team of scientists, engineers, and production personnel to bring new substances from lab to production to market.*

A Draft Curriculum

The curriculum must engage students in the subject matter of chemical engineering and its use, and cultivate along the way that mix of attributes that characterizes the engineer. To accomplish these goals we envision a four-year structure that emphasizes the themes of chemical engineering, integrates the contents of these themes into a flexible and strong understanding, and exercises the skills we want to develop. This structure is versatile, admitting a variety of materials and modes of presentation, and is thus adaptable to a range of cultures, resources, and facilities found among chemical engineering departments.

I do not have a finished structure of

a curriculum to present; we are not yet that far along. At the third workshop held on Cape Cod, however, we developed a draft curriculum as a “proof of concept” to convince ourselves that this was possible. Shown in Figure 4 is the layout for a curriculum that develops the three organizing principles—molecular transformations, multiscale analysis, and systems analysis and synthesis—in parallel throughout the undergraduate years, and shows how the three themes are integrated in chemical engineering practice.

The content must also be integrated horizontally through time, so that each principle is clearly developed. It is important to provide many opportunities for repetition of key ideas, concepts, and tools as the students move through the four years of curriculum. The reinforcement of these key elements should also be accompanied by a systematic movement from simple to complex topics as the curriculum proceeds. Content must also be integrated vertically at given times in order to avoid compartmentalization. One way to achieve this vertical integration is to use part of each year for case studies, projects, or laboratories that cut across the three themes. For example, each theme in the core curriculum could be presented in one-and-a-half-semester subjects. In the latter half of the spring semester each year, students could work in teams on intensive, integrated laboratory or design projects that enable them to take the material learned that year and apply it in projects developed by industry/academic project members. In this way, both the teaching and learning of the integrated core would be addressed. Integration could be further enhanced by a small-group seminar series (possibly appended to an existing subject) that develops important abilities of social awareness,

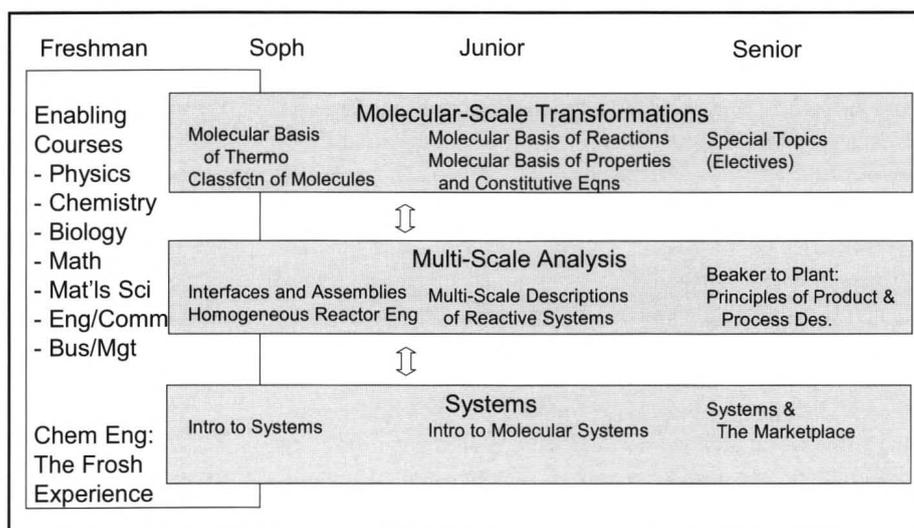


Figure 4. An example layout of a curriculum.

professional ethics, communication, business development and professional practice, and economics. By focusing each seminar series on these important nontechnical abilities, students would hone these skills and be better able to apply them as part of their spring semester integrated project work.

In summary, the material within an academic term, as well as across the four years, must proceed from simple to complex. Fundamentals must be illustrated with applications, and examples must range from the simple demonstration to the challenge of complex design or system manipulation. Finally, students must be engaged actively with this material. At the end, the curriculum must add up to a complete picture of chemical engineering. The detail given in each principle block suggests an order of topics. Detailed definition of these blocks is the subject of ongoing workshops.

CONCLUDING REMARKS

This paper proposes a vision for chemical engineering education for the future—for 2015 and beyond. To return to the Hougen analysis of the chemical engineering curriculum shown in Figure 1, I am suggesting a structure and focus for Decade XI as illustrated in Figure 5. Because we have not engaged in substantial curriculum revision in 45 years, I believe that we are best served by beginning with a clean slate. For outflow, I suggest the entire current curriculum. This is not to say that there are not key elements of what we teach today that should be retained, but rather everything in the existing curriculum must compete with new ideas to win a spot in the new curriculum. As illustrated in the figure, the Decade XI curriculum would be organized around the organizing principles of molecular transformations, multiscale analysis, and systems analysis and synthesis.

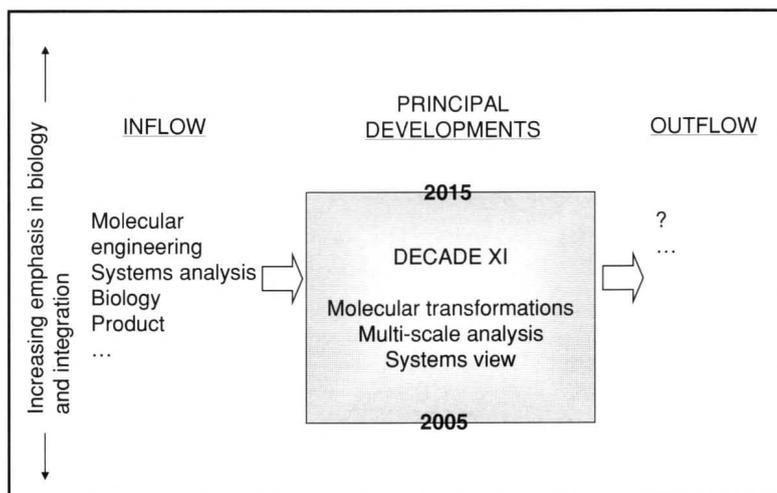


Figure 5. The proposed extension to Hougen's chart.

This radically different curriculum would produce more versatile chemical engineers, who are needed to meet the challenges and opportunities of creating products and processes, manipulating complex systems, and managing technical operations in industries increasingly reliant on molecular un-

The opportunities for reform in chemical engineering curricula are so compelling and broad that an appropriate response requires wide-ranging participation across the entire discipline.

derstanding and manipulation. Another benefit of the new curriculum is that it reconnects undergraduate education with ongoing research in chemical engineering in a way that has not been present for the past 40 years. This reconnection will serve us well as an engineering discipline in attracting the best and brightest students and in reopening the path to continual renewal of the curriculum.

ACKNOWLEDGMENTS

In writing this paper I have drawn very heavily on the collective thinking at the Frontiers Workshops. It is impossible to emphasize too strongly how much we have to learn from one another as we move forward in this great adventure. I want to give special thanks to the participants who synthesized summary reports at each of these workshops—Nick Abbott, Jeff Reimer, Jim Rawlings, Mike Thien, Greg McRae, and Bill Green—and to Barry Johnston, who prepared all of the material for the Frontiers Web site including the excellent executive summaries. Finally I thank Jeannette Gerzon who has ably helped organize and facilitate these workshops to help us be productive.

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**TEACHING ENGINEERING
IN THE 21ST CENTURY
WITH A 12TH-CENTURY TEACHING MODEL:
HOW BRIGHT IS THAT?**

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If you took a stroll down a hall of the University of Bologna in the 12th century and looked into random doorways, you would have seen professors holding forth in Latin to rooms full of bored-looking students. The professors would be droning on interminably in language few of the students could understand, perhaps occasionally asking questions, getting no responses, and providing the answers themselves. You might see a few students jotting down notes on recycled parchment, a few more sneaking occasional bites of the cold pizza slices concealed in their academic robes, some sleeping, and most just staring vacantly, inwardly cursing the fact that iPods would not become readily available for another 800 years. Toward the end of the lecture, one student would ask “Professore, siamo responábili per tutta questa roba nell’esame?” and that would be the only active student involvement in the class. Eventually the class would be released, and the students would leave grumbling to each other about the 150 pages of reading assigned for the next period and expressing gratitude for the CliffsNotes version of the text.

American engineering education doesn’t *exactly* follow that model. For one thing, the only engineering professor in the Western Hemisphere—and maybe in the world—who could lecture in Latin was Rutherford Aris, and he’s deceased. Hard drives have replaced parchment, baseball caps and jeans have replaced caps and gowns, and (this is a huge difference) students in Bologna actually had a lot of power, including the responsibility of hiring professors and the right to fire them if their performance was considered unsatisfactory. Leaving those differences aside, however, the fact is that things haven’t changed all that much since the 12th century. If you walk down the hall of an early 21st-century engineering school and look into random doorways, there’s a good chance you’ll see the descendants of those Bolognesi staring vacantly,

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snacking, and sleeping as their professors drone on incessantly in what might as well be Latin and fill the board or projector screen with Latin and Greek symbols that have little or no obvious relevance to anything the students know or care about.

Twenty years ago that's *all* you would have seen in those classrooms, with very few exceptions. Now, however, in some departments at some schools you can find a significant number of classrooms in which other things are happening. You might get the first signal of a difference before you ever get to the doorway, when from down the hall you hear things that are never heard in a traditional engineering classroom—sounds of conversation, discussion, and argument, possibly punctuated by laughter, alternating with periods of silence. If you look into the room for awhile you would see traditional classroom moments alternating with brief periods in which students are doing things individually or in pairs or small groups—answering questions, completing the next steps of derivations or problem solutions, troubleshooting, predicting, estimating, critiquing, interpreting, modeling, designing, formulating questions, and summarizing. At any given moment the professor might be in front of the class lecturing and answering questions, or quietly observing the activity, or wandering around the room interacting with individual students and student groups. Unlike the situation in the traditional classroom, many people—including the professor—would appear to be enjoying themselves. Also unlike the traditional classroom, most of the students enrolled in the course would actually be there.

If you inquired further into how courses are run in that department, you would see further evidence of two competing models—one that would seem familiar to our 12th-century scholars and one dramatically different. In one set of courses, the professor would spend a great deal of class time lecturing on the basic facts, formulas, and problem-solving algorithms that comprise the course material, and would then give assignments and tests calling on the students to demonstrate their ability to recite the facts, execute the formulas, and implement the algorithms. In the other courses, the students would be presented with problems *before* they are told everything they need to know to determine the solutions. They would then work—sometimes individually and sometimes in teams—to identify what they know and what they need to find out, do research, formulate and test hypotheses, and arrive at solutions. The professor would still be there to provide information and guidance, but formal instruction would

only occur when the students had established a need to know something to progress with their work.

So why the change? What is the answer to the traditional professor's traditional defense of tradition: "It's been done this way for decades or centuries and has worked fine," or implicitly, "This is how I was taught, and look how well I turned out!"

There are several answers, which would take much longer to present completely than I have in this little piece, so I'll only give brief suggestions of what they are and point to references where the whole story can be found. First, if "working fine" means turning out excellent engineers who have made brilliant creative contributions to industry and society, that has certainly happened over the centuries. The issue, however, is whether it happened because of traditional higher education or despite it. There is compelling evidence that the latter may be the case. Take Europe, for example. In the traditional European system of higher education that has prevailed for centuries, the professor is a godlike figure who lectures to students and has little or nothing more to do with them. The students may or may not choose to attend the lectures—if the professor is a particularly skilled lecturer they attend, otherwise most don't.

You might argue that this system led to the wondrous scientific advances of the Renaissance and the Enlightenment and the giant technological leaps of the industrial revolution, but I would quarrel with that argument. If you admit only the cream of the crop of a nation's youth (which universities in Europe and America did until fairly recently), it almost doesn't matter what you do or don't do in the classroom. You could simply hand out syllabi and lists of references and tell the students that they will be examined at the end of the year, and then do nothing else—no lectures, no homework, no tests except the final exam—and most students would manage to learn the material and pass the exam, and the few geniuses among them would go on to make their brilliant contributions, especially if they were clever enough to apprentice themselves to masters from the previous generation.

In short, professors who provide only traditional lecture-based instruction are largely irrelevant to the real learning process for top students. Good lecturers can certainly enrich their classroom experience, but they will learn with or without that enrichment. On the other hand, if you are trying to educate a broad segment of the population—as we are now doing in the United States—many students can't make it with

If you have been firmly entrenched in the traditional paradigm I would encourage you to try branching out, but I would also suggest taking it easy.

only the support that traditional instruction provides, and the consequence is the attrition of 50% and higher that we routinely see in engineering.

Another argument for change is that unlike our antecedents in the Middle Ages, we now know a lot from cognition research about how people learn and the instructional conditions that facilitate learning [see the reference by Bransford, *et al.*, in the bibliography], and everything we know supports the proposition that the traditional lecture-homework-test paradigm of engineering education is simply ineffective—good students learn despite it, and weaker students who could make excellent engineers frequently cannot survive it. The alternative instructional environment supported by the research is quite different. Here are some of the things teachers do in that environment, contrasted with what they do in the traditional approach.

- **T:** (Traditional) Establish a syllabus assuming that all necessary prerequisite knowledge is known, and march through it.

A: (Alternative) Find out at the beginning of a course what most of the students know and don't know and what misconceptions they have about the subject, and start teaching from that point. (This approach is known as *constructivist teaching*.)

- **T:** Assume all students with the ability to succeed in the profession for which they are being educated are basically alike (specifically, like the professor) and learn in the same way, and teach accordingly.

A: Recognize that good students vary considerably in motivation, cultural background, interests, and learning style, and teach accordingly.

- **T:** Focus on facts, formulas, and algorithms for solving well-structured closed-ended single-discipline problems.

A: Supplement the traditional content with training in critical and creative thinking, methods of solving ill-structured open-ended multidisciplinary problems (which tend to be what practicing engineers spend most of their time dealing with), and professional skills such as communication, teamwork, and project management.

- **T:** Cover basic knowledge (facts, algorithms, and theories) in lectures, then assign problems

that call for implementation of the knowledge, then illustrate the knowledge in laboratories.

A: Recognize that students learn best when they perceive a need to know the material being taught. Start with realistic complex problems, let students establish what they know and what they need to find out, and then guide them in finding it out by providing a combination of resources (which may include mini-lectures and integrated hands-on or simulated experiments) and guidance on performing library and Internet research. This is *inductive teaching* and has a number of variations, including *problem-based learning*, *project-based learning*, *guided inquiry*, *discovery learning*, and *just-in-time teaching*.

- **T:** In class, present information, derive formulas, and illustrate problem-solving procedures in lectures, boardwork, and overheads or PowerPoint images, occasionally asking questions and responding to questions students might ask.

A: In addition to lecturing, have students work individually and in small groups on brief course-related activities, such as answering questions, setting up problem solutions, completing steps in derivations, interpreting observations or experimental data, estimating, predicting, brainstorming, troubleshooting . . . Call on several students for responses at the conclusion of each activity, then invite volunteers to provide more responses to open-ended questions, and proceed with the lesson when the desired points have been made. This is *active learning*.

- **T:** Require students to do all of their work individually.

A: Assign a combination of individual work and teamwork, structuring the latter to provide assurances of individual accountability for all the work done and following other procedures known to promote good teamwork skills (including communication, leadership, project management, time management, and conflict resolution skills). This is *cooperative learning*.

- **T:** Tell the students they are responsible for everything in the text, lectures, and homework, and make up exams that draw on those sources, including some problems with twists that the

students have not seen before and have to figure out on the spot. (Those problems are there to see if the students “know how to think.”) It is up to the students to guess what the instructor thinks is important enough to include on a test.

A: Write comprehensive *instructional objectives* that list the things the students should be able to do (identify, explain, calculate, model, design, critique . . .) to demonstrate that they have satisfactorily mastered the knowledge and skills the instructor wants them to master, including high-level thinking and problem-solving skills. Make the objectives available to the students, ideally in the form of study guides for tests. Design in-class activities and homework to provide practice in the desired skills, and make the tests specific instances of a subset of the instructional objectives.

Instructors who are unfamiliar with the latter approach imagine that they will have to list thousands of objectives to be comprehensive, but this is not the case—a two-sided sheet of paper is normally sufficient to list all of the objectives that might be drawn upon to construct a midsemester test.

Entire articles and books can be—and have been—written on each of the given alternative teaching methods, describing how to implement them and summarizing the research base that demonstrates their superiority to the traditional approach. The bibliography at the conclusion of this paper suggests starting points for interested readers.

If you have been firmly entrenched in the traditional paradigm I would encourage you to try branching out, but I would also suggest taking it easy. Going directly from a traditional teaching model to a full-bore active/cooperative/problem-based learning paradigm starting next Monday is probably not a good idea—the amount of preparation required and the student resistance that might erupt could be overwhelming. A better approach is to make the change gradually, perhaps by doing a few small-group exercises in lectures, using a problem-based approach to teach one or two topics, and writing instructional objectives for one midterm test. In subsequent courses, increase your use of the new methods, never departing too much from your comfort zone, and you should see your students’ learning steadily increasing. After all, it took us 800 years to get from Bologna to where we are now; if it takes you a few years to get where you want to be, the sky won’t fall.

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A DIFFERENT CHEMICAL INDUSTRY

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An **Altered Industry.** The chemical industry today is completely different from the chemical industry of 25 years ago. The clearest evidence comes from the jobs taken by graduating chemical engineers. Twenty-five years ago, 80 percent of these graduating students went to the commodity chemical industry, exemplified by Dupont, Exxon, Shell, and Dow. Occasionally they went to international companies such as Bayer and ICI, though this was less common. The remaining 20 percent were roughly divided into equal groups. Some, perhaps 10 percent, went to product-oriented businesses such as PPG, Upjohn, or 3M. A similar number, perhaps another 10 percent, went to everything else, including consulting, government, and academia. This older chemical industry, dominated by large-commodity chemical companies, was very familiar and dependable.

