



## Dennis J. Miller

... of Michigan State University



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## Author Guidelines for the LABORATORY Feature

The laboratory experience in chemical engineering education has long been an integral part of our curricula. CEE encourages the submission of manuscripts describing innovations in the laboratory ranging from large-scale unit operations experiments to demonstrations appropriate for the classroom. The following guidelines are offered to assist authors in the preparation of manuscripts that are informative to our readership. These are only suggestions, based on the comments of previous reviewers; authors should use their own judgment in presenting their experiences. A set of general guidelines and advice to the author can be found at our Web site: <<http://che.ufl.edu/~cee/>>.

- c Manuscripts should describe the results of original and laboratory-tested ideas. The ideas should be broadly applicable and described in sufficient detail to allow and motivate others to adapt the ideas to their own curricula. It is noted that the readership of CEE is largely faculty and instructors. Manuscripts must contain an abstract and often include an Introduction, Laboratory Description, Data Analysis, Summary of Experiences, Conclusions, and References.
  - An Introduction should establish the context of the laboratory experience (e.g., relation to curriculum, review of literature), state the learning objectives, and describe the rationale and approach.
  - The Laboratory Description section should describe the experiment in sufficient detail to allow the reader to judge the scope of effort required to implement a similar experiment on his or her campus. Schematic diagrams or photos, cost information, and references to previous publications and Web sites, etc., are usually of benefit. Issues related to safety should be addressed as well as any special operating procedures.
  - If appropriate, a Data Analysis section should be included that concisely describes the method of data analysis. Recognizing that the audience is primarily faculty, the description of the underlying theory should be referenced or brief. The purpose of this section is to communicate to the reader specific student-learning opportunities (e.g., treatment of reaction-rate data in a temperature range that includes two mechanisms).
  - The purpose of the Summary of Experiences section is to convey the results of laboratory or classroom testing. The section can enumerate, for example, best practices, pitfalls, student survey results, or anecdotal material.
  - A concise statement of the Conclusions (as opposed to a summary) of your experiences should be the last section of the paper prior to listing References.

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# *Dennis J. Miller*

## *of Michigan State University*



*Dennis with post-doctoral associate Navin Asthana in 2006.*

BY DAINA M. BRIEDIS WITH JANE L. DEPRIEST

**D**edicated and resolute. If taken without energy, innovation, and relationships, these attributes suggest routine, even monotony, in life. But for Dennis Miller, professor of chemical engineering at Michigan State University (MSU), life is anything but monotonous. His love of discovery and creative spirit energize him to constantly seek new opportunities both professionally and personally, and his dedication and resolve have led to a life that is full of diverse experiences and accomplishments. With these traits, Dennis Miller is exemplary in how a typical kid from Toledo, Ohio, can become a respected and accomplished teacher, researcher, and community servant.

Dennis has been a faculty member in the Department of Chemical Engineering and Materials Science at MSU in East Lansing, Michigan, since completing his doctorate in 1982. He has had the same “job” for his entire academic career. During that time, Dennis has been successful in cultivating his passion for teaching and research, while maintaining a hefty measure of service in the academic and local communities. He has balanced career, family, and faith—all while trying to keep a healthy perspective on time and resource challenges. His energy, enthusiasm, and selfless commitment in all aspects of life have earned him the affectionate title of “The “Energizer Bunny” among family and friends. His passion

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for “doing”—and doing things well—is contagious, and has benefited his students, colleagues, family, and the progress of his career.

“Dennis is an exemplary, complete faculty member,” says Martin Hawley, professor and chairperson of the MSU Department of Chemical Engineering and Materials Science. “He has a high-level and high-quality research program involving graduate students and post-docs, and he collaborates quite effectively with his colleagues. Dennis is also an outstanding educator. He incorporates new ideas related to his own experiences, is willing to try new approaches, and requires high standards in student work.”

## UPBRINGING—A STABLE FOUNDATION

Dennis has a strong family background. He was born in Toledo, Ohio, to Fred and Dorothy Miller, who still live in the same house to which they moved when Dennis was six months old. His father attended the University of Toledo from 1946-1949 on the GI Bill and graduated as an electrical engineer. That started a tradition for the Miller family. Dennis and his two brothers all are engineering graduates of the University of Toledo. Fred Miller worked for Toledo Edison for his entire career (1949-1987) and was involved in a variety of jobs that culminated with the engineering of the safety systems for the Davis-Besse Nuclear Power Plant in Oak Harbor, Ohio, about 20 miles southeast of Toledo.

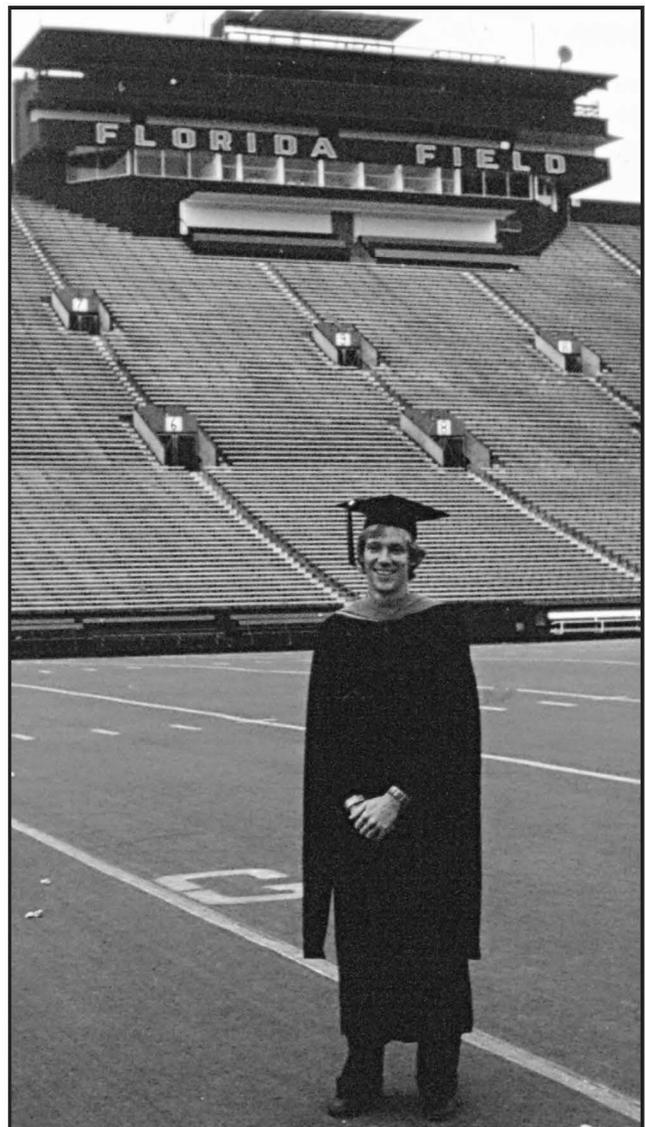
The opportunity to observe the nuclear plant construction during his high school and early college years triggered Dennis’s interest in science and engineering. His AP chemistry teacher at Thomas A. DeVilbiss High School, Ethyl Molnar, helped to ignite his passion for chemistry because she challenged her students to think through problems; his high school math teachers demanded systematic effort and correct answers and helped Dennis begin to think like an engineer.

Following his high school graduation, Dennis proceeded immediately to the University of Toledo (which was nearly as close to his house as his high school) to study chemical engineering. His favorite courses were kinetics and transport phenomena, clearly evidenced by the direction his career has taken. “I had an excellent experience as an undergraduate,” Dennis remembers. “The professors were great, especially Ken DeWitt, James Lacksonen, and Joe Boston, and the classes were small, and so there was a lot of interaction.”

Dennis was able to couple his coursework with a student internship at Owens-Illinois Glass Company, where he worked on a research project with Millard Jones, another University of Toledo faculty member and a consultant for Owens-Illinois. Dennis worked on heat transfer in glass bottle manufacturing. This involved bench-scale experimentation, computer modeling, and pilot plant testing, which provided good exposure to the research environment. This experience, along with the support of his college professors, was influential in encouraging Dennis to go on to graduate studies.



*Above: Early evidence of a lifelong love of fishing, Dennis displays a trophy walleye taken from Georgian Bay, Lake Huron (1967). Below: Graduation day at the University of Florida.*



As a teenager, Dennis spent many hours working on cars, where he fine-tuned his appreciation for problem solving and developed skill in working with his hands. He and his friends took apart and assembled VW Beetles, and, most infamously, two Triumph Spitfires. One of the Triumphs had significant front-end damage and the other was smashed in the back. After filling the garage floor with car parts for months at a time and visiting every foreign car shop and junkyard in town, Dennis successfully assembled the two wrecks into one working vehicle that ended up serving him well through college. The Triumph experience, however, was not without trouble. The serial number of the car used for the title was on the damaged car body that was disposed of, so when Dennis sold the car, the serial number did not match the one on the title. Dennis had to do some serious explaining to the buyer and the police that the car wasn't stolen.

That same Triumph was also the victim of a practical joke by Steve Le Blanc and other chemical engineering classmates at the University of Toledo, who lifted and wedged the light vehicle sideways between two other parked cars, leaving only inches at the front and rear of the Triumph. When Dennis left the engineering building that evening, he was trapped between the two other cars with no way to move his Triumph. Only by pleading with his thoroughly amused "friends" was the car finally rescued from its predicament.

Of all Dennis's hobbies and interests, his favorite as a youth and as an adult has been fishing. His father's fascination with the sport meant that most family vacations involved angling in some way, from Alaska to the Florida Keys, and many places in between. When salmon were first planted in the Great Lakes in 1967, Dennis and his father quickly joined in this exciting, new sport-fishing adventure. That excitement has persisted to the present, and Great Lakes and inland lake fishing remain an integral part of what Dennis does for enjoyment, relaxation, and fellowship. He shares his interest with family and friends; if anyone even mentions fishing, Dennis is the first in planning where and when. Dennis jokingly boasts about the time that he caught a salmon barehanded. That sounds impressive until you hear the real story! The spawning run was so thick on Michigan's Platte River that a poor salmon trapped itself between the Miller boat and the shore. Dennis simply jumped out of the boat and scooped up the 15-pound fish.