Today, as Figure 1 shows, the situation is completely different. The percentage of graduates going to the commodity chemical companies has dropped dramatically, perhaps to a quarter of the total. Simultaneously, the percentage going to consulting has risen to around another quarter. This consulting includes functions such as process engineering, now contracted out rather than performed within the engineering laboratories of the commodity chemical companies.

The bulk of new graduates, however, now goes to industries where products are most important. Some of these products, such as pharmaceuticals, are familiar; others, such as foods, have existed previously but have not involved significant numbers of chemical engineers; still others such as electronics represent new efforts.

WHAT PRODUCTS ARE IMPORTANT

In this altered chemical industry, we must first ask what are the products that we are going to produce. I believe there are three types of these products, each with different characteristics. The first and most obvious are the familiar com-

modities—the same products which used to dominate the chemical engineering enterprise. The key for producing these new products is their cost. Styrene produced by Dow and styrene produced by BASF are chemically identical; the issue is who can produce large quantities at the lowest possible price.

The second and third types of products may be less familiar. The second type involves molecules with molecular weights of 500-700 and with specific social benefits. The most obvious examples are pharmaceuticals. The key to the production of pharmaceuticals is not their cost but rather their time to market, *i.e.*, the speed of their discovery and production. The first-to-market tends to get at least two-thirds of the eventual sales for the molecule, even after patents on the particular molecule expire. These products are normally not made in dedicated equipment but rather in whatever reactors are available at that specific time. Thus, process optimizations tend to be less important than questions of scheduling: If the equipment is being used for many different products, when can you get in to make yours?

The third product type includes those for which the value is added by processing to make a specific nanostructure. The key to these products is their function. For example, I don't

Edward L. Cussler, currently distinguished institute professor at the University of Minnesota, received the B.E. with honors from Yale University in 1961, and his M.S. and Ph.D. in chemical engineering from the University of Wisconsin in 1963 and 1965, respectively. Soon after, he went to teach in the Department of Chemical Engineering at Carnegie Mellon University. In 1980, Cussler joined the faculty at the University of Minnesota. He is the author of Multicomponent Diffusion, published in 1976, and Diffusion, published in 1984 with a second edition published in 1997. He is the co-author of Membrane Separation Systems, Bioseparations, and most recently, Chemical Product Design, the English edition of which was published in 2001.

care why my shoes shine after I have applied polish; I only care that they do shine. It is the shine, not the molecule that produces the shine, that is important. Customers are often willing to pay a premium for such a function, be it in a coating, in a food, or in a cleaner.

I find it helpful to think about these three types of products using the summary shown in Table 1. For commodity products, the key factor as stated previously is the cost of the product. The basis for producing the product will continue to be unit operations—unit ops—the familiar core of chemical engineering. Our action in this area should be to sustain the commodity industry. We are certainly not currently carrying out unit operations in the best way possible, but we are probably close to the limit of what is economically attractive.

With the key factor of the second type of molecular products being time to market, the major cost of products of this type, such as drugs, is not the process engineering but the cost of their discovery. At best, only one in a thousand drug candidates is commercially successful. This enormous drop-out rate is the reason drugs are expensive. The key to discovery normally comes from chemistry and microbiology, not from chemical engineering. As a result, it is not clear whether traditional process engineering has a major role to play in molecular products.

For nanostructured products, the third type, whose key factor comes from their superior function, the added value comes from the process rather than from the chemical synthesis. Their desired function is the shine of the polish or the cleaning of the detergent. Studies in this area seem to lack any unifying intellectual core. Flavor release in food science takes no advantage of what is known about controlled drug release in pharmaceuticals. Micelle formation in latex paint is an independent topic from micelle formation in detergents. I believe there is a genuine need for a general theory of nanostructured products. Such a theory could be part of a required course common to departments including chemical engineering, food science, and pharmacy.

IMPLICATIONS FOR EDUCATION

Faced with this altered chemical industry, we must ask whether the skill set currently mastered by chemical engineers is appropriate for the future. This skill set consists of three roughly equal parts, based in physics and mechanics, in chemistry and biology, and in chemical engineering. I don't think this skill set is inappropriate for the future. The ideas of reaction engineering and separation processes will continue to be central to what chemical engineers do. Within these areas, some topics will recede and other topics will become more important, but the core will remain.

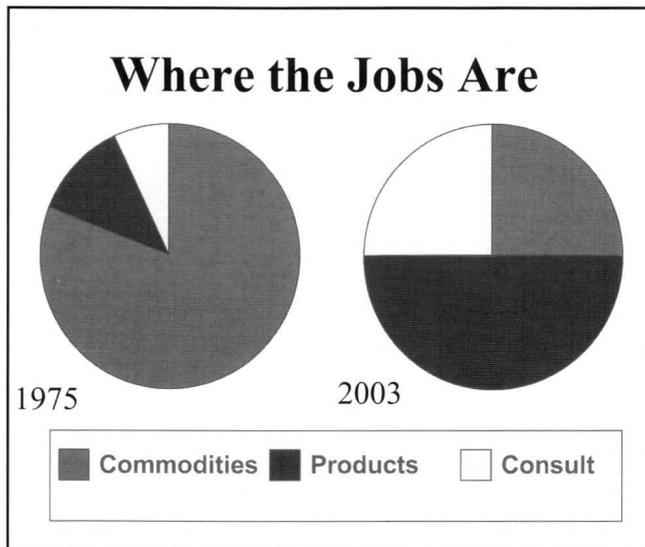


Figure 1. Where the jobs are in chemical engineering.

I do think that there may be a partial problem with the courses that present these topics. At the moment, these courses are biased heavily toward the commodity chemical industry. This bias includes such classical chemical engineering courses as transport phenomena and thermodynamics. In the future, new courses, including those based on biology, on polymer science, and on product design, must become more central to the chemical engineering curriculum. We require three such courses at the University of Minnesota precisely because we believe the content of those courses will better prepare our students for the new chemical industry.

Some may find this description of a changed chemical industry depressing. I don't. I think it is simply different. For example, it means that we may now work more on crystallization and less on fugacity, but I don't think that is a problem. In many ways, the reemergence of an emphasis on products and the corresponding de-emphasis of a few commodity chemicals suggests a broader intellectual challenge for chemical engineering. That challenge is interesting. I welcome it. I think it is exciting. And I think all of us will discover that excitement together. □

	Commodities	Molecules	Nanostructures
Key	Cost	Speed	Function
Basis	Unit Ops	Discovery	f (Properties)
Action	Sustain	Chemistry Key	Unified Theory

CRYSTAL ENGINEERING: *From Molecules To Products*

Preamble • According to many contemporary scientists, engineers, policy-makers, and business leaders, the future belongs to biotechnology, nanotechnology, and information technology. Chemical engineering research and teaching are being changed by these fields, as discussed in this series of articles and elsewhere. Change is happening at a measured pace, and biology has joined chemistry, physics, and mathematics as a fourth foundation discipline of the chemical engineering curriculum. I have little to offer that has not already been said about bio, nano, and info. However, there are other subjects that are of vital interest to society that are squarely in the domain of chemical engineering and that have received less attention than their worth. Among these, energy and crystalline solids rank high. I would like to say something about both these topics, but I will confine myself to crystalline solids—particularly organic materials. My goal is to highlight the importance of the solid state and to show how easily it can be incorporated into the chemical engineering curriculum.

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Crystalline organic solids are ubiquitous as either final products or as intermediates in the specialty chemical, pharmaceutical, and home and personal-care industries. Virtually all small molecular-weight drugs are isolated as crystalline materials,^[1] and more than 90% of all pharmaceutical products are formulated in particulate, generally crystalline, form.^[2] Crystalline chemical intermediates, such as adipic acid, are produced in large amounts to make polymers and specialty products. Skin creams and other personal-care product formulations contain crystalline solids. In most cases the properties of the crystalline solid have a major impact on the functionality of the product as well as the design and operation of the manufacturing process.

Crystal size (or size distribution), shape, enantiomorph, and polymorph all influence product functionality. For example, even a 50 micron particle in a hand cream makes the cream feel gritty.^[3] Size distribution is important in the manufacture of beta-carotene, which is virtually insoluble in water and only sparingly soluble in vegetable oils, and is used as a food colorant. The color shade given to the food is determined by the narrow size distribution, which must be in the submicron range.^[3] Crystal shape and polymorph influence solubility, dissolution rate (which influences bioavailability), compress-

ibility (important for tableting), and stability. The crystal enantiomorph is of vital importance in the manufacture of chiral materials, which has become a \$150 billion industry in recent years. The choice of solvent, along with the design and operation of the manufacturing process, determines the crystal properties. Moreover, crystal size, distribution, and shape have a major impact on the design of the manufacturing process since small crystals are difficult to separate from solution, and needle-like crystals or plate-like crystals can be difficult to filter and dry.

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Many important compounds exhibit polymorphism, *i.e.*, the existence of more than one crystal structure. Different polymorphs can have very different physical properties, including color, hardness, and stability. Therefore, control of which polymorph crystallizes in an industrial system is of vital importance. For example, since bioavailability can vary greatly among polymorphs of the same drug,^[4] the U.S. Food and Drug Administration requires the registration of each drug polymorph and the strict production of only that form. It can be difficult to control which polymorph crystallizes, even to the extent that production output can change unexpectedly from one form to another. This can be catastrophic, *e.g.*, halting production until the process can be altered to produce the original polymorph.^[5] Many in industry, particularly the pharmaceutical industry, are now undertaking exhaustive polymorph screening to identify all possible/likely polymorphs before beginning to scale up crystallization processes.^[6]

The importance of crystal shape to processing and product quality/functionality has been discussed in the context of ibuprofen.^[7] The primary interest in this system is the existence of high-aspect ratio needles when grown from nonpolar hydrocarbon solvents such as hexane or heptane. Equant (*i.e.*, low aspect ratio crystals with roughly equal sides) are formed when grown from polar solvents such as methanol or ethanol. This was discovered by researchers at the Upjohn Company,^[7] who patented the change in solvent as a process improvement.

The structure of this article is as follows. It begins by highlighting some of the advances made in the fundamentals of crystallization during the last decade, together with recommendations for where these topics can be inserted into the curriculum. Next is a brief review of recent improvements in CFD and population balance modeling for crystallizers. Third are descriptions of new methods for process synthesis of flowsheets containing crystallization steps. Last are some recommendations for incorporating crystal engineering into the core of chemical engineering education and research.

FUNDAMENTALS OF CRYSTAL ENGINEERING

Crystal Structure

A crystal is an ordered three-dimensional array of molecules, and represents one of nature's most remarkable examples of self-assembly. This definition contains the concept of periodicity. A solid material that has disordered structure, or that displays no long-range order (although it may possess short-range order) is called amorphous.

All crystals have translational symmetry, *i.e.*, repetition of motifs by translational displacement in space. Each crystal can be decomposed into a collection of unit cells, which are the smallest structural units that re-create the entire three-

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dimensional crystal structure when they are repeated in space by simple translation in every direction. Unit cells are parallelepipeds, the vertices of which constitute a grid of points called a lattice with its own periodicity and symmetry. The unit cell also defines three sets of planes in space, each set being parallel and equally spaced—the distance between the planes in each set is called the interplanar spacing, which is an important concept in crystal growth models. Within the cell, symmetry operations relate the molecules that constitute the contents of the cell. An asymmetric unit is the smallest structural unit (*e.g.*, a nonsymmetrical dimer, a single molecule, or part of a molecule) within which no symmetry elements operate. The collection of symmetry elements belonging to a crystal structure is called a space group. Therefore, a space group is the set of geometrical symmetry operations that brings a three-dimensional periodic crystal into itself. There are a total of 230 unique space groups. The number of symmetry elements in a space group must be equal to the number of asymmetric units in the cell.

It is important to realize that unit cells do not physically exist in a lattice and the lattice does not physically exist in the solid. These are mental constructs to help visualize the solid structure. There are several different lattice arrangements and unit cells that can be constructed—but only 14 possible lattices that fill three-dimensional space. These lattices can be further divided into seven crystal systems; each has a fixed relationship between the cell's spatial dimensions and angles. The seven systems are: cubic, tetragonal, orthorhombic, hexagonal, trigonal, monoclinic, and triclinic. Most organic molecules have uneven molecular shape that leads to low-symmetry crystal systems. The crystallographic systems with uneven unit-cell parameters are the monoclinic, triclinic, and orthorhombic. The majority of organic structures reported (approximately 95%) belong to these systems.

Molecules arrange themselves in crystals in such a way that the whole spatial arrangement must belong to one of the 14 Bravais lattices. The total number of independent ways in which molecules can decorate these lattices is 230 (corresponding to the total number of independent space groups).

Fortunately, only a few of these space groups are important in solid state chemistry. A more in-depth view of crystallography is available from many sources, including Cullity,^[8] Stout and Jensen,^[9] and the International Tables for X-Ray Crystallography.

Crystal structure and x-ray crystallography are well suited for inclusion in the undergraduate physical chemistry sequence. Gavezzotti^[10] has created an excellent visual introduction to crystal symmetry, written in a tutorial style suitable for undergraduates.

Nucleation

Crystals are born by nucleation, which may be defined as the formation of molecular solute clusters in solution that are in dynamic contact with the solute molecules dissolved in the solution. When the clusters reach a critical viable size they become a crystalline particle that grows by the addition of solute material on the crystal faces. Faces may appear or disappear during growth depending on the relative growth velocities of adjacent faces.

Nucleation can be divided into two types: primary and secondary. Primary nucleation is the formation of nuclei in solution whether or not suspended crystals are present. It is further subdivided into homogeneous and heterogeneous. Homogeneous nucleation is the formation of nuclei in previously crystal-free solution. Primary heterogeneous nucleation requires the preexistence of foreign bodies or catalytic surfaces in the solution. Foreign bodies can be dust particles, nuclei of substances different from the solute, etc. Catalytic surfaces may be roughness on the vessel walls, or a surface that was designed specifically for this purpose, such as a compressed surfactant monolayer (Langmuir) film or a self-assembled monolayer. Secondary nucleation is used to describe any nucleation mechanism that requires the presence of suspended solute crystals. Secondary nucleation may take place by several mechanisms: seeding, breakage, attrition due to collision (collision nucleation), or removal of surface layers through surface shear. Collision nucleation is the dominant mechanism of secondary nucleation, whereby growing crystals collide with the container walls, with a stirrer, or with other crystals.

Homogeneous nucleation from clear solution is of special interest because it is an important pathway in which the crystal polymorph (crystalline packing structure) is created—see the section below on Solution Mediated Polymorphism. The classical view of this process is that it occurs from the solute species clustering together in solution and then adopting the ordered arrangement of the crystalline state to minimize the free energy. The Gibbs-Thomson theory for the critical cluster size, r_c , is also based on free energy minimization. Clusters larger than r_c must grow in order to reduce the free en-

ergy of the total system (solute cluster + solution) while clusters smaller than the critical size dissolve in order to reduce the free energy of the system.

In the Gibbs-Thomson theory, it is assumed that only solute transfers to the nucleus from a supersaturated solution (the composition of which is located in the metastable region of the phase diagram). It is also supposed that the mass of the nucleus phase is so small that the composition of the solution phase is constant during the nucleation event. The total free energy change, ΔG , consists of three terms: a change in bulk free energy of the solution, a change of bulk free energy of the nucleus, and a change of surface free energy of the nucleus. The resulting expression for a spherical nucleus is

$$\Delta G = -\frac{4}{3}\pi r^3 \frac{\Delta\mu_{\text{solute}}}{v_{\text{solute}}} + 4\pi r^2 \gamma \quad (1)$$

where $\Delta\mu_{\text{solute}}$ is the difference in chemical potential of the solute in the supersaturated solution and in the nucleus (this term is always positive); v_{solute} is the molar volume of pure solute in the nucleus phase. The chemical potential difference can be written

$$\Delta\mu_{\text{solute}} = RT \ln(1 + \sigma) \quad (2)$$

where σ represents the relative supersaturation $(C^{\text{supersat}} - C^{\text{sat}})/C^{\text{sat}}$. The major assumption in Eq. (2) is that the activity coefficient of the supersaturated solution is equal to that in the saturated solution—a reasonable approximation in most cases. The leading term in Eq. (1) is always negative and represents the decrease in bulk free energy due to phase change. The second term in this equation contains the quantity γ , which is the surface free energy per unit area of nucleus (always a positive quantity) and represents the increase in free energy due to surface formation. The sum of these two terms produces a free energy plot with a single maximum that defines the size of a critical nucleus, as shown in Figure 1 for the alpha polymorph of the simplest amino acid, glycine, nucleated from aqueous solution at room temperature.

The critical nucleus size is given by

$$r_c = \frac{2\gamma v_{\text{solute}}}{\Delta\mu_{\text{solute}}} \quad (3)$$

This theory predicts that typical values for a characteristic length (diameter) of a critical nucleus are in the size range of hundreds of nanometers. For α -glycine, the critical diameter is approximately 600 nm. Recent computer simulations on small molecules predict critical nucleus sizes of 3-6 nm. The reason for the large discrepancy is currently unknown.

Using atomic-force microscopy *in situ* during the crystallization of the protein apoferritin from its aqueous solution, Yau and Vekilov^[11, 12] have directly measured the crystalline

packing structure and critical nucleus size of this material. They found critical nucleus sizes in the range of a few tens of nanometers (depending on the level of supersaturation). A typical value is 40 nm for the cluster shown in Figure 2—two orders of magnitude smaller than expected from traditional nucleation theory for large molecules. The molecular arrangement within the nuclei were observed to be similar to that in the bulk crystal, indicating that the crystal polymorph is already established at these small length scales. Moreover, the authors state, “Contrary to the general belief, the observed nuclei are not compact molecular clusters, but are planar arrays of several rods of 4-7 molecules set in one or two mono-

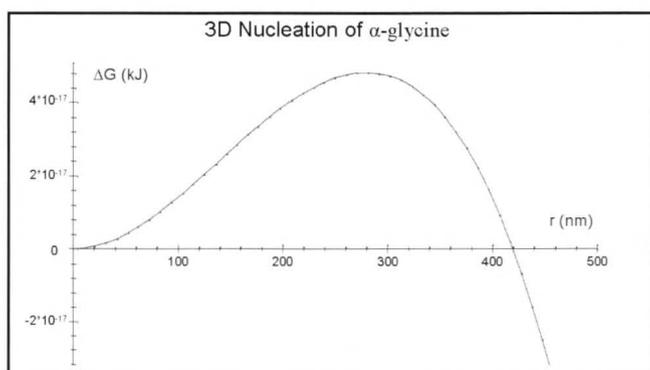


Figure 1. Change in free energy as a function of nucleus size for α -glycine grown from aqueous solution at room temperature, where $v_{\text{glycine}} = 46.71 \text{ cm}^3/\text{mol}$, $\gamma = 148.1 \text{ erg/cm}^2$, $\sigma = 0.02$, and $RT = 2.5 \text{ kJ/mol}$.

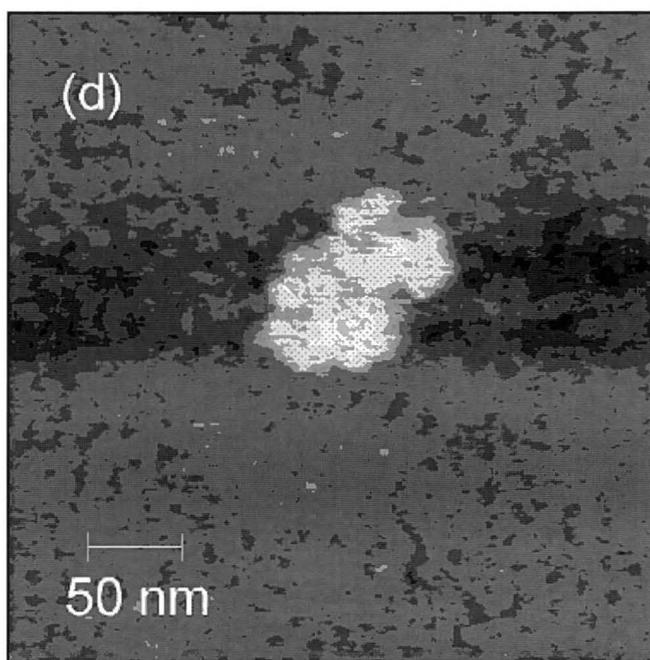


Figure 2. A flat, near-critical-sized cluster consisting of approximately 20 apoferritin molecules.^[12]

molecular layers. Similarly unexpected nuclei structures might be common, especially for anisotropic molecules. Hence, the nucleus structure should be considered as a variable by advanced theoretical treatments.”

Using small-angle neutron scattering, Lefebvre, *et al.*,^[13] determined the critical length scales in phase separating polymer blends of polymethylbutylene-polyethylbutylene. They obtained results similar to those reported for proteins, namely, critical diameters in the range of 20-50 nm.

Therefore, the current status of classical nucleation theory is that it predicts critical nucleus sizes that are about two orders of magnitude too high compared to the most recent measurements by Balsara’s group at UC Berkeley and Vekilov’s group at the University of Houston. Moreover, classical theory does not provide the molecular arrangement within the nucleus—this is an “input to” rather than an “output from” the theory. There are opportunities here for major improvements in nucleation theory that could have significant impact on crystal engineering.

Nucleation is an excellent topic to include in the undergraduate Solution Thermodynamics course. I like to teach the two-dimensional theory in which the solid nucleus is taken to be a rectangular lozenge of fixed thickness with variable length and width (the number of dimensions in the theory is equal to the number of independent lengths that are needed to characterize the shape and size of the nucleus). This model is much richer than the traditional one-dimensional spherical nucleus described above, which is characterized by only one spatial variable: diameter. In the two-dimensional nucleation theory, the critical nucleus corresponds to a *saddle-point* in the Gibbs free energy surface, which is easy to calculate and visualize for undergraduates. Therefore, the expected nucleation path corresponds to a trajectory through the free energy landscape over a saddle-point barrier. This provides a nice analogy to transition state theory and the reaction coordinate over a saddle-point barrier in chemical reaction rate theory. Moreover, it is easy to show that the shape of the critical two-dimensional nucleus satisfies the Wulff construction for a two-dimensional equilibrium shape. That is, the two-dimensional critical nucleus attains a shape that minimizes its total surface energy for the given (faceted) volume. Teaching this material to undergraduates also provides a good vehicle for explaining the difference between surface energy¹ and surface stress.¹¹ In the case of liquids, all processes of interest

¹ The reversible work per unit area needed to create a surface—if the variation in surface area does not change the surface density of molecules, then the specific surface work is surface energy.

¹¹ The reversible work per unit area needed to elastically stretch a preexisting surface—if the variation in surface area changes the surface density of molecules, then the specific surface work is surface stress.

involve variations in area without varying the surface density, and the surface work represents a surface-free energy. The traditional processes involving surface energy are creating a soap bubble and cleaving a solid into two parts, while the traditional example of a process involving surface stress is blowing up a rubber balloon. Both types of energy are expected to play a part in creating a solid nucleus, yet there is no theory that accounts for this. Finally, a good reason for teaching this material to undergraduates is to show them that not all is known, even in traditional areas of science that have been studied for a long time.

Growth Models

Evidence suggests that crystal faces grow by one of three mechanisms: a screw dislocation mechanism, a two-dimensional nucleation mechanism, or by rough growth. It is also known that different faces of a crystal may grow by different mechanisms, according to the solute-solvent interactions at the interface (surface-free energy) and the level of supersaturation. At low supersaturation levels, or large surface-free energies, the screw dislocation mechanism is normally operative. The original theory, developed by Burton, Cabrera, and Frank,^[14] proposed that screw dislocations, which exist on real crystal faces at all supersaturation levels, provide an infinite source of steps onto which oncoming particles can be incorporated. According to this theory, growth occurs by the flow of steps across the surface, which forms a spiral. Spirals have been observed on many faces of many crystals^[15-17] (see Figure 3). At moderate levels of supersaturation, the two-dimensional nucleation mechanism may apply. Above a critical level of supersaturation, the face is roughened and growth proceeds at a high rate.

The BCF expression for the rate of growth normal to a surface is:

$$R_{hkl} = \frac{v_{hkl} h_{hkl}}{y_{hkl}} \quad (4)$$

where v_{hkl} is the lateral step velocity, h_{hkl} is the step height, which can be approximated by d_{hkl} (the interplanar spacing) for monolayer height, and y_{hkl} is the distance between steps. Since growth occurs at kink sites (vacancies in steps where solute growth units can incorporate—see Figure 1 in Chen and Vekilov^[18] for a beautiful image of kink sites on a step of crystallized ferritin), the lateral step velocity depends mainly on the density of kink sites. In the simplest case, molecules along the edges of a spiral are found in one of three microstates: a positive kink site, a negative kink site, and no kink site. The energy for each of these microstates can be calculated, and if we assume that they occur in their most probable configuration, then the probability of finding a kink site along an edge is given by the Boltzman distribution. This

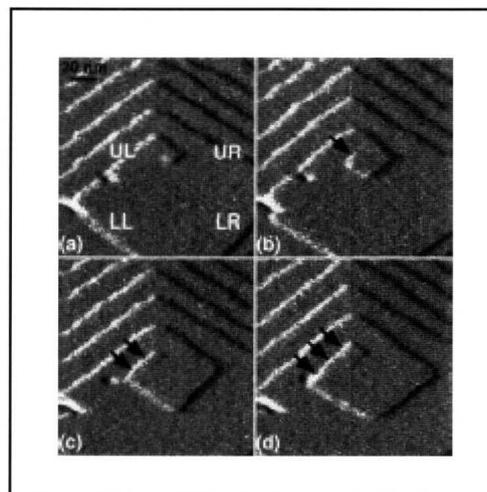


Figure 3. Four consecutive images of a spiral growing from a screw dislocation on a calcite crystal face.^[17]

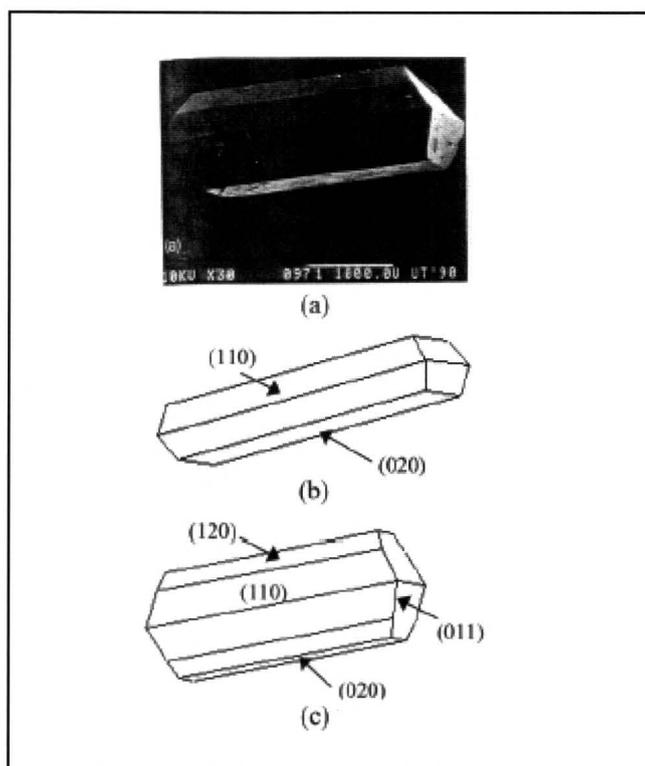


Figure 4. Reported and predicted morphologies for α -glycine crystallized from aqueous solution. (a) Experimentally grown crystal from Boek, et al.^[27] (b) Predicted shape using the form of the BCF model in Eq. (4) with a dimer growth unit. (c) Shape predicted by Eq. (4) using a modified monomer growth unit.^[26]

result provides a nice link between elementary statistical mechanics and the kinetics of crystal growth. (In my experience, if you want to teach undergraduates the methods of statistical mechanics so that they understand, use the textbook by Kittel and Kroemer.^[19])

Crystal Shape

It is well known that crystals grow in a variety of shapes in response to both internal and external factors. Some of these factors can be manipulated (*e.g.*, solvent type, solution temperature, and supersaturation) by crystal engineers to steer crystals toward a target shape or away from undesired shapes.

Experiments performed on the growth of crystals from spherical seeds have shown that flat faces appear during growth. Some of the faces that appear eventually disappear, while others grow in size, eventually leading to a fully faceted stationary (steady state) shape. The shape of crystals at thermodynamic equilibrium can be determined using Gibbs' approach of minimality of the total surface-free energy per unit volume. This thermodynamic equilibrium condition leads to the Wulff construction to determine crystal shape

$$\frac{\gamma_i}{h_i} = \text{constant}, \quad i=1, \dots, N \quad (5)$$

where γ_i is the specific surface-free energy of face i , h_i is the perpendicular distance between the origin and face i , and N is the number of faces. Only very small particles (nanoparticles) can undergo rapid shape change to reach equilibrium, during which the size change is not substantial. For larger particles, however, the number of elementary transport processes that have to occur to achieve significant changes in shape is so large compared with the lowering of the surface-free energy that the rate of equilibration becomes negligible.^[20] For crystals grown from seeds, steady state shapes (that have self-similar growth) are therefore observed more often than the equilibrium shapes. Wulff's condition was modified by Chernov^[21] (also see Cahn, *et al.*,^[22]) to determine the crystal shape at steady state, given as:

$$\frac{R_i}{h_i} = \text{constant}, \quad i=1, \dots, N \quad (6)$$

where R_i is the perpendicular growth velocity of face i . As noted in the previous subsection, many mechanisms and models are available to estimate the perpendicular growth velocities of facets, but in most solution crystallizations only one model—the screw dislocation model [BCF model, Eq. (4)]—has the proven capability to correctly estimate the relative growth rates of crystals grown from solution. A comprehensive validation of this modeling approach is given by Liu, *et*

al.,^[23] Winn and Doherty,^[24, 25] and Bisker-Leib and Doherty.^[26]

The shapes of many organic crystals have been successfully predicted with this approach, *e.g.*, urea grown from aqueous solution, ibuprofen grown from methanol and from hexane, adipic acid grown from water. Figure 4 compares the experimental and predicted steady state growth shapes of α -glycine crystallized from aqueous solution. This is a particularly sensitive test of the approach due to the complex network of hydrogen bonds that are formed in the solid state. Although there are many aspects of this modeling approach that need improvement, such as *a priori* identification of the nature of the growth units that incorporate into the growing crystal faces, the approach is already sufficiently well developed for immediate application to engineering design.

Although significant progress has been made recently on predicting the steady state shapes of organic materials crystallized from solution, there is less to report on the important related matter of predicting shape evolution from an initial seed or nucleus shape through to the final steady state shape. The only evolution models reported in the literature are for two-dimensional crystals, which apply to materials that crystallize in flat plate-like shapes, such as succinic acid grown from water (flat hexagonal crystals), and L-ascorbic acid (vitamin C) grown from water (flat rectangular crystals). The dynamics of shape evolution for three-dimensional crystals are quite complicated as faces, edges, and vertices appear or disappear during growth. The definitive study is yet to be done.

Although some may disagree with me, I think the topic of crystal growth and crystal shape as outlined above is good material for inclusion in an undergraduate transport course.

Solution Mediated Polymorphism

The phenomenon of polymorphism—a solid crystalline phase of a given compound resulting from the possibility of at least two crystalline arrangements and/or conformations of the molecules of that compound in the solid state—has been known to exist for over two centuries.^[28] Despite this, its prevalence presents one of the greatest obstacles to the solids-processing industry today. To obtain the desired properties of the product, the correct polymorph must be obtained since they have different physical properties: melting points, solubilities, bioavailabilities, enthalpies, color, and many more. Differences between polymorphs are crucial for industries such as the pharmaceutical industry, where differences in dissolution rates between two polymorphs may mean that one polymorph is a potential product because of its high dissolution rate (high efficacy) while another is not due to its negligible dissolution. A dramatic example of this phenomenon is provided by the Ritonavir polymorphs.^[5]

Paracetamol (acetaminophen) is an analgesic drug that is used worldwide as a pain reliever. Due to its commercial importance, acetaminophen has been subject to many crystallization experiments and, in particular, polymorph studies. Paracetamol has three known polymorphs. Monoclinic paracetamol is the thermodynamically stable form at room temperature and, therefore, it is the commercially used form. Unfortunately, it is not suitable for direct compression into tablets, since it lacks slip planes in its structure, which are necessary for the plastic deformation that occurs during compaction. Consequently, it has to be mixed with binding agents, which is costly in both time and material. Crystallization of the orthorhombic polymorph (form II) of paracetamol from solution is more desirable since it undergoes plastic deformation and is therefore suitable for direct compression. In addition, it is believed to be slightly more soluble than form I. Until 1998 there was no reproducible experimental procedure available for the crystallization of form II from solution. The only method that had been reported for bulk preparation of form II was to grow it as polycrystalline material from fused form I.

In 1998, Gary Nichols from Pfizer and Christopher Frampton from Roche^[29] described a laboratory-scale process to crystallize form II from solution. They found that the orthorhombic polymorph of paracetamol could be crystallized from supersaturated solution of industrial methylated spirits (ethanol with approximately 4% methanol) by nucleation with seeds of form II, maintaining crystallization at a low temperature of 0 °C and collecting the crystals within one hour after nucleation began. The typical yield achieved was less than 30%, but they proposed that when the process was optimized, a commercial application was possible. By having better control over the crystallization process, they managed to crystallize only the orthorhombic polymorph and to have the desired crystal shape.

Ostwald noted in his Rule of Stages describing phase transitions that it is not the most thermodynamically stable state that will normally appear first but that which is the closest, in

free energy, to the current state.^[30,31] In accordance with this rule, crystallization of a compound having two polymorphs will often proceed first with the growth of the metastable form until the solution composition achieves the equilibrium solubility of this form. When the saturation concentration of the metastable form is reached it will stop growing. The stable form may have nucleated at any point, determined by relative kinetics, up to and including when the saturation of the metastable form is reached. The stable form will then grow, thus causing the solution to be undersaturated with respect to the metastable form, causing it to begin to dissolve. Once the metastable form has completely dissolved at the expense of the growing stable form, the stable form will grow until the solution reaches its equilibrium solubility with respect to the stable form.^[32] For example, a snapshot of the polymorphic transformation of glycine crystallized from a water/ethanol mixture is shown in Figure 5. At the beginning of the crystallization, beta-glycine (needle) crystals form first. This is the

less stable polymorph. After 10 minutes, the more stable polymorph, alpha-glycine (shaped as a coffin), grows at the expense of the beta-glycine, which dissolves.

A more complete understanding of solution-mediated polymorphism will involve appropriate integration of nucleation, growth, and dissolution, with the thermodynamic equilibrium phase diagram for the polymorphs.^[34]

Crystallizer Design

Crystallization processes are designed to achieve specific material properties in the final solid product, which are normally determined by the crystal purity, polymorph, mean particle size, size distribution, and crystal habit. The design decisions that influence these material characteristics include: choice of solvent, tailor-made surface-active modifiers,^[35-37] fines removal system, and the temperature and supersaturation fields inside the crystallizer (which are determined by the solute feed concentration and temperature, crystallizer temperature, vessel volume and geometry, agitation rate, and/or antisolvent feed rate or evaporation rate, as appropriate). Buildup of impurities in the recycle streams also has the potential to significantly influence crystalline material properties.