## GRADUATE STUDIES—FRAMING THE FUTURE

After working the summer of 1977 at the Exxon Research and Development Laboratory in Baton Rouge, La., Dennis headed to graduate school at the University of Florida in Gainesville for a change of scenery. "I wanted to go to a different part of the country for graduate school and at that time, the University of Florida was in the process of expanding its faculty and research efforts," says Dennis. He chose to work with Hong Lee, who had just arrived at Florida from Westvaco Corp. "As Hong's first student, I spent a lot of time setting up the lab and assembling equipment, which was something I

was pretty comfortable with," says Dennis who helped build a high-pressure thermobalance for coal hydrogasification studies and constructed an enclosure around it in case something exploded. Ultimately, their kinetics work on the role of alkali carbonate catalysts in gasification fueled Dennis's broader interest in catalysis, kinetics, and alternate energy sources that drives his current research.

Lest the reader think that Dennis suddenly neglected his hobbies, he also balanced the rigorous demands of graduate studies and research with outside activities that included salt-water fishing and playing beach volleyball and softball with the department's graduate students and younger faculty. Among the latter was a long-haired assistant professor shortstop named Tim Anderson, who has remained a lifelong friend.

The graduate experience in Florida included another component that strongly influenced Dennis's future—good teaching experiences as an assistant to both Professors Lee and Ray Fahein. "I taught a good part of the transport phenomena course one year for Dr. Fahein because he was experiencing some health issues," says Dennis. "That really perked my interest in teaching. I enjoyed interacting with students and seeing them get interested in the course material."

After receiving a Ph.D. in chemical engineering in 1982 and with encouragement from Ray Fahein and John O'Connell, Dennis applied for both academic and industrial positions. "As graduation neared, job interviews and plant trips had been scheduled, but the '82 recession led to hiring freezes at many companies. In the end, Michigan State offered a balance of teaching and research, along with plans for significant department growth that sounded promising. Don Anderson, the chair of the chemical engineering department at that time, was a real advocate for young faculty members."

## CAREER—RELATIONSHIPS BUILT TO LAST

The early years at MSU were full of the typical heavy workload and stresses of an assistant professor's job. "I most enjoyed being in front of students in the classroom, but I knew I had to develop a research program to stay in the academic world," says Dennis. "Those years were definitely a struggle in terms of research funding, but enough came through for promotion and tenure."

The early toils were shared by a fellow assistant professor, Daina Briedis, who had also started working at Michigan State in 1982. They became friends through shared hours of commiseration about the life of a young faculty member, racquetball matches at the local gym, and teaming up in mixed doubles beach volleyball, where the couple even advanced as far as winning 2nd place in a tournament. The strong friendship led to a permanent "arrangement," and Dennis and Daina were married in 1985.

While Dennis's original work focused on carbon gasification chemistry and pyrolysis, by 1985 the focus of the work done in Dennis's research program shifted to catalytic conversions of



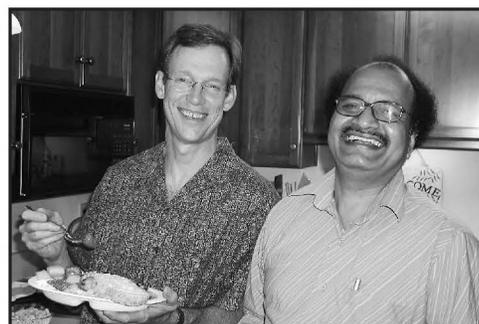
*Clockwise from lower left:  
A chemical engineering wedding; Dennis  
along with colleagues Ned Jackson (left)  
and Carl Lira (2nd from left), and Michigan  
Governor Jennifer Granholm, during her  
visit to MSU chemical engineering follow-  
ing the awarding of \$7 million for Michi-  
gan 21st Century Jobs Fund; with UICT  
professor G.D. Yadav at the Miller home  
during one of his visits to MSU.*

renewable feedstocks. “Having the Michigan Biotechnology Institute come to East Lansing brought a number of pioneers in the field to MSU,” Dennis recalls. “They started talking about sugars, organic acids, and alcohols as chemical feedstocks, so we started looking at the types of catalytic conversion chemistry we could do with those molecules.”



Dennis may have been a few years ahead of the curve. “At a couple of Catalysis Society meetings in those years, people would ask why we were wasting our time looking at obscure compounds like lactic acid,” says Dennis. “It seemed that most people were studying single crystal surfaces in high vacuum or surface reactions of simple hydrocarbons, so our work appeared somewhat unwieldy because we were dealing with multiple reaction pathways, carbon deposition on the catalyst, and closing the material balance.”

His research efforts took a positive turn in 1989 when he partnered with James E. (Ned) Jackson, a physical organic chemist and, at that time, assistant professor in the MSU Department of Chemistry. Ned and Dennis enjoyed immediate success in securing research funding from the U.S. Department of Energy (DOE) and the U.S. Department of Agriculture (USDA). A prolific partnership was born. “Ned and I are a great team because we complement each other so well. He studies mechanisms; I study kinetics and transport phenomena. He is a thinker; I am a doer,” says Dennis. Together the two have published more than 20 papers, garnered several million dollars of research funding, have 10 joint patents, and have studied numerous chemical systems in-depth. Much



of the work has focused on aqueous phase hydrogenation. “Most biorenewable feedstocks are water-soluble, and they need to be deoxygenated en route to becoming replacements for petrochemicals, so aqueous phase reactions are a natural,” says Dennis.

The Miller-Jackson collaboration is now approaching 20 years of research with no end in sight. Ned is now a professor of chemistry.

“Working with Ned has been a real professional and personal benefit for me,” says Dennis. “It’s a marriage, in a sense, because we know each other’s strengths and weaknesses so well and we can take advantage of that to maximize our productivity.” Ned agrees. “Our collaboration has been a continuous learning experience. It’s been very healthy for me and my students to learn about not only large-scale chemistry but also the economics and even politics of the massive flows of chemical matter that we transform and traffic through the world,” says Ned, who believes that chemistry students should learn more about the significance of the field in (and between) natural and human environments. “Hopefully the learning exchange has gone the other way too, with engineering students gaining some appreciation of the rules governing reactions at the molecular scale, to bolster their insights into transport, reactor design, thermochemistry, stoichiometry, kinetics, and economics.”

With the blossoming of the ethanol industry and emerging interests in renewable feedstocks, the Miller research group has expanded significantly in the past 10 years to include efforts in reactive separations and, more recently, biofuels. “Michigan State is a national leader in biorefinery development, and it also is, and always has been, an excellent place to collaborate on research,” says Dennis. “I have been fortunate to have the chance to work with a number of

Clockwise from right: On vacation at the family's lake cottage; coaching girls' volleyball at Lansing Christian School; the Miller family posing in front of a 12th-century Roman Bridge during a 2007 mission trip to Spain.



outstanding individuals across this campus and within the College of Engineering, and those partnerships have nearly always led to synergies that outweigh any possible advantages of working alone.” Colleagues Carl Lira, Ramani Narayan, Kris Berglund, and Robert Ofoli in chemical engineering, and Harold Schock in mechanical engineering along with Jackson create combined expertise that makes proposals competitive in most venues.”

In addition, Dennis has worked with a group of postdoctoral associates from the Mumbai (India) University Institute of Chemical Technology (UIC). “They have been great colleagues and have generated many ideas and intellectual property,” explains Dennis. These former students of M.M. Sharma and G.D. Yadav have really jump-started the reactive distillation program in Dennis’s lab. Dennis maintains close contact with UIC, having visited there twice and having hosted Professor Yadav at MSU during the 2001-2002 academic year.

Today Miller’s research group, which includes six graduate students and three postdoctoral associates, is active in multiple research projects funded by DOE, USDA, private industry, and national laboratories.

Besides research accomplishments and his advancement through the faculty ranks, Dennis finds even more satisfaction in educating students. “My early experiences in teaching at

the University of Florida are what stimulated me to consider an academic career,” says Dennis. “The university is all about students, and my responsibility in educating them is equally, if not more, important as advancing knowledge through research. I ascribe to the motto of Michigan State—*Advancing Knowledge. Transforming Lives.* And I believe I can help influence the lives of our undergraduates.”

Dennis’s love of teaching has garnered him awards in education. These include the Martin Best Paper Award in the Chemical Engineering Division of ASEE, the Amoco Foundation Excellence in Teaching Award (MSU), the Michigan State University Teacher-Scholar Award, and five Withrow Teaching Excellence Awards (1991, 1994, 1995, 1996, 2000) given by the college for outstanding instruction in engineering. The reason for these awards and esteem is clear: Dennis has been an early adapter of the principles of active learning and engaging students in the classroom. He has a friendly, collegial manner, but also sets high expectations. His office door is always open for student questions and conversations, and they are not afraid to talk with him.

One student notes, “Dr. Miller’s office hours are worth it because you actually get something out of them. He really takes the time to help his students understand. After the office hours of some other professors, I’ve left just as confused as when I came in. Dr. Miller really puts things into ways that I can understand. He knows how to connect with students,

which makes us enjoy him as a teacher.” Another student has this perspective: “I really enjoyed taking ChE 210 (Transport) with Dr. Miller because he doesn’t alienate his students by making them feel stupid. He takes the time to explain concepts slowly and thoroughly to make sure that every student understands completely.”

Every year engineering undergraduate students work in Miller’s research laboratory. “This gives students a background in research, so they can make an intelligent choice of whether they would like to go on for graduate studies,” says Dennis. One of the students, a junior who worked in the pilot plant during the summer of 2008, writes, “When I worked with Dr. Miller, I gained so much practical work knowledge. It was a hands-on internship where I really got a better understanding of what chemical engineers do. Also, Dr. Miller took the time to explain the organic chemistry behind the experiments, so I actually understood what was going on in the reactors.”

His dedication to improving the student learning environment is also evident in Dennis’s long years of service on the college’s and department’s curriculum committees. He helped steer the college and his department through the transition from quarters to semester, and has been a strong advocate of many curricular innovations. He was the first faculty member in chemical engineering to develop a freshman seminar course that included hands-on activities, unique problem-solving scenarios, guest speakers, and a variety of contemporary issues. This course contributed to a dramatic increase in enrollments in chemical engineering at MSU at a time when enrollments nationwide were plummeting. He and his colleagues both at MSU and in India at UICT developed a course in “green” engineering that was several years ahead of its time. This course has become a mainstay of the chemical engineering program and has broad appeal across the College of Engineering for both graduate students and undergraduates.