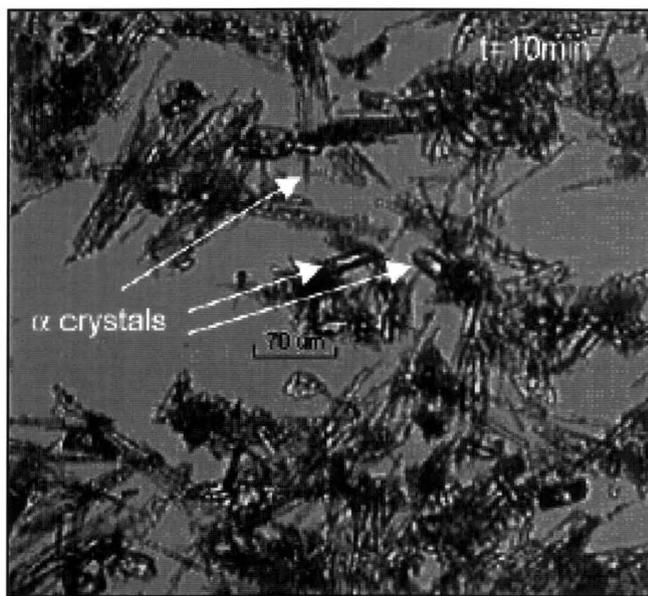


Figure 5. Two polymorphs of glycine in water-ethanol solution: alpha-glycine (shaped as a coffin) and beta-glycine (needles).^[33]

Considering the fundamentals of crystallization, it is tempting to envision crystals growing quietly in a uniform medium. This is an ideal seldom if ever realized in industrial crystallization. In most industrial crystallization processes, crystals grow suspended with myriad similar crystals in large, vigorously agitated vessels. Frequently, the solution composition in the vessel is nonuniform both temporally and spatially. Growing crystals are subject to collisions with other crystals, the vessel agitator, wall, and internals. These phenomena have a significant, sometimes profound, effect on the properties of the resulting crystals. Crystallizer and crystallization process design attempt to reconcile and manage these competing effects to produce adequate, even superior crystals.

Modeling crystallizer flows is critically important and presents many difficulties, such as concentrated two-phase flows, turbulent flow, complicated geometries, and a particle phase that is changing in concentration and properties over time. Despite these challenges, advances in closure modeling, numerical solution techniques, and computational power are beginning to make computational fluid dynamics (CFD) a useful tool for characterizing crystallizer flows. Advances have also been made incorporating the effect of the suspended particles on the flow field.

Currently, there is great hope for Lattice Boltzmann techniques to simplify the computational treatment of the equations of motion, making numerical solution much more efficient. The techniques are also amenable to including the effect of solids^[38] and are becoming commonly used. Because they are so much more efficient than traditional solution techniques, significantly more complicated and consequently more realistic problems can now be solved. It remains a challenge to incorporate changing particle size distribution (PSD) into these models, but this is an area of current research and progress is being made.^[39]

The ultimate goal is to combine transport and population balance modeling. Only then will realistic PSD predictions be possible for a wide variety of nonideal systems. Progress has been made, but a model applicable to a wide variety of conditions remains elusive.

SYSTEMS DESIGN / PROCESS SYNTHESIS

Normally, large amounts of dissolved solute remain in solution in the effluent stream of a continuous crystallizer, or at the end of a batch crystallization. In either case, the crystals are separated from the solution, and the liquor is recycled. The crystallizer, therefore, is part of a larger flowsheet, which may involve reactors, dissolvers, additional crystallizations, various kinds of separators, heaters and coolers, etc. Both the structure of the flowsheet and the devices and their operating

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policies influence the recycle flow rate and composition, which in turn influence the performance of the crystallizer. Surface active impurities and their buildup in recycle loops can have a major impact (often adverse) on crystallizer performance.

In recent years geometric methods have proven to be useful for the systematic generation of process flowsheets. One such tool, the crystallization path map, is useful for finding feasible flowsheets in which crystallization steps occur. These maps are closely related to residue curve maps for the synthesis of azeotropic distillation systems.^[40] The crystallization paths are trajectories of the liquid composition in a crystallizer as the solid is formed and removed from solution.^[41, 42] The presence of eutectics and compounds causes the presence of crystallization boundaries, which divide the map into distinct crystallization regions. These regions are nonoverlapping and mutually exclusive; that is, a liquid trajectory that starts in one region cannot cross a boundary (except by noncrystallization means) into an adjacent region. Within each region there is one and only one crystal product, which may be a pure component, a eutectic, or a compound.

Crystallization maps are useful for synthesizing flowsheets for adductive crystallization (where a compound is the desired crystal product), extractive crystallization, and many other embodiments.^[43-45] Although these maps are valuable for laying out process flowsheets, the accumulation of impurities associated with process recycle and the effect on crystal properties both remain difficult to predict. Therefore, integrated pilot-scale testing including all recycle streams is still required for confident system design, but there are significant modeling opportunities here that will enable more reliable and rapid development of process flowsheets.

SUMMARY AND CONCLUSIONS

During the last decade there have been significant advances made in every aspect of crystal engineering. New experimental techniques, such as atomic force microscopy, allow us to

explore crystal surfaces and embryonic nuclei to learn about their formation and growth, infrared and Raman spectroscopy allow us to follow supersaturation changes and polymorphic transformations *in situ* while crystallization is taking place. New models have been developed to predict the influence of both internal and external factors on crystal polymorph and shape. Molecular templates are being developed to control crystal form and structure. Advances in fluid mechanics and transport phenomena have added greatly to our understanding of mixing patterns and particle trajectories inside crystallizer vessels of realistic geometry. These and other advances not mentioned or not yet even anticipated, are expected to continue.

Most of these advances are not being made by chemical engineers, however. And moreover, they are taking place in isolation. There is a large disconnect, for example, between the microscopic models for growth of individual crystal faces and the macroscopic models for CFD and PSD prediction. Perhaps the larger question is, "How do we incorporate our rapidly advancing knowledge and modeling capability to make better products?"

There are major opportunities here for chemical engineers who must be encouraged to take up the challenge. Specific recommendations for incorporating crystal engineering into chemical engineering research and undergraduate education include:

Education

- (1) Crystalline solids should be one of the core themes throughout the chemical engineering curriculum. Topics include: *Thermodynamics course*- thermodynamics of solid-liquid phase diagrams and solubility curves, spinodal curve and metastable zone curve, traditional nucleation theory. *Transport course*- diffusion of solute through a solution to a growing crystal surface, estimates of characteristic times for bulk diffusion, surface diffusion and integration of solute at kink sites on a crystal surface, models for flow of steps across crystal surfaces. *Reaction Engineering course*- simultaneous reaction and crystallization (*i.e.*, precipitation). *Separation course*- design of batch and continuous crystallizers. *Design course*- simultaneous product and process design for crystalline products (*e.g.*, a dye, a pigment, or a simple pharmaceutical such as paracetamol—trade name Tylenol).
- (2) Solid state chemistry should be part of the undergraduate chemistry sequence. Topics include: crystal structure and crystallography, nucleation (both traditional and statistical mechanics models), solid state bonding and bond chains, and surface growth models—especially the spiral dislocation model.

There are numerous useful monographs and textbooks available on the subject of crystallization that may be used for teaching undergraduates. These include: Randolph and Larson,^[46] Mullin,^[47] and Davey and Garside.^[48] The last of these is short, inexpensive, and extremely well written. Undergraduates should be happy to purchase this book.

Research Topics

- (3) New models and experiments for understanding, directing, and controlling nucleation and polymorph selection
- (4) Models for understanding and predicting polymorphic phase transitions—both solution mediated and solid state transformations
- (5) Models and experiments for predicting the effect of additives and impurities on crystal properties (*e.g.*, crystal shape, size, polymorph)
- (6) Improved models for CFD of dense suspensions of crystals that are growing inside a solution crystallizer
- (7) Improved procedures for simultaneous product and process design for crystalline particulate products; application and testing of the procedures in such product sectors as: chiral and pharmaceutical products, home and personal care (*e.g.*, skin creams, suntan lotions), food (*e.g.*, margarine, chocolate, ice cream), dyes and pigments, bulk chemicals (*e.g.*, adipic acid), and specialty chemicals

ACKNOWLEDGMENT

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INSIDE THE CELL

A New Paradigm for Unit Operations and Unit Processes?

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Traditionally the chemical engineering paradigm for designing industrial plants has been to separately consider unit operations and unit processes. Although these terms are not prevalent in current curricula, courses in separations, reaction engineering, polymer engineering, etc., reflect this traditional view.

The usual scheme of process development starts at the laboratory bench. And with experimentation and exploration, conditions are optimized and then the process goes through a scale-up procedure to reach commercial production needs. Recent advances in MEMS technologies, however, have led to the implementation of Lab-On-a-Chip devices such as the integrated DNA analysis chip developed by Burns, *et al.*^[1] (see Figure 1). These analytical devices bring together various elements of unit processes such as separation steps, reaction steps, and process control (detection and sensing procedures). The capability for miniaturization and integration has led some chemical engineers (*e.g.*, Klavs Jensen) to envision an entirely new paradigm for production methods, *i.e.*, scaling down instead of scaling up. Figure 2 from Professor Jensen's Web site succinctly illustrates this contrast in paradigms.

Given the immense efforts in MEMS and nanotechnology toward miniaturization and integration, one can readily speculate about potential future methods for carrying out chemical processes through the application of these technologies. The

organizational structure of biological cells could have important lessons and impact in this regard. As the extensive structural and operational characteristics of the biological cell are being revealed, it is becoming clear that biological systems have evolved with a much more integrated design paradigm of processes and operations than the traditional chemical engineering approach.

Jerome Schultz received his B.S. and M.S. in chemical engineering from Columbia University, and his Ph.D. in biochemistry from the University of Wisconsin in 1958. He started his career in the pharmaceutical industry (Lederle Laboratories) then joined the University of Michigan, where he was chairman of the Department of Chemical Engineering. He spent two years at the National Science Foundation as deputy director of the Engineering Centers Program. In 1987 he joined the University of Pittsburgh as director of the Center for Biotechnology and Bioengineering, and was the founding chairman of the Department of Bioengineering—a nationally ranked degree program in bioengineering. He recently spent a year at NASA's Ames Research Center as a senior scientist in their Fundamental Biology Program. In 2004 Dr. Schultz joined the faculty at the UC Riverside as the director of the newly formed Bioengineering Program and the Center for Bioengineering. He is a member of the National Academy of Engineering, a Fellow of the American Association for the Advancement of Sciences, Editor of Biotechnology Progress, and was a founding Fellow and President of the American Institute for Medical and Biological Engineering.

New advances in genomics, proteomics, metabolomics, cell signaling, and control have allowed the documentation of the thousands of species and interactions that comprise the internal milieu of cells. This vast amount of information has allowed the harnessing of biological cells for many purposes such as preparation of many biologics (*e.g.*, insulin and EPO [erythropoietin, monoclonal antibodies]), as well as the use

of cells for detoxification of herbicides.

Much of our thinking related to the future of biotechnology is based on our appreciation of biological systems deduced from the dissection and separation of the components of cells such as enzymes, signaling proteins, antibodies, RNA, and DNA. Much of the richness of biological systems, however, resides in the structural features of cells. To date, many of the structural elements that have been deduced from electron micrographs are categorized as organelles. Some of the classes of organelles that have been identified include the nucleus, mitochondria, lysosomes, peroxisomes, vesicles, chloroplasts, and golgi (Figure 3). It is clear that cells are not a bag of enzymes and substrates, *i.e.*, a CSTR.

Although the morphology of these structural elements is fairly well characterized by electron microscopic methods, the functional and dynamic biological/chemical processes that are taking place in these structures are not well understood at all. Early hints from the study of some of these organelles have revealed that biology does not separate unit processes from unit operations, but rather integrates them. For example, in chloroplasts the capture of photons and fixation of carbon dioxide into carbohydrates simultaneously results in photolysis—the separation of protons and oxygen evolution. Ribosomes integrate the genetic code and protein synthesis.

Most organelles are known to be complex multi-membranous structures, but the composition and detailed organization of these units are not known. One reason for the lack of detailed understanding is that the typical dimensions of these structures is on the order of nanometers and thus below the resolution of optical microscopes. So they cannot be visualized in detail while in a normal functional mode. This lack of

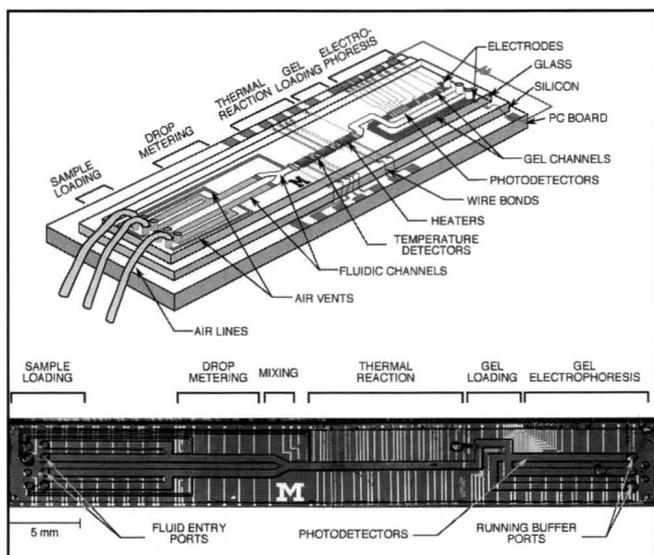


Figure 1. An example of a Lab-On-a-Chip device. This is a DNA analysis system devised by Mark Burns and associates.^[1] Various “unit operations” including metering, mixing, reactions, separations, and detection are combined in a single device.

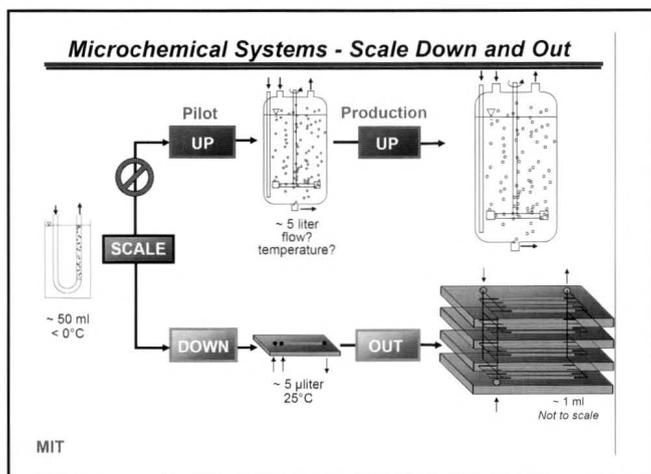


Figure 2. Klavs Jensen’s concept for a new paradigm in chemical process development that utilizes the multiplexing capabilities of MEMS technology to carry out integrated synthesis and separation operations in the same unit.

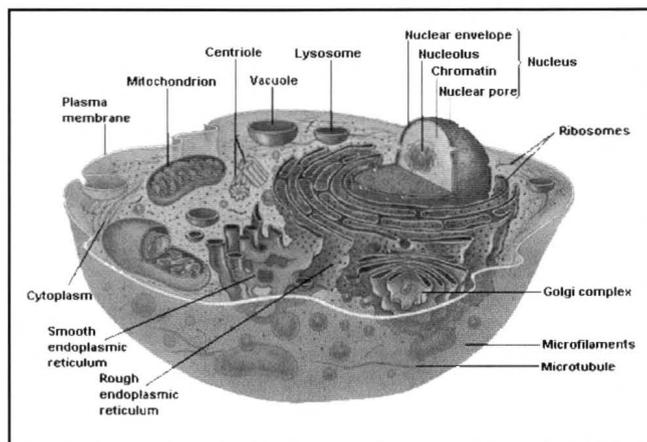


Figure 3. Diagrammatic illustration of the various structures within a cell illustrating the complex structures inside of cells that are responsible for much of the biosynthetic activities of living systems.

The Next Millennium in ChE

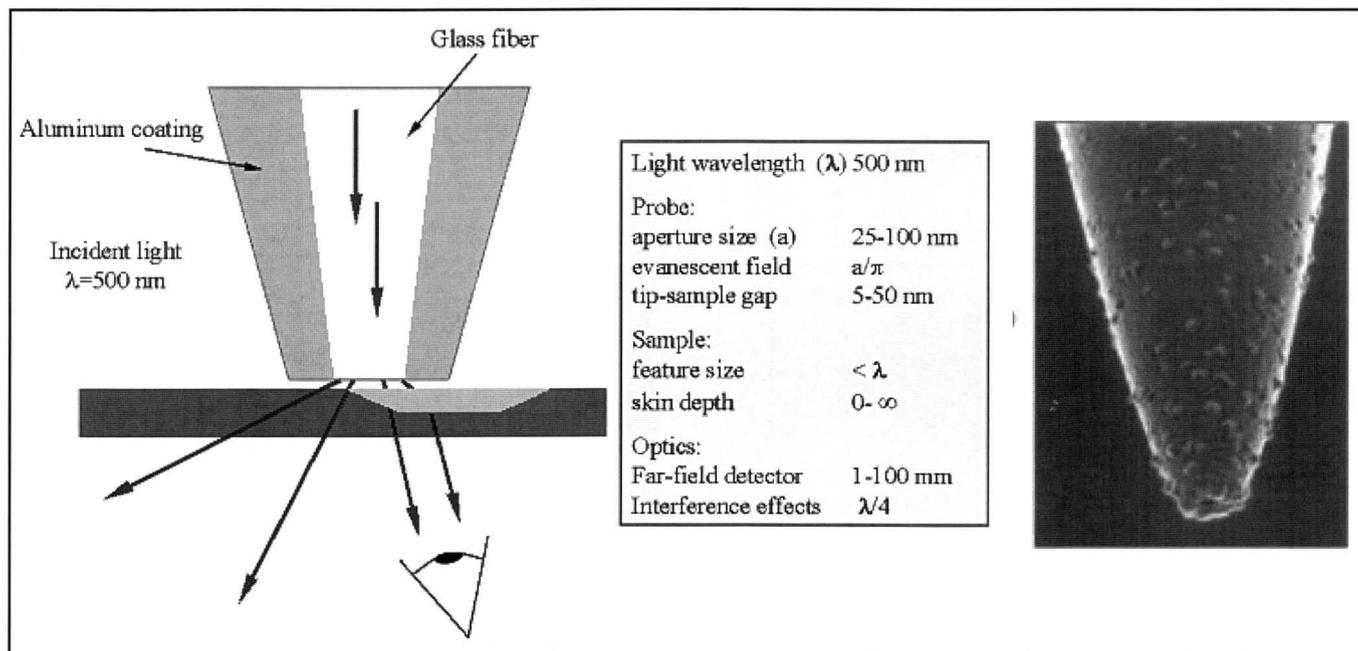


Figure 4. Operational characteristics of near field microscopy (left). Close-up of the optical scanning probe (right). This is one of the devices that will allow the visualization of structures within living cells and their behavior.

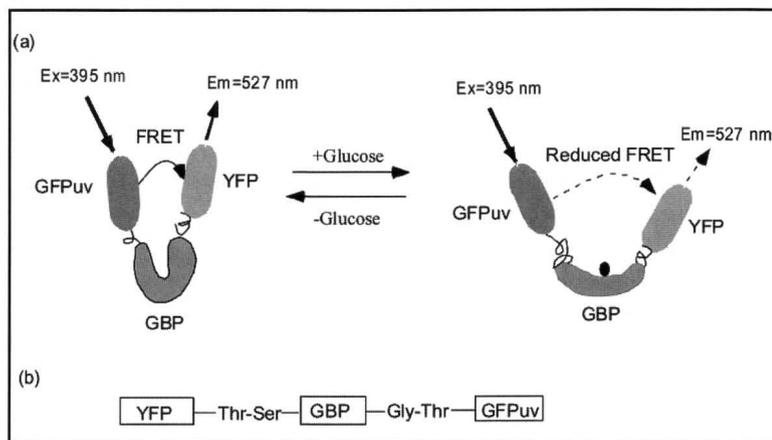


Figure 5. Glucose-responsive protein engineered from a glucose binding protein from *E. coli*, and two different green fluorescent proteins. This type of structure can be introduced into a cell via a plasmid to result in the biosynthesis of the sensor protein within the cell. (a) In the absence of glucose the two fluorophores are in close proximity and exhibit fluorescent energy transfer (FRET) (left). In the presence of glucose the protein opens, and FRET is reduced. (b) Structure of the fusion protein.^[10]

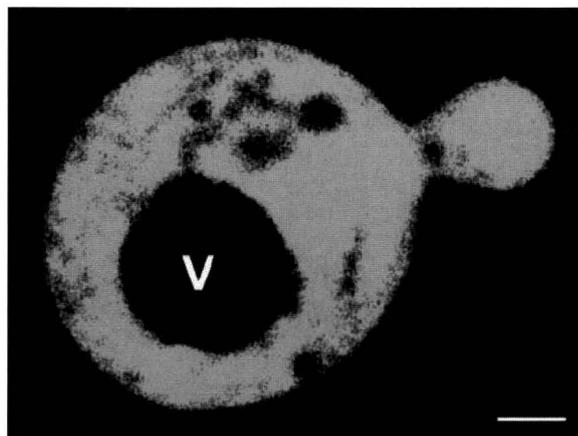
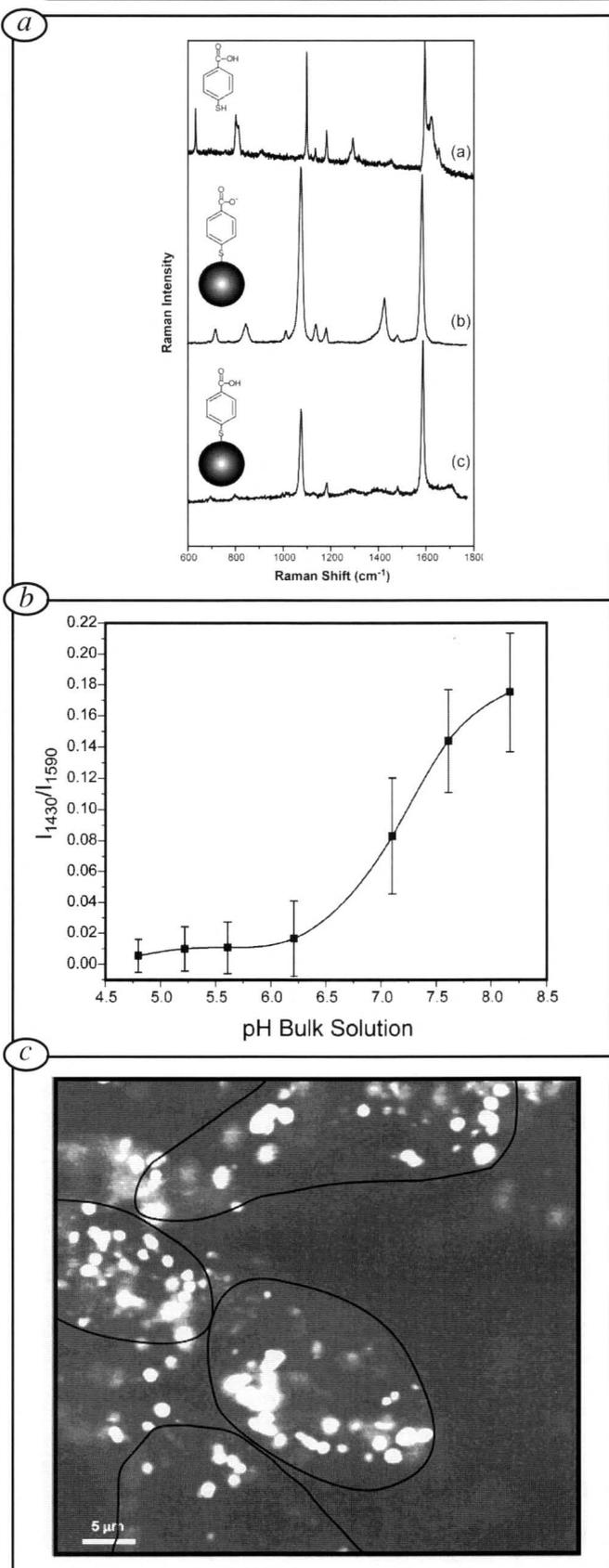


Figure 6. Confocal image of a yeast cell containing a maltose responsive protein similar to that illustrated in Figure 5. The intensity of fluorescence is indicative of the concentration of maltose in various regions of the cell. By incorporating various indicator proteins of this type within cells, one could monitor the dynamics of biosynthesis of specific biomolecules in space and time. V is a vacuole. (Bar = 1 micron).^[11]

knowledge has hampered our ability to mimic these biological systems for chemical processes.

Hope is on the way, however. To deal with this issue, indirect methods are under active development to elucidate mechanisms of the functioning of organelles.

Many new instrumental techniques are being developed to provide some real-time measurements of the behavior of sub-cellular structures. These techniques include confocal microscopy,^[2] two-photon microscopy,^[3] and optical coherence tomography.^[4] Near field microscopy,^[5] Figure 4, allows the



visualization of structural elements near the surface of the cell. Basically an optical fiber is drawn down to diameters less than the wavelength of light and placed in contact with the cell's outer membrane. The probe is scanned across the cell membrane to provide a map of structures just beneath the membrane surface.

Several clever concepts based on various reporter techniques have also been described recently that are beginning to give specific dynamic data on intracellular events. The rapidly expanding knowledge base on the structure and properties of green fluorescent proteins has opened up many opportunities for the protein engineering of intracellular probes. A multitude of techniques is available for incorporating plasmids for these proteins into cells. These reporter indicators can be either freely mobile within the cell or localized in specific structures.^[6, 7]

Roger Tsien and his group^[8, 9] have pioneered the use of green fluorescent proteins as functional probes for biomolecules within cells based on the technique of fluorescence energy transfer (FRET). One recent application of this approach has been to monitor sugar concentrations within cells. We^[10] engineered a fusion protein consisting of a glucose-binding protein and two different green fluorescent proteins as shown in Figure 5. The sugar-binding moiety undergoes a conformational change when glucose binds, such that it changes the distance between the GFP and YFP in a manner that results in a change in FRET. Fehr, *et al.*,^[11] incorporated a similar maltose-binding protein into yeast cells. Using confocal microscopy, they were able to monitor the distribution of maltose throughout the cell, Figure 6.

Other techniques for monitoring the concentration of materials within cells are based on inserting tiny "biosensor" particles within cells. Raoul Kopelman and colleagues^[12] have designed various materials called "PEBBLES" for measuring oxygen, sugars, and pH within cells by optical techniques. Talley, *et al.*,^[13] have extended this approach by inserting functionalized gold particles within cells that showed changes in the Raman spectrum with local pH changes. Again, these particles could be placed within cells to measure the distribution in acidity within cells, Figure 7. In order to measure

Figure 7. Use of particles placed within cells to monitor intracellular analyte concentrations by surface-enhanced Raman spectroscopy. In this example of intracellular monitoring, a compound that shows different Raman spectra in its two ionic forms, is used to monitor the pH distribution within cells.^[13] (a) Structure of the probe particle and Raman spectra at different pH's. (b) The pH behavior of Raman spectra. (c) Distribution of nanoparticles within cells.

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local enzyme activity within cells, Weissleder, *et al.*,^[14] incorporated a probe polymer with an enzyme hydrolysable link between two fluorophores (see Figure 8).

With the increased amount of information afforded by these imaging techniques, software to manage and display this data in a meaningful fashion has become important. Several groups are developing appropriate software for this purpose.^[15-18]

Government agencies are targeting technologies for improvement in intracellular imaging sensitivity. For example, the NIH recently funded nine centers to develop cellular imaging techniques. Descriptions of these research efforts as reported on the NIH Web site (<<http://www.nigms.nih.gov/cellularimaging/index.html>>) are quoted below.

OVERVIEW

The Exploratory Centers for the Development of High Resolution Probes for Cellular Imaging support multi-investigator teams to develop new technologies that enable higher-sensitivity biological imaging in living cells. Each of the nine centers will focus on different strategies for probe development, cellular delivery, probe targeting, and signal detection to improve detection schemes by a factor of 10 to 100. A major emphasis of this initiative is to apply novel, high-risk approaches to create fundamentally new probes with enhanced spectral characteristics. The ultimate goal is to develop probes and imaging systems that can be used to routinely achieve single-molecule sensitivity for imaging dynamic processes in living cells.

The centers are funded in conjunction with the NIH Roadmap for Medical Research as part of the "New Pathways to Discovery," an effort to advance our knowledge of biological systems by building a better toolbox for medical research. This initiative originated in NIGMS and was later adopted by the Roadmap. NIGMS currently supports seven of the centers as Roadmap-affiliated grants. Funding for all nine centers is expected to total approximately \$25 million over four years (\$6.8 million the first year).

1. **Fluorescent Probes for Multiplexed Intracellular Imaging.** Kevin Burgess, Ph.D., Principal Investigator, Texas A&M University

Researchers from Texas A&M University and the University of Pennsylvania plan to create novel probe sets composed of multiplexed "through-bond energy transfer cassettes," using multiple, linked, donor-acceptor dye pairs that are optimized for cellular imaging. These probes, which efficiently absorb light at one wavelength, emit amplified fluorescent signals at different, resolvable wavelengths close to the red-infrared region, far removed from cellular autofluorescence. The dye cassettes will be specifically adapted for tracking interactions

of proteins in cells, ultimately with single-molecule detection.

2. **Sub-nm Dendrimer-Metal Nanoclusters as Ultrabright, Modular Targeted in vivo Single Molecule Raman and Fluorescence Labels** • Robert M. Dickson, Ph.D., Principal Investigator, Georgia Institute of Technology

Metal nanoclusters, composed of silver and gold atoms stabilized on organic dendrimers, exhibit strong, size-dependent emission throughout the visible and near-infrared spectrum. The spectral characteristics of these clusters—their small size (< 1 nm) and short and highly radiative

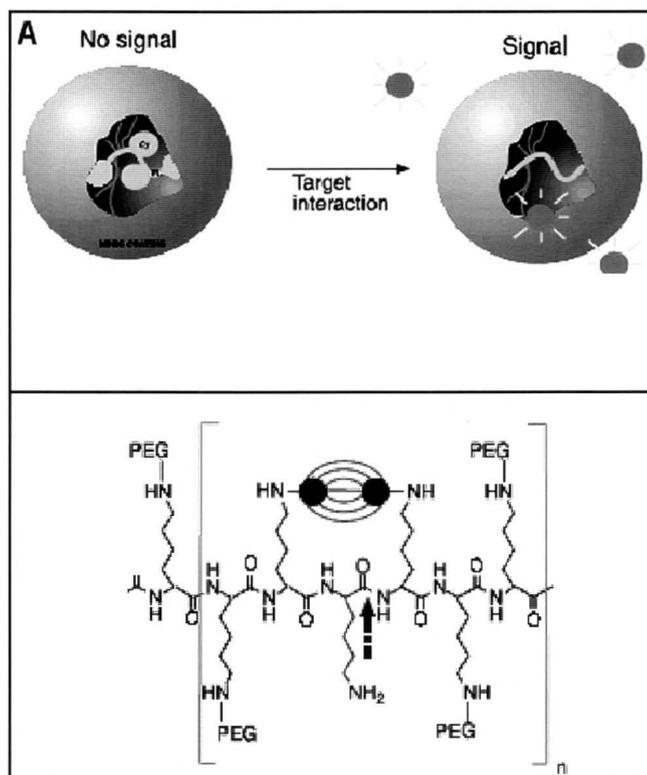


Figure 8. Example of a polymer probe to determine enzyme activity within a cell. In this case the purpose was to monitor the activity of a proteolytic enzyme within cells. A special polymer substrate was created that contained the peptide bond that the enzyme cleaves and fluorophores (indicated by the circles) that self-quench when in close proximity. When the peptide bond is cleaved by the enzyme of interest, the fluorophores are separated and quenching is prevented. Thus, monitoring the appearance of fluorescence gives a measure of local enzyme activity. Upper panel: Schematic of the concept. Lower Panel: Example structure of the probe polymer to measure enzyme activity.^[14]

lifetimes—create signals that have the potential to be several orders of magnitude higher than conventional labels. Grantees from the Georgia Institute of Technology and Emory University plan to functionalize the nanoclusters for attachment to different biological targets and to develop single molecule imaging methods to facilitate detection of the signal inside cells.

3. **Single-Molecule Fluorophores for Cellular Imaging** • William E. Moerner, Ph.D., Principal Investigator, Stanford University

A group from Stanford and Kent State University plans to synthesize and characterize a new class of highly emissive (dicyanodihydrofuran) fluorophores that exhibit large increases in signal when bound to rigid surfaces. The strategy for incorporating the probes into cells will be based upon the genetically encoded tetracysteine-biarsenical targeting system and then tested for single molecule specificity and detection in bacteria.

4. **Bioaffinity Nanoparticle Probes for Molecular/ Cellular Imaging** • Shuming Nie, Ph.D., Principal Investigator, Emory University and Georgia Tech

A collaborative group will develop a new class of polymer-encapsulated bioconjugated luminescent nanoparticles with enhanced optical properties, cellular delivery, and targeting/binding functions for real-time and multicolor imaging in living cells. The focus will be on core-shell semiconductor quantum dots because of their improved brightness, resistance against photobleaching, and simultaneous multicolor excitation. The researchers will test the probes and their ability to detect them in studies aimed at finding the subcellular locations of p53, nuclear factor B, and androgen receptor in living cells.

5. **Probes for Quantitative Optical and Electron Microscopy** • David W. Piston, Ph.D., Principal Investigator, Vanderbilt University Medical Center

A group from Vanderbilt will develop new fluorescent probes in the visible and infrared spectral regions based on three approaches: genetically encoded proteins, lanthanide chelates, and nanocrystals (quantum dots). Each approach will be tested for imaging of a protein in the plasma membrane as well as an intracellular target. Subcellular resolution fluorescence imaging by widefield, deconvolution, confocal, and multi-photon excitation microscopy will be used to implement and test the new detection schemes based on spectral and time-gated resolution. To reach the highest resolution, the researchers will determine the utility

and limitations of using the new probes for direct detection by electron microscopy for correlative imaging.

6. **Imaging Single Proteins in vivo with Quantum Dots** • Sanford Simon, Ph.D., Principal Investigator, Rockefeller University

Researchers from the Rockefeller University plan to extend and optimize an in vivo trans-splicing and expressed-protein ligation approach to ligate quantum dot derivatives to cytosolic or integral membrane proteins. Their strategy includes development of a conditional protein trans-splicing approach that will allow probes to be ligated to the target following a designated functional interaction. The cellular fate of “activated” proteins will thus be monitored by a change in the signal emitted by the probe. The team intends to use these tools to study exocytosis and transport through nuclear pores.