Dennis shares his enthusiasm for chemical engineering and education through many outreach activities. He has been an instructor numerous times in the MSU Summer High School Institute, a program designed to educate high school students about the principles of engineering. He is active as a volunteer in middle school and high school classrooms and can often be seen heading to a high school chemistry class with his Dewar flask of liquid nitrogen and a boxful of hands-on demos tucked into his briefcase.

## **FAMILY AND FAITH—A STRONG STRUCTURE**

Dennis views the balancing of priorities in life as coming in seasons. “First there is education, then establishing oneself in the professional community. When you are raising children, your family must be a priority because most of us only get one chance to do that,” says Dennis. He and Daina have two daughters (Mara, 20, and Anna, 15).

Dennis’s and Daina’s involvement in their church community has helped establish the foundation of their priorities. Among

other activities, Daina and their two daughters participate on the church’s worship team, and Dennis has taught Sunday school and is a member of the church’s leadership team. He has also led or participated in two major mission trips with adults and youth—to Renosa, Mexico, and to Camp L’Arcada Banyoles, Spain—the latter of which included the whole family.

A major stress relief for the family has been their traditional summer escapes to a small Northern Michigan lake cottage. That is the place where work is truly left behind, and time is spent enjoying all kinds of water sports, visits from extended family, youth retreats, and (of course) fishing.

Another pastime Dennis still enjoys is volleyball, which he’s coached at the middle school, junior varsity, and varsity levels at his daughters’ school. “These kinds of activities help me feel connected not only with my own kids, but with other young people who, in a few short years, will be the ones sitting in our university classrooms. I love coaching volleyball, and it also helps me to be aware of how kids this age think. Although,” he quips, “I don’t think I will ever understand teenage girls completely.”

A dual-career family life has offered its share of challenges and true tests of communication and time-management skills. Daina and Dennis both consider themselves fortunate to work in an environment where administration and colleagues understand the importance of family and where faculty schedules, as grueling as they can be, allow some measure of flexibility. This has enabled the couple to share responsibilities of home and family, particularly when their daughters were young. In addition, both Dennis’s and Daina’s parents provided continual, active support and encouragement. “We couldn’t have gotten through those early years without them,” affirms Dennis.

## **OPENING DOORS FOR OTHERS—THE KEY**

Dedication and resoluteness have gotten Dennis to this point in his career. He prefers to emphasize relationships over the job. “The key to academic success for me is to build genuine long-term relationships with as many people as possible,” says Dennis. “It doesn’t matter if they are students, colleagues, program managers, or funding agents—valuing people, treating them respectfully, being responsible, and working really hard for them is a sure route to success.”

Ned Jackson, Dennis’s longtime collaborator, amplifies this point. “The greatest pleasure in working with Dennis is that the better I know him, the more I admire him,” says Ned. “He is a man of integrity, humility, and creativity; one who seeks to make a real difference by bettering the world and the life of those around him.” Ned believes this is evident in the calm passion Dennis brings to his research and his teaching, his deep caring for his students, his dedication to honest and thorough experimentation and reporting, and the zest he radiates for all these parts of his work. “His ego is not built on having to be more ‘right’ than others, but in sharing his unique talents to map out the way as we all stumble, imperfectly, toward deeper knowledge.” □

# *Chemical Engineering at . . .*

## *South Dakota School of Mines and Technology*

KENNETH M. BENJAMIN  
AND ROBB M. WINTER

The year was 1921, and the South Dakota Board of Regents (SDBOR) authorized a degree program in chemical engineering at the South Dakota School of Mines—a new field that had been birthed from applied chemistry a few decades earlier. A vision had emerged to bring this growing field to the Great Plains. Dr. **Andrew Karsten** (1922–1960), the first professor of chemical engineering at the South Dakota School of Mines (as the institution was named at this time), single-handedly brought the school's chemical engineering program into existence. Dr. Karsten would then shape and sustain the department for the next 20 years, along with chemistry colleagues Drs. **G.G. Osterhof** and **G.W. Bond**.

In 1935 several Master of Science (M.S.) programs were authorized by the SDBOR, including one in chemical engineering. During the early years, the Department of Chemical Engineering was the sole source of M.S. graduates on campus, establishing a culture of graduate education in the program. In 1943 South Dakota School of Mines was renamed the South Dakota School of Mines and Technology (SDSM&T) to signify this institution's expansion from its mining heritage to a broad array of engineering and science offerings. Dr. **Warren E. Wilson**, the fifth President of SDSM&T (serving in the role from 1948 to 1953), urged the chemical engineering program to become accredited, and this prompted the hiring of **R.L. Sandvig**, who would lead the department in the decades to come. A new Chemistry and Chemical Engineering building designed by chemistry and chemical engineering faculty Osterhof and **R. Heckman** (1953–1977), respectively, was dedicated in 1957. It included a state-of-the-art chemical engineering unit operations laboratory—a crowning achievement for Karsten. In classic pioneering fashion the laboratory was designed and fabricated by chemical engineering students with the help of



*Where it all began: The Chemistry and Chemical Engineering Building, photographed shortly after its completion in 1957.*

their mechanical engineering colleagues. The unit operations laboratory would become a popular Parents' Day visitation spot in the years to come. Accreditation was achieved and the department has enjoyed accreditation status ever since.

During the '70s, faculty to join the department (with their years of service in parenthesis) included **L.G. Bauer** (1973–2002), **W.A. Klemm** (1975–1990), and **J.M. Munro** (1977–2005). In addition, the biology program was integrated into the department structure, which planted the seeds for the development of the biochemical engineering emphasis within the chemical engineering program. Faculty members **Sookie Bang** (1985–present) and **Kent Fish** (1969–1995) were brought onto the team. With the retirement of Sandvig in the late '80s came the close of an era that saw Karsten, Sandvig, and Heckman provide continuity and bold, visionary leadership over nearly seven decades, 1922 to 1987.



*Leading the way: (Left to right) Russell F. Heckman, early faculty and one of the building's designers; Andrew Karsten, the first ChE professor at the school and a key player in the department's creation; and Robert L. Sandvig, integral to the accreditation of the department and its chair for many pivotal years.*

The '90s saw a renaissance of the chemical engineering curriculum at SDSM&T. Bauer, **D.J. Dixon** (1993–present), Munro, **J.A. Puszynski** (1991–present) and **R.M. Winter** (1988–present) pursued the development of the next generation of the curriculum determined to provide SDSM&T chemical engineering graduates with a modern, industrially relevant education, including an emphasis on design and controls. Soon after, our Industrial Advisory Board agreed that the time was ripe for the chemical engineering program to develop a biochemical engineering emphasis. In this regard, the chemical engineering and biology team found Cargill, Inc., to be particularly interested in developing a unique undergraduate curriculum that would produce graduates with a practical knowledge of bioprocesses at the Bachelor of Science level. Over the next several years faculty **P. Gilcrease** (2002–present), **T. Menkhaus** (2005–present), and **R. Sani** (2006–present) developed this biochemical engineering emphasis, which integrates topics relevant to bioprocessing across the ChE curriculum, and also immerses the students in hands-on, open-ended biochemical engineering laboratory experiences. With the arrival of Dr. **Ruch** (2003-2008), the 10th president of SDSM&T, came a restructuring of the university that resulted in the formal creation of the Department of Chemical and Biological Engineering. The growth and vigor seen over the last 15 years would be the springboard for the request and approval of the Ph.D. degree in chemical and biological engineering (CBE) and the hiring of faculty **K. Benjamin** (2007–present) and **R. Shende** (2008–present), with a third faculty member yet to be hired. Over the last 20 years research has become an indispensable vehicle for education and infrastructure development. The core areas of research broadly include biochemical engineering, energy, and nano- and macro-materials.

## THE FACULTY AND STAFF IN PROFILE

The faculty of the CBE department at SDSM&T is composed of chemical engineers, biochemical engineers, biologists, and microbiologists, by training. Among the nine faculty members, seven have had industrial experience, allowing our department to provide an applied dimension to our teaching and research, in addition to engineering and scientific fundamentals.

Professor and Chair David Dixon has a long history at SDSM&T. He is an alumnus of the department, having received both his B.S. and M.S. degrees in chemical engineering from the school. He obtained his Ph.D. in chemical engineering from the University of Texas at Austin. Dixon joined the faculty at SDSM&T in 1993 and has served as chair of the CBE department since 2006. His teaching interests include thermodynamics and numerical methods, and his research interests center on supercritical fluids, polymers, and environmental and biochemical engineering. Recently, he has also been appointed site director for the new National Science Foundation Industry/University Cooperative Research Center (NSF I/UCRC), the Center for BioEnergy Research and Development.

Professor Robb Winter arrived in the CBE department in 1988. He obtained his Ph.D. in chemical engineering from the University of Utah. Winter's research centers on understanding how molecular-level chemical phenomena, particularly at interfaces, influence bulk materials properties for composite and thin film systems. The research is largely experimental, and is aided by use of an interfacial force microscope—one of few available in the country. Winter was also instrumental in the creation of the Composites and Polymer Engineering Laboratory (CAPE) on campus. In addition to research,



*The faculty of the Department of Chemical and Biological Engineering, from left to right, front row: Rajesh Shende, Sookie Bang, Pat Gilcrease, Rajesh Sani, and Robb Winter; back row: Dave Dixon, Jan Puszynski, Ken Benjamin, and Todd Menkhaus.*

Winter has helped shape the educational environment in the department by creating the polymer/materials emphasis for students within the undergraduate ChE curriculum, and by helping bring National Science Foundation (NSF) Research Experience for Undergraduates (REU) and Research Experience for Teachers (RET) sites to the SDSM&T campus.