7. **Light-Activated Gene Expression in Single Cells** • Robert H. Singer, Ph.D., Principal Investigator, Albert Einstein College of Medicine

Investigators from the Albert Einstein College of Medicine will develop a photoactivatable gene that, upon exposure to light, begins transcription of visible nascent chains of RNA. The ecdysone response element and a caged, photoactivatable ecdysone gene into which an RNA reporter has been inserted, will be used. Gene expression will be initiated by uncaging the ecdysone in vivo by conventional and two-photon microscopy. The system will be engineered into cancer cells and then imaged intravitaly in tumors. The dynamics of single RNA molecule movements and distribution will be monitored.

8. **Library-Based Development of New Optical Imaging Probes** • Alice Ting, Ph.D., Principal Investigator, Massachusetts Institute of Technology

The investigators plan three parallel approaches to generate small-molecule and genetically encoded probes that can be targeted to specific RNA or protein sequences inside living cells. In the first, libraries of fluorophores will be synthesized in a combinatorial fashion and then screened for their ability to label small peptide motifs or RNA aptamers with high specificity. In the second approach, the natural bacterial enzyme biotin transferase will be re-engineered to catalyze covalent labeling of fluorescent probes to peptides inside cells. Third, a systematic approach using a

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ENERGY CONSUMPTION VS. ENERGY REQUIREMENT

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Today, the phrase “energy consumption” is popularly spoken and written.^[1] Nevertheless, caution should be exercised for its continued use, especially in the instruction of not only thermodynamics but also various other courses in engineering, including those in chemical engineering.

The first law of thermodynamics teaches that energy is always conserved in an isolated (or closed) system; it is neither created nor destroyed by any process, system, or phenomenon.^[2-5] In contrast, the available energy analysis, which is the combination of the first and second laws of thermodynamics, indicates that in the real world the available energy is *never* conserved, even in an isolated (or closed) system. Even though in ideal circumstances available energy is only *theoretically* conserved, the reality is that it is incessantly consumed, or dissipated, by any process, system, or phenomenon.^[6-15]

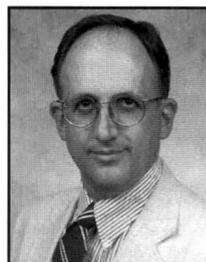
This consumption of available energy—or exergy—is accompanied by an increase in entropy, signifying the dissipation of available energy (or exergy) to the surrounding environments. The dissipation of this available energy (exergy) reduces its potential or availability to perform useful work.

Similar to enthalpy, exergy is a state property of any system. The enthalpy as well as exergy contents of materials are



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measured relative to the dead state, *i.e.*, the extended standard state. It is defined by the environmental temperature, the environmental pressure, and the datum-level substances. Any element is part of the corresponding datum-level substance, which is defined as being thermodynamically stable, existing in abundance, and containing no available energy.^[8, 11, 16-19] The environmental temperature and pressure, which vary according to time and place, are usually adopted as the datum-level temperature and pressure; despite this, they are often specified as 298 K and 1 atm, respectively, for convenience and also to be consistent with the conventionally defined standard state.

MASS, ENERGY, AND AVAILABLE ENERGY BALANCES

A system in which a phenomenon or process of interest occurs is thermodynamically defined or specified by its mass, energy, and available energy balances.^[8, 11, 13, 19-21] The following subsections outline these three balances for system A, or simply “the system,” having multiple input and output streams under the steady-state, open-flow conditions depicted in Figure 1, on the basis of a unit time, *i.e.*, the rate. Figure 1 exhibits an isolated overall system; besides system A, it encom-

passes work and heat sources and sinks, and the entire surroundings, *i.e.*, environments. It is postulated that, except *energy* (enthalpy) and *available energy* (exergy) of mass flowing through system A, other forms of energy—such as potential energy and kinetic energy—are negligible. Thus, the changes in the enthalpy and exergy are induced by the *transfer of energy* (between system A and its surroundings or other systems) as heat or work. For simplicity, the aforementioned three balances will be written around system A by referring to Figure 1 and with the notations given in the section on nomenclature.

Mass Balance

By taking into account both convective and diffusional flows, the mass balance around system A yields

$$\sum_i M_i = \sum_e M_e \quad (1)$$

In terms of the molar flow rate, the above expression can be rewritten as

$$\sum_i \left[\sum_k (M_w)_k n_k \right]_i = \sum_e \left[\sum_k (M_w)_k n_k \right]_e \quad (2)$$

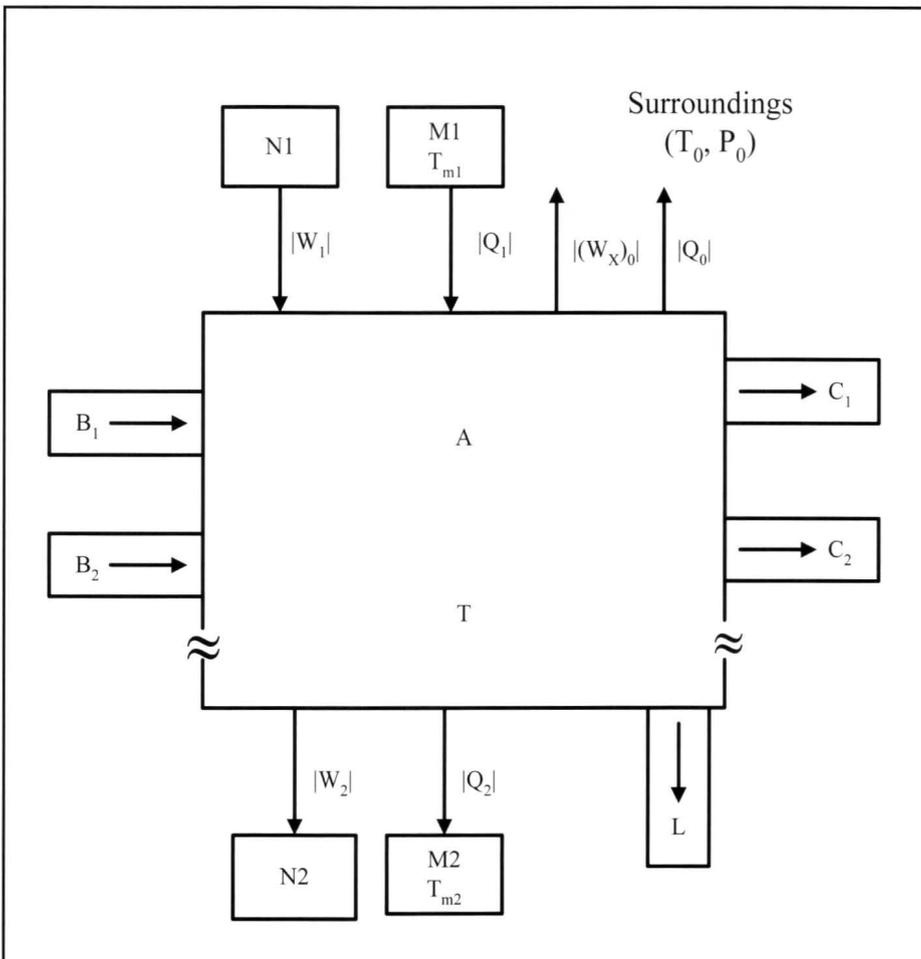


Figure 1. Schematic diagram of an isolated overall system encompassing a steady-state, open-flow system (system A), a heat source at temperature T_{m1} (system M1), a heat sink at temperature T_{m2} (system M2), a work source (system N1), a work sink (system N2), and the entire surroundings at the environmental temperature of T_0 and the environmental pressure of P_0 . In the text, entering streams B_1, B_2, \dots are designated by subscript i ; and exiting streams C_1, C_2, \dots, L —the last being the leaking stream (leakage)—are designated by subscript e ; the useful and leaking streams among the exiting streams are differentiated by additional subscripts u and l , respectively.

Energy Balance

The energy balance around system A yields

$$\left\{ \left[\sum_i \left(\sum_k \bar{\beta}_k n_k \right)_i \right] + [W_1 + |Q_1|] \right\} = \left\{ \left[\sum_e \left(\sum_k \bar{\beta}_k n_k \right)_e \right] + [W_2 + |Q_2|] + [(W_x)_0] + |Q_0| \right\} \quad (3)$$

Even under steady-state flow conditions, some parts of the system, such as the surface of a rotating shaft of any pump, do the work against the surroundings, or continuously generate electric charges which are discharged to the surroundings. This leads to the work loss, $|(W_x)_0|$, which will be transformed into thermal energy and be transferred to the surroundings as heat. The term, $|(W_x)_0|$, therefore, can be combined with the heat loss, $|Q_0|$, thereby constituting the total heat loss to the surroundings, $|Q_{0w}|$; thus,

$$|Q_{0w}| = |Q_0| + |(W_x)_0|$$

This renders it possible to rewrite Eq. (3) as

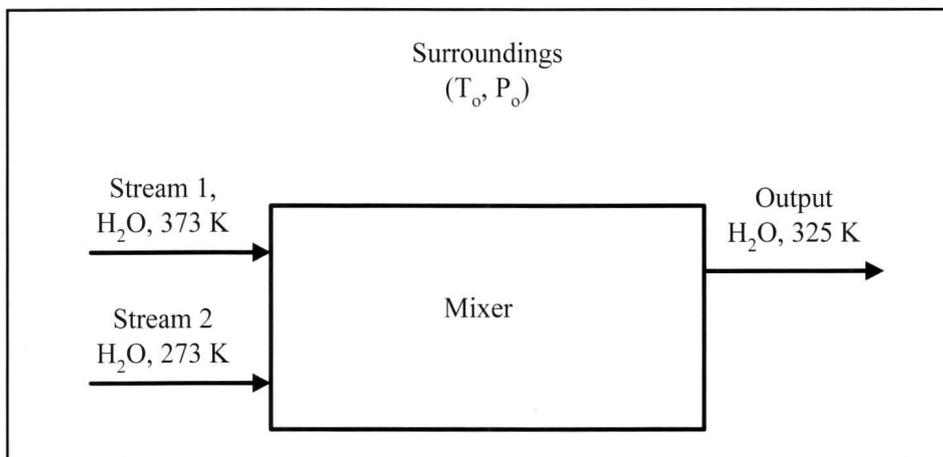
$$\left\{ \left[\sum_i \left(\sum_k \bar{\beta}_k n_k \right)_i \right] + [W_1 + |Q_1|] \right\} = \left\{ \left[\sum_e \left(\sum_k \bar{\beta}_k n_k \right)_e \right] + [W_2 + |Q_2|] + |Q_{0w}| \right\} \quad (4)$$

Note that the energy content of the isolated overall system remains invariant regardless of whether the analysis for system A is under steady-state or unsteady-state flow conditions.

Entropy Balance

The principle of the increase of entropy, which is a mani-

Figure 2. Schematic diagram of a steady-state thermal mixing system, where a stream of water at 373 K and 1 atm entering the system at the rate of $0.5 \text{ kg}\cdot\text{s}^{-1}$ is mixed adiabatically and isobarically with another stream of water at 273 K and 1 atm entering the system at the rate of $0.5 \text{ kg}\cdot\text{s}^{-1}$; the resultant stream of water exits from the system at the rate of $1.0 \text{ kg}\cdot\text{s}^{-1}$ at 1 atm and 323 K, resulting from the energy balance that yields $\{(0.5 \times 1.0 \times 373 + 0.5 \times 1.0 \times 273) / [(0.5 + 0.5) \times 1.0]\}$.^[13, 21]



festation of the second law of thermodynamics, states: "The entropy of an isolated system increases or in the limit remains constant."^{12, 16]} Consequently,

$$\left(\frac{dS}{dt} \right)_{\text{iso}} \geq 0$$

The above equation can be rewritten as^[2]

$$(\Delta S)_{\text{iso}} \geq 0 \quad (5)$$

In this expression, subscript iso stands for the isolated system. The overall system depicted in Figure 1 is one such system as previously indicated: It encompasses system A and its surroundings. It is often convenient to transform Eq. (5) into an equality by introducing a nonnegative quantity, σ , defining the rate of entropy creation in the isolated overall system; this gives rise to

$$(\Delta S)_{\text{iso}} \equiv \sigma \quad (6)$$

By considering all the quantities that lead to the change in entropy, we obtain

$$(\Delta S)_{\text{iso}} = \sigma = \left\{ \left[\sum_e \left(\sum_k \bar{r}_k n_k \right)_e \right] + \frac{|Q_2|}{T_{m2}} \right\} - \left\{ \left[\sum_i \left(\sum_k \bar{r}_k n_k \right)_i \right] + \frac{|Q_1|}{T_{m1}} \right\} + \frac{|Q_{0w}|}{T_0} \quad (7)$$

As indicated in connection with the energy balance, $|Q_{0w}|$ in the above expression includes the work loss $|(W_x)_0|$ as well as the heat loss $|Q_0|$ to the surroundings.

Available Energy Balance

Combining the energy balance, Eq. (4), and the entropy creation, Eq. (7), gives rise to

$$\left\{ \sum_i \left[\sum_k (\bar{\beta} - T_0 \bar{\gamma})_k n_k \right]_i + \left[|W_1| + |Q_1| \left(1 - \frac{T_0}{T_{m1}} \right) \right] \right\} \quad (8)$$

$$= \left\{ \sum_e \left[\sum_k (\bar{\beta} - T_0 \bar{\gamma})_k n_k \right]_e + \left[|W_2| + |Q_2| \left(1 - \frac{T_0}{T_{m2}} \right) \right] \right\} + T_0 \sigma$$

In light of the aforementioned definitions of $\bar{\beta}$ and $\bar{\gamma}$, term $(\bar{\beta} - T_0 \bar{\gamma})$ in the above equation has a connotation of the available energy of molar species, for which symbol $\bar{\epsilon}$ is coined; it is defined as the partial molar exergy. Thus,

$$\bar{\epsilon} = \bar{\beta} - T_0 \bar{\gamma} \quad (9)$$

Hence, Eq. (8) can be rewritten as

$$\left\{ \sum_i \left(\sum_k \bar{\epsilon}_k n_k \right)_i + \left[|W_1| + |Q_1| \left(1 - \frac{T_0}{T_{m1}} \right) \right] \right\} \quad (10)$$

$$= \left\{ \sum_e \left(\sum_k \bar{\epsilon}_k n_k \right)_e + \left[|W_2| + |Q_2| \left(1 - \frac{T_0}{T_{m2}} \right) \right] \right\} + T_0 \sigma$$

The quantities in the brace on the left-hand side of Eq. (10) have an implication of the total available energy input to system A. Note that they are not equal to the quantities in the brace on the right-hand side of Eq. (10) that have an implication of the total available energy exiting from the system. Their difference, $T_0 \sigma$, signifies the available energy dissipated by all types of irreversibility, which is transferred as thermal energy or heat from the system to its surroundings under the environmental conditions, as elaborated earlier.

The partial molar enthalpy relative to the dead state, $\bar{\beta}$, in Eq. (4), the partial molar entropy relative to the dead state, $\bar{\gamma}$, in Eq. (7), and the partial molar exergy relative to the dead state, $\bar{\epsilon}$, in Eq. (10) can be estimated from the following equations.^[7-11, 17, 23]

$$\bar{\beta} = \bar{\beta}_o + \int_{T_o}^T \bar{c}_p dT + \int_{P_o}^P \left[\bar{v} - T \left(\frac{\partial \bar{v}}{\partial T} \right)_P \right] dP \quad (11)$$

$$\bar{\gamma} = \bar{\gamma}_o + \int_{T_o}^T \frac{\bar{c}_p}{T} dT - \int_{P_o}^P T \left(\frac{\partial \bar{v}}{\partial T} \right)_P dP \quad (12)$$

$$\bar{\epsilon} = \bar{\epsilon}_o + \int_{T_o}^T \bar{c}_p \left(1 - \frac{T_o}{T} \right) dT + \int_{P_o}^P \left[\bar{v} - (T - T_o) \left(\frac{\partial \bar{v}}{\partial T} \right)_P \right] dP \quad (13)$$

Many of their values can also be found in various sources.^[11, 17, 22, 23]

THE MIXER EXAMPLE

This illustration is based on an extremely simple example. It is well suited, however, for effectively conveying the main theme of the current contribution. This example is an extension of the well-known one^[13, 21] in which: no work or heat is transferred from the system of concern to other systems and vice versa; no work or heat is lost from the system to its surroundings; no moving mechanical parts are visible on the system; and no changes in the chemical compositions of the streams passing through the system are detectable. Nevertheless, simply mixing two streams of water at different temperatures internally leads to significant reduction of the available energy (exergy) of the system. Figure 2 illustrates the system, which is a steady-state, thermal-mixing device, or simply "the mixer."

Mass Balance

The term, $\sum_{e,l} M_{e,l}$, in the mass balance equation, Eq. (1), vanish for the mixer; thus,

$$\sum_i M_i = M_{e,u} \quad \text{or} \quad M_{e,u} - \sum_i M_i = 0 \quad (14)$$

Since $M_{e,u} = 1.0 \text{ kg}\cdot\text{s}^{-1}$ and $\sum_i M_i = 0.5 + 0.5 = 1.0 \text{ kg}\cdot\text{s}^{-1}$, we have

$$M_{e,u} - \sum_i M_i = 1.0 - 1.0 = 0 \text{ kg}\cdot\text{s}^{-1} \quad (15)$$

As expected, the mass is conserved in the mixer and its surroundings, collectively constituting the isolated overall system: Water entering the mixer from its surroundings,

$$\sum_i M_i,$$

balances out exactly the water exiting from the mixer to its surroundings, $M_{e,u}$.

Energy Balance

The terms, $\sum_{e,d} (\beta n)_{e,d}$, $\sum_{e,l} (\beta n)_{e,l}$, $|W_1|$, $|W_2|$, $|Q_1|$, $|Q_2|$, and $|Q_{0w}|$, in the energy balance equation, Eq. (4), vanish when applied to the mixer; thus,

$$\sum_i (\beta n)_i = (\beta n)_{e,u} \quad \text{or} \quad (\beta n)_{e,u} - \sum_i (\beta n)_i = 0 \quad (16)$$

On the basis of mass flow M , instead of molar flow n , the terms in the above expression are evaluated as

The first law of thermodynamics teaches that energy is always conserved in an isolated (or closed) system; it is neither created nor destroyed by any process, system, or phenomenon.^[2-5] In contrast, the available energy analysis, which is the combination of the first and second laws of thermodynamics, indicates that in the real world the available energy is never conserved . . .

$(\beta M)_{e,u} = (25.0)(1.0) = 25.0 \text{ kcal}\cdot\text{s}^{-1}$, in which

$$(\beta)_{e,u} = \beta_o + \int_{T_o}^T c_p dt + \int_{P_o}^P \left[v - T \left(\frac{\partial v}{\partial T} \right)_P \right] dP$$

$$= 0 + (50.0 - 25.0)(1.0) + 0 = 25.0 \text{ kcal}\cdot\text{kg}^{-1}$$

and similarly

$$\sum_i (\beta M)_i = (-25.0)(0.5) + (75.0)(0.5) = 25.0 \text{ kcal}\cdot\text{s}^{-1}$$

Consequently,

$$(\beta M)_{e,u} - \sum_i (\beta M)_i = 25.0 - 25.0 = 0 \text{ kcal}\cdot\text{s}^{-1} \quad (17)$$

Obviously, the energy in the mixer and its surroundings—collectively constituting the isolated overall system—remains unchanged; energy is conserved, *i.e.*, never consumed. The energy entering into the mixer from its surroundings with the flow of water,

$$\sum_i (\beta M)_i,$$

balances out the energy exiting from the mixer to its surroundings with the flow of water, $(\beta M)_{e,u}$. Naturally, the first-law efficiency of the mixer in terms of energy conservation is $(25.0/25.0)$ or 100.0%.

Entropy Balance

The terms,

$$\sum_{e,d} \left(\sum_k \gamma_k n_k \right), \sum_{e,l} \left(\sum_k \gamma_k n_k \right), \left| \frac{Q_1}{T_{m1}} \right|, \left| \frac{Q_2}{T_{m2}} \right|,$$

and $|Q_{ow}|/T_0$, in the expression for entropy creation, Eq. (7), vanish when applied to the mixer and its surroundings, *i.e.*, to the isolated overall system; thus,

$$(\Delta S)_{iso} = \sigma = (\gamma n)_{e,u} - \sum_i (\gamma n)_i \quad (18)$$

On the basis of mass flow M , instead of molar flow n , the terms in the right-hand side of the above expression are evaluated as

$$(\gamma M)_{e,u} = (0.080)(1.0) = 0.08 \text{ kcal}\cdot\text{s}^{-1}\cdot\text{K}^{-1}$$

in which

$$(\gamma)_{e,u} = \gamma_o + \int_{T_o}^T \frac{c_p}{T} dT - \int_{P_o}^P T \left(\frac{\partial v}{\partial T} \right)_P dP$$

$$= 0 + 1 \cdot \ln \left(\frac{323}{298} \right) - 0 = 0.080 \text{ kcal}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$$

and similarly

$$\sum_i (\gamma M)_i = (-0.088)(0.5) + (0.224)(0.5) = 0.068 \text{ kcal}\cdot\text{s}^{-1}\cdot\text{K}^{-1}$$

As a result, we have

$$(\Delta S)_{iso} = \sigma$$

$$= (\gamma M)_{e,u} - \sum_i (\gamma M)_i$$

$$= 0.012 \text{ kcal}\cdot\text{s}^{-1}\cdot\text{K}^{-1}$$

or, equivalently expressed as the most diffused form of thermal energy under the environmental conditions,

$$T_0 (\Delta S)_{iso} = T_0 \sigma$$

$$= (298)(0.012)$$

$$= 3.576 \text{ kcal}\cdot\text{s}^{-1}\cdot\text{K}^{-1} \quad (19)$$

This ascertains that the entropy change of the isolated overall system, accompanying whatever process or phenomenon is occurring in the mixer, is destined to be nonnegative.

Available Energy Balance

The terms,

$$\sum_{e,d} \left(\sum_k \epsilon_k n_k \right), \sum_{e,l} \left(\sum_k \epsilon_k n_k \right), |W_1|, |W_2|, |Q_1|(1 - T_0/T_{m1}),$$

and $|Q_2|(1-T_0/T_{m2})$, in the available energy balance equation, Eq. (10), vanish when applied to the mixer; thus,

$$\sum_i (\varepsilon n)_i = (\varepsilon n)_{e,u} + (T_0 \sigma) \quad \text{or} \quad (\varepsilon n)_{e,u} - \sum_i (\varepsilon n)_i = -(T_0 \sigma) \quad (20)$$

On the basis of mass flow M , instead of molar flow n , the terms in the above expression are evaluated as

$$(\varepsilon M)_{e,u} = (1.160)(1.0) = 1.160 \text{ kcal}\cdot\text{s}^{-1}$$

in which,

$$\begin{aligned} (\varepsilon)_{e,u} &= (\beta)_{e,u} - T_0(\gamma)_{e,u} \\ &= (25.0) - (298)(0.088) = 1.160 \text{ kcal}\cdot\text{kg}^{-1} \end{aligned}$$

and similarly

$$\sum_i (\varepsilon M)_i = (1.224)(0.5) + (8.248)(0.5) = 4.736 \text{ kcal}\cdot\text{s}^{-1}$$

Hence,

$$(\varepsilon M)_{e,u} - \sum_i (\varepsilon M)_i = 1.160 - 4.736 = -3.576 \text{ kcal}\cdot\text{s}^{-1} = -(T_0 \sigma) \quad (21)$$

Note that Eq. (21) is totally unlike Eqs. (15) and (17): Exergy is not conserved. No work is performed on the surroundings by water passing through the mixer and no heat is lost to the surroundings from water passing through the mixer. In fact, it is even assumed that the flow of water does not even encounter any friction during the passage through the mixer. Nevertheless, the available energy (exergy) entering into the mixer from its surroundings with the flow of water,

$$\sum_i (\varepsilon M)_i,$$

does not balance with the available energy (exergy) exiting from the mixer to its surroundings with the flow of water,

$$(\varepsilon M)_{e,u}$$

In fact, it decreases, thereby correctly reflecting the irreversibility of the thermal mixing of two water streams inside the mixer. The difference signifies the dissipation of available energy, evaluated by Eq. (21) as $-3.576 \text{ kcal}\cdot\text{s}^{-1}$: Available energy (exergy) is always consumed, or dissipated, in the real world. Naturally, this dissipation of available energy is the only source of the entropy increase or creation in the isolated overall system, whose thermal equivalent is evaluated by Eq. (19) as $+3.576 \text{ kcal}\cdot\text{s}^{-1}$. In essence, the energy of water streams “available” to perform useful work is lost to its surroundings in the most diffused form—thermal energy under environmental conditions—which is totally unavailable to do any work. This results in entropy creation in the isolated over-

all system, which can be the universe itself. In drastic contrast to the first-law efficiency, the second-law efficiency in terms of available energy (exergy) conservation is merely $(1.160/4.7361)$ or 24.5%.

Now suppose that the mixer is externally heated at the rate, $|Q_1|$, of $50 \text{ kcal}\cdot\text{s}^{-1}$ by a heater at the temperature, T_{m1} , of 800 K. Naturally, the temperature and the corresponding energy (enthalpy) of water exiting from the mixer increase to 373 K and $[1.0 \times (100 - 25)] \times 1.0 \text{ kcal}\cdot\text{s}^{-1}$, *i.e.*, $75 \text{ kcal}\cdot\text{s}^{-1}$, respectively. The energy balance around the mixer yields the first-law efficiency of $[75/(25+50)] \times 100\%$ or 100%, thereby indicating that it is not affected by external heating. The concomitant change in the available energy (exergy) of water exiting from the mixer is from $1.160 \text{ kcal}\cdot\text{s}^{-1}$ to $[75 - (298 \times 0.224)] \times 1.0 \text{ kcal}\cdot\text{s}^{-1}$, *i.e.*, $8.248 \text{ kcal}\cdot\text{s}^{-1}$. This is obviously an increase rather than a decrease without external heating, thus indicating the possibility of enhancing the mixer’s second-law efficiency. In reality, however, the opposite is the case: simply adding external heating reduces the second-law efficiency from 24.5% to $\{8.248/[4.736 + 50 \times (1 - 298/800)]\} \times 100\%$, *i.e.*, 22.8%. Regarding the first law, Seider, *et al.*,^[21] state, “. . . it can not even give a clue as to whether energy is being used efficiently” Moreover, according to Reistad and Gaggioli,^[24] “The second-law efficiency is the performance parameter which indicates the true thermodynamic performance of the system.”

CONCLUDING REMARKS

With the aid of a deceptively simple example, it has been unequivocally demonstrated that energy *is* conserved, *i.e.*, never consumed; what is always consumed, or dissipated, is available energy (exergy), which is the essence of this brief contribution. This simple example also succinctly indicates that an attempt to rigorously assess the sustainability of any process or system should be based firmly upon the thermodynamics, in general, and the evaluation of the system’s second-law efficiency based on available energy (exergy), in particular, as practiced in the EU community^[25] and the Canton of Geneva in Switzerland.^[26]

ACKNOWLEDGMENT

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NOMENCLATURE

- A system A
- \bar{c}_p specific heat, $\text{J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$
- M mass flow rate including both convective and diffusional flows, $\text{kg} \cdot \text{s}^{-1}$
- Mw molecular weight, $\text{g} \cdot \text{mol}^{-1}$
- N molar flow rate including both convective and diffu-

sional flows, mol · s⁻¹

P pressure, atm

$|Q_0|$ heat loss to the environment per unit time, J · s⁻¹ or kcal · s⁻¹

$|Q_{0w}|$ total heat loss to the environment per unit time, J · s⁻¹ or kcal · s⁻¹

$|Q_1|$ heat transmitted from system M1 to system A per unit time, J · s⁻¹ or kcal · s⁻¹

$|Q_2|$ heat transmitted from system A to system M2 per unit time, J · s⁻¹ or kcal · s⁻¹

S entropy, J · K⁻¹

\bar{s} partial molar entropy, J · mol⁻¹ · K⁻¹

T temperature of system A, K

T_{m1} temperature of system M1, K

T_{m2} temperature of system M2, K

v volume, m³

$|W_0|$ work lost to the surroundings per unit time, J · s⁻¹ or kcal · s⁻¹

$|W_1|$ work supplied from system N1 to system A per unit time, J · s⁻¹ or kcal · s⁻¹

$|W_2|$ work supplied from system N2 to system A per unit time, J · s⁻¹ or kcal · s⁻¹

$|W_x)_0|$ work lost to the surroundings except that due to expansion of the boundary of system A per unit time, J · s⁻¹ or kcal · s⁻¹

Greek letters

$\bar{\beta}$ partial molar enthalpy relative to the dead state, J · mol⁻¹ or kcal · kg⁻¹

$\bar{\beta}_0$ partial molar chemical enthalpy, J · mol⁻¹ or kcal · kg⁻¹

\bar{e} partial molar exergy, J · mol⁻¹ or kcal · kg⁻¹

\bar{e}_0 partial molar chemical exergy, J · mol⁻¹ or kcal · kg⁻¹

$\bar{\gamma}$ partial molar entropy relative to the dead state, J · mol⁻¹ · K⁻¹ or kcal · kg⁻¹ · K⁻¹

$\bar{\gamma}_0$ partial molar chemical entropy, J · mol⁻¹ · K⁻¹ or kcal · kg⁻¹ · K⁻¹

σ created entropy per unit time, J · sec⁻¹ · K⁻¹ or kcal · sec⁻¹ · K⁻¹

Subscripts

0 dead state

e,u useful output streams

i input streams

iso isolated system

k material species

l leakage

Superscript

0 standard state

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Inside the Cell

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combination of rational design and screening of mutant libraries will be used to create green fluorescent proteins with improved photophysical properties.

9. **Genetically Targetable Labels for Light and EM** • Roger Y. Tsien, Ph.D., principal investigator, University of California, San Diego

A team from the University of California and the University of Illinois plans a series of approaches to generate fluorescent proteins with increased photostability and higher quantum yield, to explore quantum dot construction and targeting, and to further develop tetracysteine labeling techniques for light and electron microscopy. The team's plans also include exploring genetically targetable labels with long excited state lifetimes based on lanthanide and transition metal luminescence as well as directed evolution of fluorescent proteins to improve their photophysical properties. A major goal of this team is to enable direct visualization in the electron microscope of the same molecules that have been tagged, observed, and dynamically tracked in the light microscope.

Now that breakthroughs are under way to provide specific information on the functioning and control of organelles, a unique opportunity is evolving for chemical engineers to use this mechanistic information to design new integrated biocellular operations and processes.

It is likely that exceptional progress will be made in the next decade to reveal the physical chemical phenomena that govern the organization and behavior of the biochemical processing units within cells. Naturally then, new concepts of process design will emerge for the chemical/biochemical industry through the research efforts of biochemical engineers. As this knowledge becomes available it will be incorporated into the graduate-program courses in chemical engineering departments as an enhancement to courses such as systems biology, bio-MEMS, biochemical separations, bioprocess engineering, and pharmaceutical biotechnology. One can expect a dramatic evolution in process technology that will become an important capability for future chemical engineers, especially for high-value, low-volume products.

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The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested, as well as those that are more traditional in nature and that elucidate difficult concepts. Manuscripts should not exceed 14 double-spaced pages and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

GAS PERMEATION COMPUTATIONS WITH MATHEMATICA

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Gas separations using membranes have received increased attention by the scientific and industrial community. This technique is now at a mature stage and can compete with more common techniques used in the petrochemical industry such as cryogenic separation, gas absorption, and pressure swing adsorption. The nonporous membranes can be organic or inorganic. They are classified according to their thermal and chemical stability as well as their selectivity to different gases. The mechanism of separation is based on the differences in the dissolution and diffusion of gases in the nonporous membrane. The separation of hydrogen from other gases such as carbon dioxide and carbon monoxide in syngas plants is a very important industrial application of this technique. Acid gas (CO_2 and H_2S) elimination from natural gas is another application of membrane separations. Very often one is confronted with the separation of multicomponent mixtures. Thus, we consider a hypothetical ternary mixture, in the first part of the paper, to show how one can obtain the permeate and reject compositions as well as the membrane area.

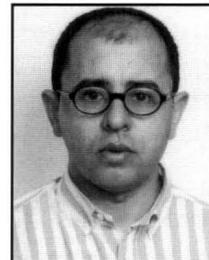
SEPARATION OF A TERNARY MIXTURE

A ternary feed mixture has the following composition and flow rate:

$$x_{fA} = 0.25, x_{fB} = 0.55, x_{fC} = 0.2 \text{ and } q_f = 1.0 \times 10^4 \text{ cm}^3 \text{ (STP)/s}$$

Since the stage cut, defined as the fraction of the feed allowed to permeate, is $\theta = 0.25$, the permeate flow rate, q_p , is equal to $0.25 \times 10^4 \text{ cm}^3 \text{ (STP)/s}$. The permeabilities, expressed in $\text{cm}^3 \text{ (STP) cm}/(\text{s cm}^2 \text{ cmHg})$, of components A, B, and C

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are equal to

$$P'_A = 200 \times 10^{-10}, P'_B = 50 \times 10^{-10}, \text{ and } P'_C = 25 \times 10^{-10}.$$

This mixture is to be separated by a membrane with a thickness $t = 2.54 \times 10^{-3}$ cm. Pressures on the feed and permeate sides are $p_h = 300$ cmHg and $p_l = 30$ cmHg. We will use the complete-mixing model to compute the permeate and the reject compositions as well as the membrane area. The three rate-of-permeation equations are:

$$q_p y_{pi} = \frac{P'_i}{t} A_m (p_h x_{Oi} - p_l y_{pi}) \text{ for } i=1,2,3 \quad (1)$$

The three material balances equations written for components A, B, and C are:

$$x_{Oi} = \frac{1}{1-\theta} x_{fi} - \frac{\theta}{1-\theta} y_{pi} \text{ for } i=1,2,3 \quad (2)$$

Finally, we have an additional relation that is the summation rule for mole fractions:

$$\sum_{i=1}^3 y_{pi} = 1 \quad (3)$$

Equations 1 through 3 are labeled rate, matbalance, and summation, respectively. We need to enter these equations in the Mathematica notebook^[2] and call *FindRoot* as follows:

```
FindRoot[{rate1, rate2, rate3,
matbalance1, matbalance2, matbalance3,
summation1}, {yPA, 0.2}, {yPB, 0.2}, {yPC,
0.2}, {Am, 106}, {xOA, 0.2}, {xOB, 0.2},
{xOC, 0.2}]
```

FindRoot uses different root search techniques that can be selected by the user. If one specifies only one starting value of the unknown, *FindRoot* searches for a solution using Newton methods. If the user specifies two starting values, *FindRoot* uses a variant of the secant method, which does not require the computation of derivatives. All this is handled internally by *Mathematica*, making the solution of complex systems of nonlinear algebraic equations very easy. We get the following solution for the permeate and reject compositions and the membrane area labeled A_m :

$$\begin{aligned} \{y_{PA} \rightarrow 0.455281, y_{PB} \rightarrow 0.450286, \\ y_{PC} \rightarrow 0.0944335, \\ A_m \rightarrow 3.54176 \times 10^6, x_{OA} \rightarrow 0.181573, \\ x_{OB} \rightarrow 0.583238, x_{OC} \rightarrow 0.235189\} \end{aligned}$$

which is in agreement with results using a tedious iterative technique.^[1]