Professor **Jan Puszynski** joined the CBE department in 1991. He obtained his Ph.D. in chemical engineering from the Institute of Chemical Technology in Prague. Puszynski's research foci include heterogeneous (gas-solid) combustion, nanoenergetic powders, densification of nanocomposites, and ceramic synthesis. His research spans experimental investigations as well as mathematical modeling and simulation. Puszynski has played integral roles in both undergraduate and graduate education in the CBE department and on the SDSM&T campus. He led the incorporation of Aspen software across the undergraduate curriculum, and has helped in the formation of two Ph.D. programs on campus, in nanoscience and nanoengineering and in chemical and biological engineering.

Sookie Bang, professor of biology in the CBE department, has been at SDSM&T since 1985. She holds a Ph.D. in microbiology from the University of California, Davis. Bang's

research interests are focused on environmental/molecular microbiology and biotechnology, with current emphasis on deep underground geomicrobiology and the use of extremophiles for biomass degradation. Her teaching interests include general and molecular biology and industrial microbiology. Bang has been consistently devoted to introducing undergraduates to the research environment, as evidenced by the fact that she has had NSF/REU recipients nearly continuously from 1995-2008, many from disciplines outside biology.

Associate Professor Patrick Gilcrease has been a member of the SDSM&T CBE faculty since 2002. He obtained his Ph.D. in chemical engineering from Colorado State University. His research activities include biomethane production from coal, biomass pretreatment, fermentation, and biocatalysis of solid substrates. Gilcrease's teaching activities complement his research well, as he has been the lead force behind the development of biochemical engineering curriculum and laboratories within the CBE department. He also serves as advisor of the AIChE student chapter, which was just selected as an Outstanding AIChE Chapter for 2007-2008.

Assistant Professor Todd Menkhaus joined the CBE department in 2005. Prior to that, he completed his Ph.D. in

chemical engineering at Iowa State University. His major research area is bioseparations, and his teaching interests span separations and biochemical engineering as well as developing and delivering new bioseparations courses as part of the CBE curriculum. Menkhaus is active in integrating teaching and research, highlighted by his roles as acting director of the NSF RET program at SDSM&T and as advisor for the ChE Car Team.

Rajesh Sani is an assistant professor of biology within the CBE department. He joined the CBE department in 2006, and received his Ph.D. in environmental biotechnology from the Institute of Microbial Technology at Punjab University, Chandigarh, India. Sani's current research interests include thermophilic bioprocessing for bioenergy and biomediated transformations of metals and radionuclides. His teaching interests include microbiology, environmental engineering, and biochemical engineering.

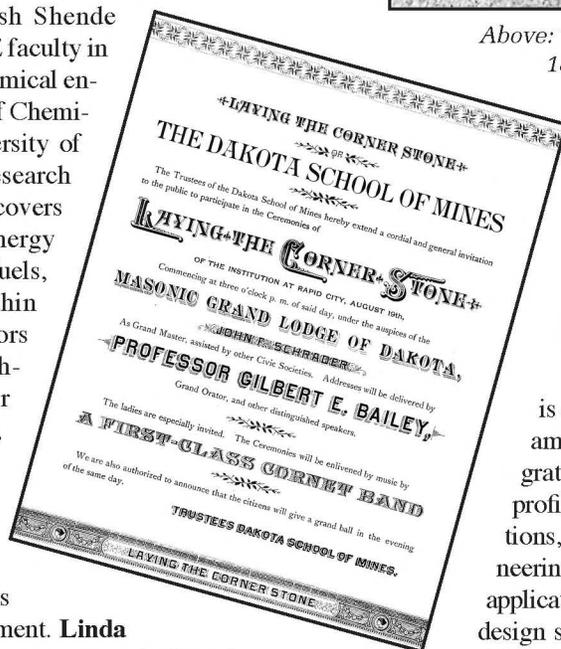
Assistant Professor Ken Benjamin joined the CBE faculty in 2007. Prior to arriving at SDSM&T, he completed a post-doctoral rotation at SUNY-Buffalo and received his Ph.D. in chemical engineering from the University of Michigan. Benjamin's teaching interests include thermodynamics and process modeling. His current research areas involve molecular and mechanistic modeling, with a focus on catalytic reactions for biorefinery and bioenergy applications, and reactions and materials processing in environmentally benign, tunable solvents.

Assistant Professor Rajesh Shende became a member of the CBE faculty in 2008. He holds a Ph.D. in chemical engineering from the Institute of Chemical Technology at the University of Mumbai, India. Shende's research portfolio is very broad, and covers areas such as sustainable energy (including solar), alternative fuels, nanostructured materials, thin films and MEMS, and sensors and therapeutics. His teaching interests include reactor design, transport phenomena, and nanomaterials.

There are two additional members of the CBE department whose contributions are integral to the success and dynamics of our environment. **Linda Embrock**, the CBE department secretary, is the primary contact within the department for all of our students and visitors, and her tireless work ensures that our department functions productively. Also, **Ivan Filipov** (M.S. chemical engineering; Bourgas Professor, Assen Zlatarov University) is the CBE department instrumentation and laboratory special-



Above: The first building on campus, completed in 1886. Center: An early document outlines the school's inception.



ist. Many students, both undergraduate and graduate, owe their enjoyable and productive laboratory experiences in large part to Filipov's continued efforts.

## UNDERGRADUATE EDUCATION: BY DESIGN AND BY CHOICE

Undergraduate ChE education at SDSM&T is driven by several principles and themes, chief among them being computer applications, integrated design, and choice. To develop a desired proficiency with computers and computer applications, freshmen students take Introduction to Engineering Modeling—a course focusing on computer applications relevant to chemical engineers, including design software for creating process flowsheets and piping and instrumentation diagrams, programming in Microsoft Excel and Visual Basic, as well as the proper use of specialized mathematical and engineering software such as MathCad, Polymath, and AspenPlus and AspenProperties. To emphasize the importance of process design and simulation to our undergraduate students, we have integrated the use of



*Begun with a state-of-the-art, pilot-plant-scale unit operations laboratory, the department has long emphasized providing students with an industrially relevant education.*



AspenPlus simulation software in nearly every ChE undergraduate course.<sup>[1-3]</sup> This feature has helped our graduates serve more effectively as practicing process engineers.

An additionally large component in our undergraduate education is the Integrated Design Project philosophy. In addition to the aforementioned integration of AspenPlus simulation software throughout the curriculum, the Integrated Design Project philosophy has one other main objective—the development of design projects that emphasize the strong linkage and interdependency of the individual ChE courses. This philosophy is a modified continuation of the original Integrated Design Project,<sup>[1]</sup> which guided students through

a three-year design project. We are currently revisiting this concept to consider how to most effectively implement such a “long-term” cohesive design project.

One last feature of our practical, design-based curriculum is the requirement that students take two process control courses. The first is taken during the junior year, and is a combination lecture/lab course that focuses more of the practical aspects of process control. The second course is taken during the senior year, and emphasizes the mathematics behind control theory. The solid foundation in controls provided by these courses complements the training our students receive in process design, and positions them well to function effectively in industry.

The emphasis on design is likewise carried through our laboratory courses. The Materials, Automation, Processing, and Simulation Laboratory (M.A.P.S), funded by the Dow Corning Foundation, exists to help teach design skills through the laboratory environment and experience. Conventional chemical engineering laboratory courses and projects involve conducting a “cookbook” experiment and performing subsequent engineering calculations to determine a parameter, or an optimal set of operating conditions. In the M.A.P.S. paradigm, however, students are asked to design a process to meet strict operating specifications using the methods learned in lecture classes, then build or assemble the equipment to meet their design, and finally to test their design by operating the process, taking relevant measurements, and conducting a critical review and comparison. Example M.A.P.S. laboratories include heat exchangers and heat exchanger networks, gas absorption,<sup>[4]</sup> piping networks, and tank-level control. Also, it should be mentioned that this open-ended approach to laboratory experiments is employed in all department laboratory classes. Other unique characteristics of the ChE laboratory courses includes the total number required for the B.S. degree (6—spread out from the freshman through the senior year), the availability of pilot-scale equipment for experiments (and the need to modify equipment for experiments), and the integration of automated process control into many laboratory experiments.<sup>[5]</sup>

The last component of our educational philosophy is that of choice. Students in our program can add specialization to their degree, by selecting curriculum options that emphasize materials/polymers, environmental engineering, or biochemical engineering. (It is worth noting that the ChE department is the founding member, and plays a continued, integral part, of the environmental engineering degree program on our campus.) Students in the materials/polymer concentration take advantage of SDSM&T’s Composite and Polymer Engineering Laboratory (CAPE), a 9,500-plus-square-foot facility that houses state-of-the-art equipment for cutting-edge research and development of polymer and composite processing, prototyping, and tooling. For those concentrating on biochemical engineering, the Cargill Biochemical Engineering Laboratory (established with generous support from Cargill, Inc.) provides students access to state-of-the-art bioprocessing equipment at the bench and pilot scale, such as fermentors, centrifuges, and chromatography for analysis and purification. In addition, all ChE majors are required to take a microbiology course, and topics particularly relevant to bioprocessing (such as stirred tank design and the use of plate and frame heat exchangers) have been integrated into a number of core ChE courses.

## STUDENT AWARDS AND RECOGNITIONS

Students in the SDSM&T chemical engineering program have participated in many opportunities to enrich their formal engineering education. They maintain an active student

**The steady and planned growth of the CBE research enterprise culminated in the formation of the Ph.D. program in chemical and biological engineering in 2007. The program currently supports 10 Ph.D. students, with the ultimate goal of growing to 20–25 students by 2010.**

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chapter of the American Institute of Chemical Engineers (AIChE) and a ChE Car Competition team—a multi-disciplinary team including environmental, metallurgical, mechanical, and electrical engineering, and computer science, students. At regional and national AIChE meetings, SDSM&T ChE students participate and compete with peer ChE students from other universities in such activities as research paper presentations, process designs, and the ChE Car Competition. As noted previously, the AIChE Student Chapter was designated one of 15 AIChE Outstanding Student Chapters for the 2007–2008 school year. ChE students have been recognized for outstanding academics by receiving national scholarships and fellowships from AIChE and Tau Beta Pi, the engineering honor society. During Summer 2007, **Travis Walker**, a ChE junior, was selected as the AIChE representative for the Washington Internships for Students of Engineering (WISE). In 2008, AIChE Student Chapter President **Ben Bangasser** was awarded the Dr. Harry West Student Paper Award from the AIChE Fuels and Petrochemicals Division. The ChE Car Team has competed in the regional AIChE Student Chapter Competitions every spring over the 10-year history of the competition. Additionally, they have qualified and participated as one of the top 31 teams in the national ChE Car Competition numerous times.

## GRADUATE EDUCATION: A PROUD HISTORY AND NEW ENDEAVORS

Graduate education in chemical engineering has been part of the department since 1935, when the Master’s program was added. In 1986, the Ph.D. program in materials engineering and science was formed on campus, which provided a natural mechanism for facilitating Ph.D. research for CBE faculty involved in polymer/materials research. Then, in 2005, the Ph.D. program in nanoscience and nanoengineering was started on campus, which augmented the existing department research in nanocomposites, nano-structured materials, and combustion synthesis of ceramic and intermetallic powders. During

**Current research activity in the CBE department at SDSM&T covers a range of areas, including bioenergy, biofuels, polymers/nanocomposites, combustion synthesis of ceramic and intermetallic powders, biochemical engineering and bioseparations, bioremediation and extremophiles, nano-structured materials, catalysis and reaction engineering, and molecular modeling.**

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the past 10 years, the diversity of research in the department has grown considerably. The steady and planned growth of the CBE research enterprise culminated in the formation of the Ph.D. program in chemical and biological engineering in 2007. The program currently supports 10 Ph.D. students, with the ultimate goal of growing to 20-25 students by 2010. The SDSM&T CBE program is different in nature from what one finds most often in chemical and biological/biomolecular engineering (*i.e.*, CBE) departments across the country. Generally, CBE departments require Ph.D. students to take the core chemical engineering graduate courses for their degree, and provide elective courses in biology, microbiology, biotechnology, etc., to supplement the training of those students focusing on biological-related dissertations. In our CBE Ph.D. program, students are required to take both chemical engineering and biology/biological engineering graduate courses to fulfill their degree requirement. At a minimum, SDSM&T CBE Ph.D. students will take two courses from the following biological engineering topics: biochemical engineering, industrial microbiology and biotechnology, metabolic engineering, biocatalysis, bioseparations, and molecular biology. This structure ensures that the SDSM&T CBE Ph.D. graduate has the foundation and skill set to be proficient as both a chemical and biological engineer.

## **OUTREACH**

Over the years, outreach to both our local and global communities has been a continuous theme. The goal of drawing more women into chemical engineering was a major thrust begun in the '70s by Sandvig. This initiative, which received a majority of its funding from the Dow Corning Corporation

and Dow Chemical, USA, was a great success, resulting in a steady and persistent increase of female students pursuing a degree in chemical engineering at SDSM&T — from 2 percent to 35 percent. The '80s and '90s saw several interrelated activities to provide Native American middle and high school students and their teachers with insight to the opportunities that a chemical engineering degree can afford. Dow Chemical, USA, provided the majority of the funds for one initiative—the Dow Chemical Native American Studies Workshop for High School Teachers. The National Science Foundation All Nations – Alliance for Minority Participation program supported three initiatives, the Native American Summer Engineering Bridge program, the SDSM&T – Oglala Lakota College AISES Leadership initiative, and the Native American Summer Research Program. These programs were envisioned and developed to inform Native American students and teachers of opportunities in engineering and science in general. The result of these efforts has been a growing number of Native American students pursuing engineering and science degrees at SDSM&T. In the '90s and '00s as the research efforts within the department grew, National Science Foundation support was sought and acquired to develop a Research Experience for Undergraduates (REU) site within the Department of Chemical and Biological Engineering. This site was successfully expanded to a sister international site at the Mongolian University of Science and Technology in Ulaanbaatar, Mongolia, where REU research assistants investigated topics in materials and environmental. To provide the regional K–12 community with opportunities to enhance their chemical engineering and science skills and knowledge, an NSF-funded Research Experience for Teachers (RET) site was established. It too was expanded internationally, to Pontificia Universidad Católica De Valparaíso in Valparaíso, Chile. Both efforts have been timely, with the recent realization of the importance of globalization and the development within the United States of a globally competent society.

## **DEPARTMENT RESEARCH**

The research environment of the SDSM&T CBE department is vibrant and growing, and holds more promise with the recently formed Ph.D. program in chemical and biological engineering. Simultaneous with the new Ph.D. program was the creation of the Center for Bioprocessing Research and Development, a 2010 Research Center of the State of South Dakota. The focus of CBRD is on research that leads to new technologies for processing plant-derived lignocellulose materials into biomaterials such as ethanol and key building-block chemicals. In 2008, the department was awarded status as the lead site for a National Science Foundation Industrial/University Cooperative Research Center (NSF I/UCRC), formally titled the Center for BioEnergy Research and Development (<CBERD; <http://bioenergynow.org>>). Further, the biological-research component of our department has received an additional significant boost from another recently awarded



*Envisioning future growth: The new addition to the Chemical and Biological Engineering/Chemistry building is scheduled to be completed in 2011.*

NSF center—the Deep Underground Science and Engineering Laboratory (DUSEL)—to be located in Lead, South Dakota, approximately 50 miles from the SDSM&T campus. In the area of polymers and materials, department researchers take advantage of the school's Composite and Polymer Engineering Laboratory (CAPE), a 9,500-plus square-foot facility for advanced research and development of polymer and composite processing, prototyping, and tooling. Current research activity in the CBE department at SDSM&T covers a range of areas, including bioenergy, biofuels, polymers/nanocomposites, combustion synthesis of ceramic and intermetallic powders, biochemical engineering and bioseparations, bioremediation and extremophiles, nano-structured materials, catalysis and reaction engineering, and molecular modeling. Current funding in the department exceeds \$1MM per year, with an average level of support of more than \$200K/faculty.

## THE FUTURE OF CHEMICAL ENGINEERING AT SDSM&T

The Department of Chemical and Biological Engineering at SDSM&T, coming from humble beginnings, has survived and thrived with the pioneer spirit so alive in the Great Plains. The Department of Chemical and Biological Engineering has entered the 21st Century with tremendous momentum and

promise, with a vibrant curriculum, an emerging research program, and now on the horizon a new building to be completed in 2011. We are fortunate that the vision and tenacity of Drs. Karsten, Sandvig, Bond, and Osterhof has propelled us to where we are today, and we look forward to making continued contributions to chemical engineering research and education locally, nationally, and globally.

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# NEWTON'S LAWS, EULER'S LAWS, AND THE SPEED OF LIGHT

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Truesdell<sup>[1]</sup> tells us that Newton listed his three laws of motion as:

Newton (1642-1727)

- I. *Every body continues in its state of rest, or of uniform motion straight ahead, unless it be compelled to change that state by forces impressed upon it.*
- II. *The change of motion is proportional to the motive force impressed, and it takes place along the right line in which the force is impressed.*
- III. *To an action there is always a contrary and equal reaction; or, the mutual actions of two bodies upon each other are always directed to contrary parts.*

Truesdell<sup>[2]</sup> also tells us that Newton never presented these ideas in the form of equations, and because of this there are differences to be found in the literature. In this work we choose “motion” to mean mass times velocity,  $m\underline{v}$ , and we choose “motive force” to be represented by  $\underline{f}$ . This leads to

$$\text{Newton I: } \quad m\underline{v} = \text{constant}, \quad \underline{f} = 0 \quad (1)$$

while the second law takes the form

$$\text{Newton II: } \quad \frac{d}{dt}(m\underline{v}) = \underline{f} \quad (2)$$

Here the “change of motion” has been interpreted as the time rate of change of the momentum,  $m\underline{v}$ . Often a precise definition of  $\underline{v}$  is not given in the discussion of Newton’s

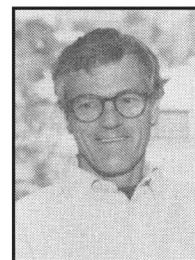
first and second laws, and we will return to this matter in subsequent paragraphs. Clearly Newton’s first law is a special case of Newton’s second law, and one can wonder why it was stated as an independent law. Physicists<sup>[3-5]</sup> have pointed out that Eq. (1) was deduced earlier by Galileo (1564-1642), thus Newton was motivated to elevate this result to the position of a “law.”

Newton’s third law for two interacting bodies can be expressed as

$$\text{Newton III: } \quad \underline{f}_{12} = -\underline{f}_{21} \quad (3)$$

in which  $\underline{f}_{12}$  is the force that body #2 exerts on body #1, and  $\underline{f}_{21}$  is the force that body #1 exerts on body #2. The most dramatic success of these laws was their use, along with the *law of gravitational attraction*, to justify Kepler’s three

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empirical laws of planetary motion. In a careful statement of Newton's laws, one often notes that they are valid in an *inertial frame*. This naturally leads to the question: What is an inertial frame? The answer is that an inertial frame is a frame in which Newton's laws are valid! We can only escape from this circular argument by noting that an inertial frame must be determined by experiment.<sup>[6]</sup> In Newton's case, the verification of Kepler's laws indicated that the sun and the "fixed stars" represented a good approximation of an inertial frame for the study of planetary motion.