ENRICHMENT OF AIR IN OXYGEN USING MEMBRANE PERMEATION

In this section, we present the study of the enrichment of oxygen in air using a single-stage membrane module. This problem has been treated first by Walawender and Stern^[3] and later by Geankoplis.^[1] The binary mixture, A (oxygen) and B (nitrogen), has an ideal separation factor, the ratio of the permeabilities of the two species, $\alpha^* = 10$. The permeability of oxygen is $P'_A = 500 \times 10^{-10}$ cm³ (STP) cm/(s cm² cmHg). The membrane is more permeable to oxygen and has

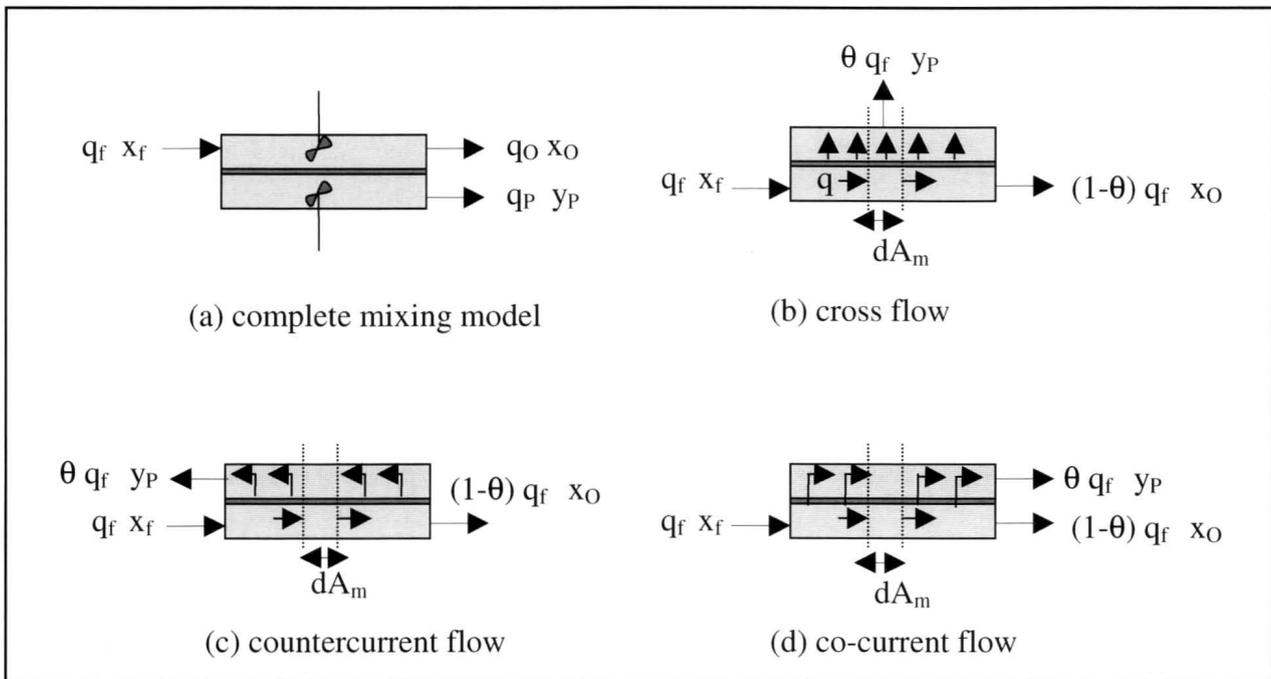


Figure 1. Flow patterns.

a thickness $t=2.54 \times 10^{-3}$ cm. The stage cut, θ , is set equal to 0.2. The values of the pressures in the feed and permeate sides chosen by Geankoplis^[1] are $p_h=190$ cmHg and $p_l=19$ cmHg, which give a ratio of pressures, r , equal to 10. The feed rate and composition are given by:

$$x_{fA}=0.209, x_{fB}=0.791 \text{ and } q_f=1.0 \times 10^6 \text{ cm}^3 \text{ (STP)/s.}$$

The different flow patterns, shown in Figure 1 (previous page) and considered in this study, are complete mixing, cross-flow, countercurrent flow, and co-current flow. Calculations for each flow pattern will be presented in a separate subsection.

1. Complete-Mixing Case

The permeate mole fraction, y_p , is the solution of the following quadratic equation:

$$\frac{y_p}{1-y_p} = \frac{\alpha^* \left[x_O - \left(\frac{P_l}{P_h} \right) y_p \right]}{\left(1-x_O \right) - \left(\frac{P_l}{P_h} \right) (1-y_p)} \quad (4)$$

where the reject composition, x_O , is given by the mass balance:

$$x_O = \frac{x_f - \theta y_p}{1-\theta} \quad (5)$$

We also define α^* and r by $\alpha^* = P'_A/P'_B$ and $r=P_h/P_l$.

The membrane area is then obtained using Equation (6):

$$A_m = \frac{\theta q_f y_p}{\left(\frac{P'_A}{t} \right) (P_h x_O - P_l y_p)} \quad (6)$$

For our particular problem, we find the following results using Mathematica:

$$y_p=0.5067, x_O=0.1346, \text{ and } A_{sol}=3.228 \times 10^8 \text{ cm}^2.$$

These results are in agreement with those found by Geankoplis.^[1]

2. Cross-Flow Case

The local permeate rates over a differential membrane area are given by

$$-y dq = \left(\frac{P'_A}{t} \right) (p_h x - p_l y) dA_m \quad (7)$$

$$-(1-y) dq = \left(\frac{P'_B}{t} \right) (p_h (1-x) - p_l (1-y)) dA_m \quad (8)$$

In addition, we can derive Equation (9) from total and component mass balances:

$$y dq = d(qx) \quad (9)$$

These three governing equations are solved simultaneously using the Mathematica built-in function called *NDSolve*. The following boundary conditions are used:

$$q|_{A_m=0} = q_f, x|_{A_m=0} = x_{fA} \text{ and } y|_{A_m=0} = y_{Pi}$$

where y_{Pi} is obtained by solving the quadratic equation

$$\frac{y_{Pi}}{1-y_{Pi}} = \frac{\alpha^* \left[x_{fA} - \left(\frac{P_l}{P_h} \right) y_{Pi} \right]}{\left(1-x_{fA} \right) - \left(\frac{P_l}{P_h} \right) (1-y_{Pi})} \quad (10)$$

The command used in the notebook to solve the system of ODEs is:

```
myODEsoln[Ω_] :=
NDSolve[{Y[A_m] D[q[A_m], {A_m, 1}] ==
D[q[A_m] x[A_m], {A_m, 1}],
-y[A_m] D[q[A_m], {A_m, 1}] == P'_A/t (p_h x[A_m]
- p_l y[A_m]),
-(1-y[A_m]) D[q[A_m], {A_m, 1}] ==
P'_B/t + (p_h (1-x[A_m]) - p_l (1-y[A_m])), x[0]
== x_f,
y[0] == y_Pi, q[0] == q_f, {x[A_m],
y[A_m], q[A_m]}, {A_m, 0, Ω}]
```

We use *FindRoot* to get the total membrane area. In fact, we must satisfy the following condition: $\theta=0.2$ where the stage cut, θ , is given by $\theta=(q_f - q_{end})/q_f$.

The Mathematica command is written as follows:

```
qend[Ω_?NumericQ] := Flatten[{q[A_m] /.
myODEsoln[Ω]} /. A_m → Ω]
```

```
A_sol = FindRoot[(q_f - qend[Ω])/q_f == θ,
{Ω, 2 10^8, 3 10^8}, MaxIterations → 1000];
```

The final result is a membrane area and a reject composition equal to: $A_{sol}=2.899 \times 10^8$ cm² and $x_O=0.1190$. A component balance, $\theta y_p + (1-\theta)x_O = x_{fA}$, can be used to obtain the permeate mole fraction and we find that $y_p=0.5688$. Our approach gives similar results as those given by Geankoplis^[1] but is far less tedious and more accurate. We can check our results by integrating $y(A_m)$ for A_m varying from 0 to A_{sol} , achieved with the command:

```
Integrate[First[Y[A_m] /. myODEsoln[Ω /
.A_sol]] /. A_m → area,
{area, 0, Ω /. A_sol}] / Ω /. A_sol
```

We get $y_p=0.5634$, a value in agreement with the previous result. Since numerical integration is used, the later value of

y_p is less exact. In Figure 2, we plot the mole fraction in the permeate and feed sides in the membrane module. Similar figures can be easily drawn for the other flow patterns using the graphical capabilities of Mathematica. Figure 2 clearly shows that the oxygen mole fraction in the feed side of the module varies from the inlet value, $x_f=0.209$, to the reject value, $x_o=0.1190$.

3. Countercurrent-Flow Case

The flow diagram for the countercurrent-flow pattern is shown in Figure 1. Both streams are in plug flow. The two governing equations have been derived by Oishi, *et al.*,^[4] and Walawender and Stern^[3]:

$$\left(\frac{q_{O,t}}{p_1 P'_B}\right) \frac{dx}{dA_m} = \left(\frac{x-y}{y-x_O}\right) \left\{ (1-x)\alpha^*(rx-y) - x[r(1-x)-(1-y)] \right\} \quad (11)$$

$$\left(\frac{q_{O,t}}{p_1 P'_B}\right) \frac{dy}{dA_m} = \left(\frac{y-x}{x-x_O}\right) \left\{ (1-y)\alpha^*(rx-y) - y[r(1-x)-(1-y)] \right\} \quad (12)$$

where $q_o=(1-\theta)q_f$. The following boundary conditions

$$x|_{A_m=0} = x_O \quad \text{and} \quad y|_{A_m=0} = y_i,$$

are used where y_i is the solution of the quadratic equation:

$$\frac{y_i}{1-y_i} = \frac{\alpha^* \left[x_O - \left(\frac{p_l}{p_h}\right) y_i \right]}{(1-x_O) - \left(\frac{p_l}{p_h}\right) (1-y_i)} \quad (13)$$

We use L'Hopital's rule to compute the derivatives at $A_m=0$ because they become indeterminate when $x=x_O$. This is performed as follows:

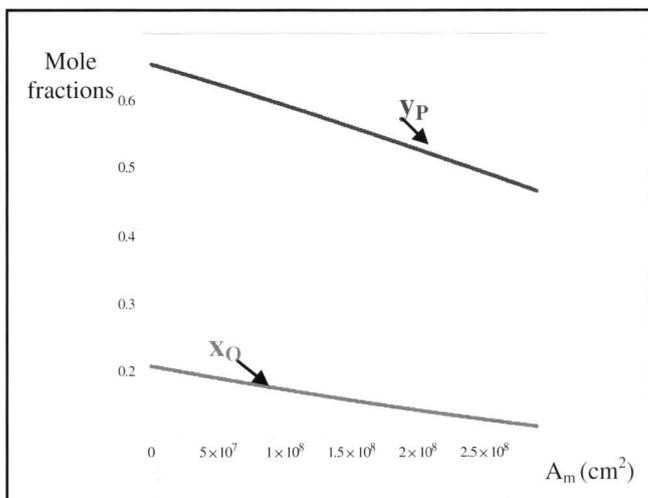


Figure 2. Mole fractions of reject and permeate.

$$\left(\frac{dy}{dA_m}\right)_{A_m=0} = \frac{(x_O - y_i)r[\alpha^* - y_i(\alpha^* - 1)]}{\left(\frac{q_{O,t}}{p_1 P'_B}\right) - \frac{\left\{ (x_O - y_i)[(\alpha^* - 1)(2y_i - rx_O - 1) - r] \right\}}{\left(\frac{dx}{dA_m}\right)_{A_m=0}}} \quad (14)$$

$$\left(\frac{dx}{dA_m}\right)_{A_m=0} = \frac{1}{\left(\frac{q_{O,t}}{p_1 P'_B}\right)} \left[\frac{\alpha^*(rx_O - y_i)(x_O - y_i)}{y_i} \right] \quad (15)$$

These two differential equations can be solved simultaneously using *NDSolve*. We enter the equations using an *If* statement to take into account the derivative expression when $A_m \rightarrow 0$:

```

eq1[a_] := D[x[A_m], {A_m, 1}] ==
If[A_m == 0,
Evaluate[
(p1 P'_B) / (q_o t) α (x_o p_h / p_l - y_i) (x_o - y_i) /
y_i /.
t -> 2.54 10^-3 /. p_h -> 190 /. p_l -> 19 /.
α -> 10 /.
P'_B -> 50 10^-10 /. q_o -> 8 10^5 /
.xo -> a],
Evaluate[
(p1 P'_B) / (q_o t) (x[A_m] - y[A_m]) / (y[A_m] -
x_o)
((1 - x[A_m]) α (p_h / p_l x[A_m] - y[A_m]) -
x[A_m] (p_h / p_l (1 - x[A_m]) - (1 - y[A_m]))) /
t -> 2.54 10^-3 /. p_h -> 190 /. p_l -> 19 /.
α -> 10 /.
P'_B -> 50 10^-10 /. q_o -> 8 10^5 /
.xo -> a]]

```

Since the value of the reject mole fraction, x_o , and the total area, A_m , are unknown, we use *FindRoot* to solve for these two unknowns so that the mole fraction of oxygen in the feed is 0.209 and that the material balance for component A is verified:

$$x|_{A_{sol}} = x_{fA} \quad \text{and} \quad \theta y_p|_{A_{sol}} + (1-\theta)x_o = x_{Af}$$

Following the treatment of Walawender and Stern,^[3] we set the area equal to zero at the outlet of the gas separation module. Thus, the sign of the membrane area obtained using this approach is negative and must be reversed. We get the following results: $A_{sol}=2.859 \times 10^8 \text{ cm}^2$, $y_p=0.5763$, and $x_o=0.1171$. We find a smaller membrane area and reject mole

fraction and a higher permeate composition.

4. Co-Current-Flow Case

The governing equations^[3] are derived in a similar fashion to the preceding case.

$$\left(\frac{q_f t}{p_1 P_B}\right) \frac{dy}{dA_m} = \left(\frac{x-y}{x-x_f}\right) \left\{ (1-y)\alpha^*(rx-y) - y[r(1-x) - (1-y)] \right\} \quad (16)$$

$$\left(\frac{q_f t}{p_1 P_B}\right) \frac{dx}{dA_m} = \left(\frac{x-y}{y-x_f}\right) \left\{ (1-x)\alpha^*(rx-y) - x[r(1-x) - (1-y)] \right\} \quad (17)$$

The following boundary conditions must be used: $x|_{A_m=0} = x_{Af}$ and $y|_{A_m=0} = y_i$. The value of y_i is a solution of the following quadratic equation:

$$\frac{y_i}{1-y_i} = \frac{\alpha^* \left[x_f - \left(\frac{p_l}{p_h}\right) y_i \right]}{(1-x_f) - \left(\frac{p_l}{p_h}\right) (1-y_i)} \quad (18)$$

Inspection of Equation (16) shows that the derivatives are indeterminate when $A_m \rightarrow 0$. We use L'Hopital's rule to get expressions for the derivatives at $A_m=0$ as follows:

$$\left(\frac{dy}{dA_m}\right)_{A_m=0} = \frac{(x_f - y_i)r[\alpha^* - y_i(\alpha^* - 1)]}{\left(\frac{q_f t}{p_1 P_B}\right) - \frac{\left\{ (x_f - y_i) \left[(\alpha^* - 1)(2y_i - rx_f - 1) - r \right] \right\}}{\left(\frac{dx}{dA_m}\right)_{A_m=0}}} \quad (19)$$

$$\left(\frac{dx}{dA_m}\right)_{A_m=0} = \frac{1}{\left(\frac{q_f t}{p_1 P_B}\right)} \left[\frac{\alpha^*(rx_f - y_i)(x_f - y_i)}{y_i} \right] \quad (20)$$

The value of the total membrane area is found using *FindRoot* to satisfy the material balance for oxygen:

$\theta y_p|_{A_{sol}} + (1-\theta)x_O = x_{Af}$. The membrane area, permeate composition, and reject mole fraction are equal to: $A_{sol} = 2.955 \times 10^8$ cm², $y_p = 0.5584$ and $x_O = 0.1216$.

5. Comparing the Different Flow Patterns

The membrane areas are equal within 10%. The smallest membrane area is obtained using the countercurrent flow pattern. The countercurrent case requires a smaller membrane area because the driving force for permeation (the composi-

tion difference between permeate and feed sides) is higher than in the other flow patterns. The complete-mixing model gives the highest membrane area. The reject mole fractions and the permeate compositions obtained for the four cases studied show similar trends. The most efficient flow pattern is the countercurrent mode. In fact, the order of efficiency is the following: countercurrent flow > cross-flow > co-current flow > complete-mixing model. Reducing membrane area has a major impact on capital investment costs. Thus, the countercurrent flow pattern is the optimal design choice. Other relevant parameters for reducing membrane area are thickness and permeability of the membrane and operating pressure, which will affect operating costs as well.

CONCLUSIONS

In this study, we showed how simple Mathematica commands^[2] can be used to solve problems that required tedious iterative techniques or complicated programming skills. We present the solutions of two problems proposed by Professor Geankoplis.^[1] We extend this author's work to the countercurrent and co-current flow patterns. These problems are given to the junior and senior students of the National Institute of Applied Sciences in Tunis as small research projects. The students excel in these type of problems despite the fact that they do not have prior knowledge of Mathematica.

NOMENCLATURE

- A_m membrane area
- P_i permeability of component i
- p_h feed side pressure
- p_l permeate side pressure
- q_f feed flow rate
- q_p permeate flow rate
- q_o reject flow rate
- t membrane thickness
- r ratio of pressures of feed and permeate sides
- x_{fi} feed mole fraction of component i
- x_o reject mole fraction
- y_p permeate mole fraction
- α^* separation factor
- θ stage cut

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