If we think about applying Eq. (2) to the motion of a body, we must wonder what is meant by the velocity,  $\underline{v}$ , since all parts of a body need not have the same velocity. Physicists often deal with this problem by arguing that Eq. (2) applies to "mass points" that are small enough so that their motion can be described by a single velocity. The statement that something is "small" always leads to the question: Small relative to what? Feynman, *et al.*,<sup>[7]</sup> touch on this problem by considering the cloud of  $N$  mass points illustrated in Figure 1. One can apply Newton's second law to the  $i^{\text{th}}$  mass point in the cloud to obtain

$$\frac{d}{dt}(m_i \underline{v}_i) = \underline{b}_i + \sum_{j=1}^{i=N} \underline{f}_{ij} \quad (4)$$

Here we have used  $\underline{b}_i$  to represent the body force exerted on the  $i^{\text{th}}$  mass point by the large, spherical body located outside the cloud in Figure 1. The force exerted by the  $j^{\text{th}}$  mass point in the cloud on the  $i^{\text{th}}$  mass point in the cloud is represented by  $\underline{f}_{ij}$ , and this force obeys Newton's third law as indicated by

$$\underline{f}_{ij} = -\underline{f}_{ji} \quad (5)$$

To obtain Newton's second law for the cloud of mass points, we sum Eq. (4) over all the mass points in the cloud<sup>[8]</sup>

$$\frac{d}{dt} \sum_{i=1}^{i=N} m_i \underline{v}_i = \sum_{i=1}^{i=N} \underline{b}_i + \sum_{i=1}^{i=N} \sum_{j=1}^{j=N} \underline{f}_{ij} \quad (6)$$

and make use of Eq. (5) to simplify this result to the form

$$\frac{d}{dt} \sum_{i=1}^{i=N} m_i \underline{v}_i = \sum_{i=1}^{i=N} \underline{b}_i \quad (7)$$

The mass of the cloud is given by

$$m = \sum_{i=1}^{i=N} m_i \quad (8)$$

while the center of mass,  $\underline{r}_{\text{CM}}$ , and the velocity of the center of mass,  $\underline{v}_{\text{CM}}$ , are defined by

$$\underline{r}_{\text{CM}} = \frac{1}{m} \sum_{i=1}^{i=N} m_i \underline{r}_i, \quad \underline{v}_{\text{CM}} = \frac{1}{m} \sum_{i=1}^{i=N} m_i \underline{v}_i, \quad (9)$$

The second of these definitions allows us to express Eq. (7) in the form

$$\frac{d}{dt}(m \underline{v}_{\text{CM}}) = \sum_{i=1}^{i=N} \underline{b}_i \quad (10)$$

We now identify the total external force acting on the cloud of mass points as

$$\underline{f} = \sum_{i=1}^{i=N} \underline{b}_i \quad (11)$$

so that Newton's second law for a cloud of mass points is given by

$$\text{Newton II:} \quad \frac{d}{dt}(m \underline{v}_{\text{CM}}) = \underline{f} \quad (12)$$

Feynman, *et al.*,<sup>[9]</sup> describe this situation by saying "Newton's law has the peculiar property that if it is right on a certain scale [*the mass point scale*], then it will be right on a larger scale [*the cloud scale*]." While this is a satisfying result, it does not explain "how small" a particle must be so that Eq. (2) can be applied with confidence. For rigid bodies the velocity  $\underline{v}$  at any point  $\underline{r}$  is given by<sup>[10]</sup>

$$\underline{v}(\underline{r}) = \underline{v}_{\text{CM}} + \underline{\omega} \times (\underline{r} - \underline{r}_{\text{CM}}) \quad (13)$$

in which  $\underline{\omega}$  represents the angular velocity. Here we see that a *single velocity* can be used to describe the motion of a rigid body whenever  $\underline{\omega} \times (\underline{r} - \underline{r}_{\text{CM}})$  is small compared to  $\underline{v}_{\text{CM}}$ , thus the constraint associated with the "mass point" assumption is given by

$$\underline{\omega} \times (\underline{r} - \underline{r}_{\text{CM}}) \ll \underline{v}_{\text{CM}} \quad (14)$$

For deformable bodies, one must replace Eq. (13) with the more general representation

$$\underline{v}(\underline{r}) = \underline{v}_{\text{CM}} + \int_{\eta=\underline{r}_{\text{CM}}}^{\eta=\underline{r}} (\nabla \underline{v})^T d\eta \quad (15)$$

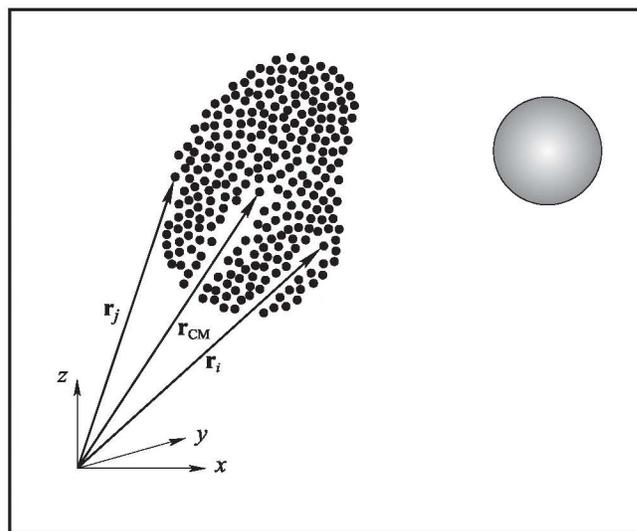


Figure 1. Cloud of mass points interacting with a body.

and then examine the velocity gradient tensor in terms of its symmetric and skew-symmetric parts.<sup>[11]</sup> In this case, the restriction<sup>[12]</sup> is obviously given by

$$\int_{\eta=\underline{\mathbf{r}}_{\text{CM}}}^{\eta=\underline{\mathbf{r}}} (\nabla \underline{\mathbf{v}})^T d\eta \ll \underline{\mathbf{v}}_{\text{CM}} \quad (16)$$

however, the associated constraint would require a more detailed analysis of the fluid deformation. If one accepts Eq. (12) as Newton's second law instead of Eq. (2), no constraint need be imposed.

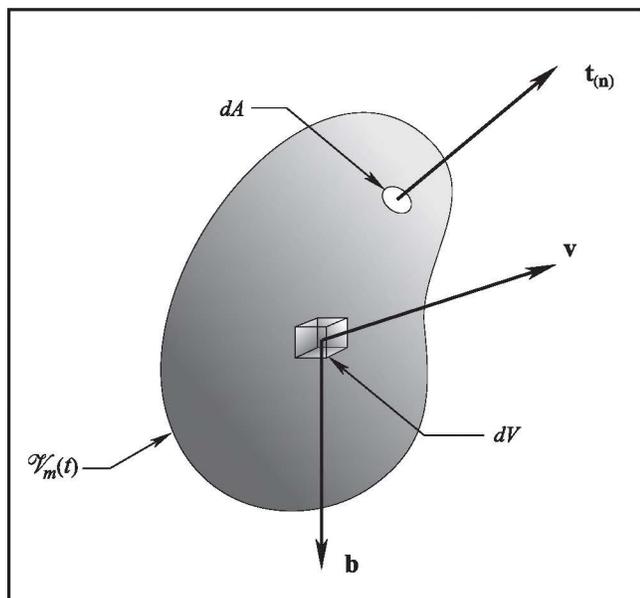


Figure 2. Moving, deformed body.

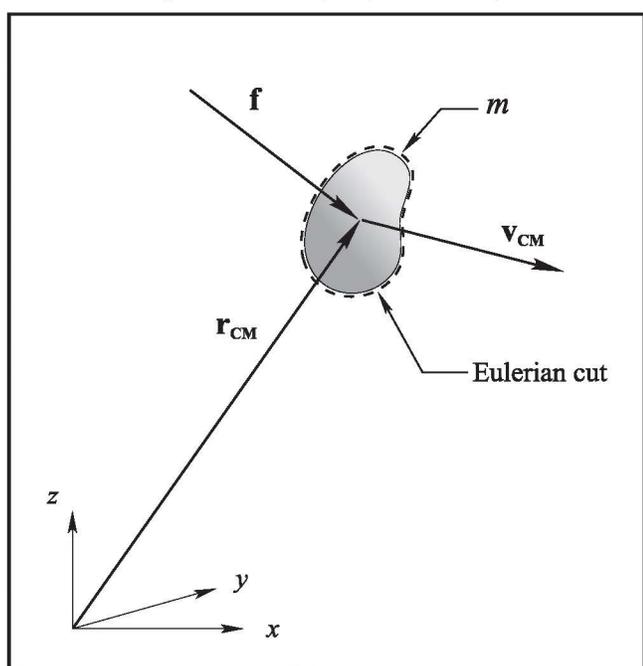


Figure 3. Motion of a body.

## EULER'S LAWS

While Newton's laws seem to be suitable for the study of mass points and clouds of mass points, they cannot be applied directly to the motion of a moving, deforming, continuous medium.<sup>[13]</sup> Regardless of what words are used to describe the laws of mechanics used by chemical engineers, those laws are indeed the laws proposed by Euler that can be stated as

Euler (1707-1783)

- I. The time rate of change of the momentum of a body equals the force acting on the body.
- II. The time rate of change of the angular momentum of a body equals the torque acting on the body, where both the torque and the moment are taken with respect to the same fixed point.

In addition to these two laws, we accept the *Euler cut principle*<sup>[14]</sup> that can be stated as:

*Not only do the laws of continuum physics apply to distinct bodies but they also apply to any arbitrary body that one might imagine as being cut out of a distinct body.*

To understand how Euler's laws are related to Newton's laws, we need to express Euler's laws in precise mathematical form. This will allow us to demonstrate that they contain Newton's laws provided that we restrict ourselves to *non-relativistic phenomena*.

For the body occupying the *material volume*,  $\mathcal{V}_m(t)$ , illustrated in Figure 2, Euler's laws are given by<sup>[15]</sup>

$$\text{Euler I: } \frac{d}{dt} \int_{\mathcal{V}_m(t)} \rho \underline{\mathbf{v}} dV = \int_{\mathcal{V}_m(t)} \rho \underline{\mathbf{b}} dV + \int_{\mathcal{A}_m(t)} \underline{\mathbf{t}}_{(n)} dA \quad (17)$$

$$\text{Euler II: } \frac{d}{dt} \int_{\mathcal{V}_m(t)} \underline{\mathbf{r}} \times \rho \underline{\mathbf{v}} dV = \int_{\mathcal{V}_m(t)} \underline{\mathbf{r}} \times \rho \underline{\mathbf{b}} dV + \int_{\mathcal{A}_m(t)} \underline{\mathbf{r}} \times \underline{\mathbf{t}}_{(n)} dA \quad (18)$$

To be clear about Euler's two laws, we need to say that the velocity,  $\underline{\mathbf{v}}$ , is determined relative to an *inertial frame* and that the position vector  $\underline{\mathbf{r}}$  is determined relative to some fixed point in an inertial frame. As mentioned earlier in connection with Newton's laws, one identifies an inertial frame by experiment. It is important to remember that these two axiomatic statements for *linear momentum* and *angular momentum* apply to any *arbitrary body* that one imagines as being cut out of a distinct body.

## EULER'S LAWS AND NEWTON'S LAWS

Given Euler's two laws of mechanics and the Euler cut principle, we need to know how they are related to Newton's three laws. To explore this problem, we consider a body of mass  $m$  illustrated in Figure 3, and we locate the center of mass of that body in terms of the position vector defined by

$$\underline{\mathbf{r}}_{\text{CM}} = \frac{1}{m} \int_{\mathcal{V}_m(t)} \rho \underline{\mathbf{r}} dV \quad (19)$$

For a sphere of uniform density, the center of mass would be located at the geometrical center of the sphere; however, the definition of  $\underline{r}_{CM}$  is completely general and Eq. (19) is applicable to any arbitrary body that is cut out of a distinct body. The velocity of the center of mass is defined in a similar manner

$$\underline{v}_{CM} = \frac{1}{m} \int_{\mathcal{V}_m(t)} \rho \underline{v} dV \quad (20)$$

and one can use a special form of the Reynolds transport theorem<sup>[16]</sup> to prove that

$$\underline{v}_{CM} = \frac{d\underline{r}_{CM}}{dt} \quad (21)$$

The definition given by Eq. (20) can be used to express the first term in Eq. (17) as

$$\frac{d}{dt} \int_{\mathcal{V}_m(t)} \rho \underline{v} dV = \frac{d}{dt} (m \underline{v}_{CM}) \quad (22)$$

As a matter of convenience, we designate the total force acting on the body by

$$\underline{f} = \int_{\mathcal{V}_m(t)} \rho \underline{b} dV + \int_{\mathcal{A}_m(t)} \underline{t}_{(H)} dA \quad (23)$$

so that Eq. (17) can be represented in the simplified form given by

$$\text{Euler Result I: } \frac{d}{dt} (m \underline{v}_{CM}) = \underline{f} \quad (24)$$

This is identical in form to Newton's second law for the cloud of mass points illustrated in Figure 1, and if the body is "small

enough" so that  $\underline{v}_{CM}$  can be replaced by  $\underline{v}$  we see that Eq. (24) is identical in form to Eq. (2) for a mass point. The similarity in form (*not content*) of Euler's first law and Newton's second law has encouraged many to think that Newton's laws and Euler's first law are essentially equivalent. This is a line of thought that should be discouraged.

## BODY FORCES

To clarify the different perspectives of physicists and chemical engineers, we apply Euler's first and second laws to the special case of three interacting bodies in a vacuum. This situation is illustrated in Figure 4 where we have shown two distinct small bodies, three Eulerian cuts (material volumes), and a distinct large body. For Cut I and Cut II, Euler's first law yields

$$\text{Cut I: } \frac{d}{dt} \int_{\mathcal{V}_I(t)} \rho_1 \underline{v}_1 dV = \int_{\mathcal{V}_I(t)} \rho_1 \underline{b}_{12} dV + \int_{\mathcal{V}_I(t)} \rho_1 \underline{b}_{13} dV \quad (25)$$

$$\text{Cut II: } \frac{d}{dt} \int_{\mathcal{V}_{II}(t)} \rho_2 \underline{v}_2 dV = \int_{\mathcal{V}_{II}(t)} \rho_2 \underline{b}_{21} dV + \int_{\mathcal{V}_{II}(t)} \rho_2 \underline{b}_{23} dV \quad (26)$$

The application of Cut III treats the two small bodies as a single body for which the time rate of change of momentum is balanced by the applied external force. This leads to

$$\begin{aligned} \text{Cut III: } & \frac{d}{dt} \left[ \int_{\mathcal{V}_I(t)} \rho_1 \underline{v}_1 dV + \int_{\mathcal{V}_{II}(t)} \rho_2 \underline{v}_2 dV \right] \\ & = \int_{\mathcal{V}_I(t)} \rho_1 \underline{b}_{13} dV + \int_{\mathcal{V}_{II}(t)} \rho_2 \underline{b}_{23} dV \end{aligned} \quad (27)$$

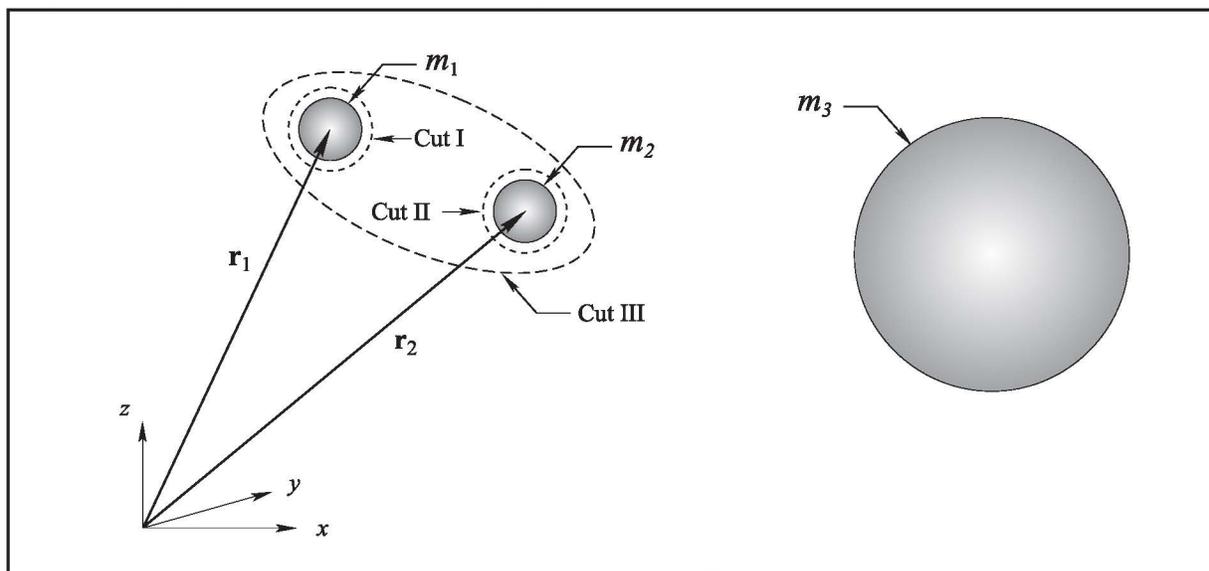


Figure 4. Three-body process.

***The similarity in form  
(not content) of Euler's first law  
and Newton's second law  
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Euler's first law are essentially  
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Substitution of Eqs. (25) and (26) into Eq. (27) leads to

$$\int_{V_1(t)} \rho_1 \underline{b}_{12} dV + \int_{V_2(t)} \rho_2 \underline{b}_{21} dV = 0 \quad (28)$$

and it will be convenient to identify these two body forces as

$$\underline{f}_{12} = \int_{V_1(t)} \rho_1 \underline{b}_{12} dV, \quad \underline{f}_{21} = \int_{V_2(t)} \rho_2 \underline{b}_{21} dV \quad (29)$$

At this point we repeat Eq. (24) as

$$\text{Euler Result I: } \frac{d}{dt}(\underline{m} \underline{v}_{CM}) = \underline{f} \quad (30)$$

And note that Eqs. (28) and (29) lead to

$$\text{Euler Result II: } \underline{f}_{12} = -\underline{f}_{21} \quad (31)$$

Eq. (30) yields Newton's second law for the cloud of mass points illustrated in Figure 3, and if Eq. (30) is applied to a single mass point it yields Newton's second law as given by Eq. (2). Eq. (31), which was derived by applying Euler's first law to the process illustrated in Figure 4, is identical to Newton's third law. Here we see that Euler's first law can be used to obtain *all three of Newton's laws*; however, the inverse is not true, *i.e.*, one cannot use Newton's laws for mass points or for a cloud of mass points to obtain Euler's first law. Euler's laws are based on the Euler cut principle and the assumption that the material under consideration can be treated as a continuum, and these constructs are not to be found in Newton's treatment of mechanics.<sup>[17]</sup>

Given that Euler's first law contains *all that is available in Newton's three laws*, one must wonder why physicists do not move forward one century and accept Euler's first law as their axiom for mechanics. The answer would appear to be associated with Euler's second law that we examine in the following paragraphs.

## CENTRAL FORCES

In the absence of any surface forces, we can express Euler's second law as

$$\frac{d}{dt} \int_{V_m(t)} \underline{r} \times \rho \underline{v} dV = \int_{V_m(t)} \underline{r} \times \rho \underline{b} dV \quad (32)$$

and for the three Eulerian cuts, or *control volumes*, illustrated in Figure 4 we have

$$\text{Cut I: } \frac{d}{dt} \int_{V_1(t)} \underline{r}_1 \times \rho_1 \underline{v}_1 dV = \int_{V_1(t)} \underline{r}_1 \times \rho_1 \underline{b}_{12} dV + \int_{V_1(t)} \underline{r}_1 \times \rho_1 \underline{b}_{13} dV \quad (33)$$

$$\text{Cut II: } \frac{d}{dt} \int_{V_2(t)} \underline{r}_2 \times \rho_2 \underline{v}_2 dV = \int_{V_2(t)} \underline{r}_2 \times \rho_2 \underline{b}_{21} dV + \int_{V_2(t)} \underline{r}_2 \times \rho_2 \underline{b}_{23} dV \quad (34)$$

$$\begin{aligned} \text{Cut III: } \quad & \frac{d}{dt} \int_{V_1(t)} \underline{r}_1 \times \rho_1 \underline{v}_1 dV + \frac{d}{dt} \int_{V_2(t)} \underline{r}_2 \times \rho_2 \underline{v}_2 dV \\ & = \int_{V_1(t)} \underline{r}_1 \times \rho_1 \underline{b}_{13} dV + \int_{V_2(t)} \underline{r}_2 \times \rho_2 \underline{b}_{23} dV \end{aligned} \quad (35)$$

Use of Eqs. (33) and (34) in Eq. (35) leads to a constraint on the body forces given by

$$\int_{V_1(t)} \underline{r}_1 \times \rho_1 \underline{b}_{12} dV + \int_{V_2(t)} \underline{r}_2 \times \rho_2 \underline{b}_{21} dV = 0 \quad (36)$$

The position vectors can be expressed in terms of the position vectors locating the centers of mass according to

$$\underline{r}_1 = (\underline{r}_{CM})_1 + \tilde{\underline{r}}_1, \quad \underline{r}_2 = (\underline{r}_{CM})_2 + \tilde{\underline{r}}_2 \quad (37)$$

and this leads to

$$\begin{aligned} & (\underline{r}_{CM})_1 \times \int_{V_1(t)} \rho_1 \underline{b}_{12} dV + \int_{V_1(t)} \tilde{\underline{r}}_1 \times \rho_1 \underline{b}_{12} dV \\ & + (\underline{r}_{CM})_2 \times \int_{V_2(t)} \rho_2 \underline{b}_{21} dV + \int_{V_2(t)} \tilde{\underline{r}}_2 \times \rho_2 \underline{b}_{21} dV = 0 \end{aligned} \quad (38)$$

Next we make use of Eqs. (28) and (29) to express this result in the form

$$\left[ (\underline{r}_{CM})_1 - (\underline{r}_{CM})_2 \right] \times \underline{f}_{12} + \left[ \int_{V_1(t)} \tilde{\underline{r}}_1 \times \rho_1 \underline{b}_{12} dV + \int_{V_2(t)} \tilde{\underline{r}}_2 \times \rho_2 \underline{b}_{21} dV \right] = 0 \quad (39)$$

In the appendix we demonstrate that the last term in this result can be neglected when the following constraint is satisfied:

$$\frac{O(\hat{\mathbf{r}}_1) + O(\hat{\mathbf{r}}_2)}{O[(\mathbf{r}_{\text{CM}})_1 - (\mathbf{r}_{\text{CM}})_2]} \ll 1 \quad (40)$$

Under these circumstances, Euler's second law leads to

$$[(\mathbf{r}_{\text{CM}})_1 - (\mathbf{r}_{\text{CM}})_2] \times \mathbf{f}_{12} = 0 \quad (41)$$

and there are three ways in which this result can be satisfied. We list the three possibilities as

$$1. \quad (\mathbf{r}_{\text{CM}})_1 - (\mathbf{r}_{\text{CM}})_2 = 0 \quad (42)$$

$$2. \quad \mathbf{f}_{12} = 0 \quad (43)$$

$$3. \quad (\mathbf{r}_{\text{CM}})_1 - (\mathbf{r}_{\text{CM}})_2 \text{ and } \mathbf{f}_{12} \text{ are parallel} \quad (44)$$

Since the first two possibilities can not be generally true, we conclude that the interaction force between two bodies must be *parallel* to the vector  $(\mathbf{r}_{\text{CM}})_1 - (\mathbf{r}_{\text{CM}})_2$ . We express this result as

$$\text{Euler Result III: } \mathbf{f}_{12} = \Omega_{12} [(\mathbf{r}_{\text{CM}})_1 - (\mathbf{r}_{\text{CM}})_2] \quad (45)$$

in which  $\Omega_{12}$  is some *scalar parameter* of the interaction force law. Eq. (45) indicates that the interaction force between two bodies subject to the constraint given by Eq. (40) must act along the line of centers, *i.e.*, it is a *central force*.

In this analysis we have shown that Euler's *first law* contains Newton's *three laws*, while Euler's *second law* provides what is known as the *central force law* for the case of mass-point mechanics. Given the power and economy of Euler's laws, one can wonder why Newton's *three laws* are not discarded in favor of Euler's *two laws*. The answer lies in the fact that the *central force law*, given by Eq. (45), represents a *non-relativistic phenomenon*. Since forces are propagated at the speed of light, the force that one body exerts on another *cannot lie along the line of centers* when the relative velocity between the two bodies approaches the speed of light. Because of this, physicists prefer to view mechanical phenomena in terms of Newton's laws and make use of the central force law as a *special case* that can be discarded when relativistic phenomena are encountered. Engineers, on the other hand, are rarely involved in relativistic phenomena and what is a *special case* for the physicist is the *general case* for the engineer. Because of this, engineers uniformly formulate their mechanical problems in terms of Euler's two laws and the Euler cut principle.

## CONCLUSIONS

Physicists, who begin teaching chemical engineering students about the laws of mechanics, are committed to a Newtonian perspective because it is consistent with relativistic mechanics and mass points. This perspective will not change.

***Physicists prefer to view mechanical phenomena in terms of Newton's laws and make use of the central force law as a special case that can be discarded when relativistic phenomena are encountered. Engineers, on the other hand, are rarely involved in relativistic phenomena and what is a special case for the physicist is the general case for the engineer.***

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Chemical engineering faculty teach chemical engineering students about Euler's laws of mechanics, regardless of what words they use to describe these laws. Chemical engineering faculty need to take responsibility for the development of a smooth transition between the perspective of physicists and the perspective of engineers. In the absence of such a smooth transition, our students will be confronted with a discontinuity<sup>[18]</sup> and will never be completely confident in the laws of mechanics that they have been given.

## ACKNOWLEDGMENT

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## NOMENCLATURE

$\mathcal{A}_m(t)$	surface area of a material volume, m <sup>2</sup>
$\mathbf{b}$	total body force per unit mass, N/kg
$\mathbf{b}_i$ , $i=1,2,\dots,N$	body force exerted by a large, external body on the $i^{\text{th}}$ mass point, N
$\mathbf{b}_{12}$	body force per unit mass exerted by body #2 on body #1, N/kg
$\mathbf{b}_{21}$	body force per unit mass exerted by body #1 on body #2, N/kg
$\mathbf{f}$	force, N
$\mathbf{f}_{12}$	force exerted by body #2 on body #1, N/kg
$\mathbf{f}_{21}$	force exerted by body #1 on body #2, N/kg
$\mathbf{f}_{ij}$	force exerted by the $j^{\text{th}}$ mass point on the $i^{\text{th}}$ mass point in a cloud of mass points, N
$m$	mass of a body or mass of a cloud of mass points, kg
$m_i$	mass of the $i^{\text{th}}$ mass point, kg
$\mathbf{n}$	unit normal vector
$\mathbf{r}$	position vector, m
$\mathbf{r}_{\text{CM}}$	position vector locating the center of mass, m
$t$	time, s
$\mathbf{t}_{(a)}$	stress vector, N/m <sup>2</sup>

- $\underline{v}_i$  velocity of the  $i^{\text{th}}$  mass point, m/s
- $\underline{v}$  velocity, m/s
- $\underline{v}_{\text{CM}}$  velocity of the center of mass, m/s
- $\frac{\partial}{\partial t}(\underline{v})$  volume of a body (material control volume),  $\text{m}^3$

### Greek Letters

- $\rho$  total mass density,  $\text{kg}/\text{m}^3$
- $\rho_i$  total mass density of the  $i^{\text{th}}$  body,  $\text{kg}/\text{m}^3$
- $\underline{\omega}$  angular velocity,  $\text{rad}/\text{s}$

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### APPENDIX: CENTRAL FORCE LAW

Deciding when some quantity is "small enough" so that it can be discarded is not always an easy task. Here we consider the simplification that led from Eq. (39) to (40) and the central force law represented by Eq. (45). We begin with Eq. (A1)

$$\left[ (\underline{\mathbf{r}}_{\text{CM}})_1 - (\underline{\mathbf{r}}_{\text{CM}})_2 \right] \times \underline{\mathbf{f}}_{12} + \left[ \int_{\mathcal{V}_1(t)} \underline{\mathbf{r}}_1 \times \rho_1 \underline{\mathbf{b}}_{12} dV + \int_{\mathcal{V}_2(t)} \underline{\mathbf{r}}_2 \times \rho_2 \underline{\mathbf{b}}_{21} dV \right] = 0 \quad (\text{A1})$$

and use the following nomenclature

$$\left[ (\underline{\mathbf{r}}_{\text{CM}})_1 - (\underline{\mathbf{r}}_{\text{CM}})_2 \right] = \underline{\mathbf{R}} \quad (\text{A2a})$$

$$\underline{\mathbf{f}}_{12} = \underline{\mathbf{F}} \quad (\text{A2b})$$

$$\int_{\mathcal{V}_1(t)} \underline{\mathbf{r}}_1 \times \rho_1 \underline{\mathbf{b}}_{12} dV + \int_{\mathcal{V}_2(t)} \underline{\mathbf{r}}_2 \times \rho_2 \underline{\mathbf{b}}_{21} dV = \underline{\mathbf{D}} \quad (\text{A2c})$$

to express Eq. (A1) as

$$\underline{\mathbf{R}} \times \underline{\mathbf{F}} + \underline{\mathbf{D}} = 0 \quad (\text{A3})$$

Here we would like to know when the vector  $\underline{\mathbf{D}}$  can be discarded in order to simplify this result. A plausible intuitive hypothesis<sup>[19]</sup> associated with this simplification is given by

$$\text{Assumption:} \quad \underline{\mathbf{R}} \times \underline{\mathbf{F}} = 0 \quad (\text{A4})$$

however, we cannot discard  $\underline{\mathbf{D}}$  as being small compared to  $\underline{\mathbf{R}} \times \underline{\mathbf{F}}$  since Eq. (A3) requires that  $\underline{\mathbf{D}}$  and  $\underline{\mathbf{R}} \times \underline{\mathbf{F}}$  be the same order of magnitude. This type of problem has been considered before,<sup>[12]</sup> and we will follow the procedure suggested in that earlier work. This requires that we decompose  $\underline{\mathbf{F}}$  into a part that is parallel to  $\underline{\mathbf{R}}$  and a part that is perpendicular to  $\underline{\mathbf{R}}$  as indicated by<sup>[20]</sup>

$$\underline{\mathbf{F}} = \underbrace{\underline{\mathbf{F}}_{\parallel}}_{\text{parallel part}} + \underbrace{\underline{\mathbf{F}}_{\perp}}_{\text{perpendicular part}} \quad (\text{A5})$$

On the basis of this decomposition, we see that Eq. (A3) provides the two results given by

$$\underline{\mathbf{R}} \times \underline{\mathbf{F}}_{\perp} = 0 \quad (\text{A6a})$$

$$\underline{\mathbf{R}} \times \underline{\mathbf{F}}_{\parallel} + \underline{\mathbf{D}} = 0 \quad (\text{A6b})$$

This allows us to estimate as  $\underline{\mathbf{F}}_{\perp}$

$$\underline{\mathbf{F}}_{\perp} = \frac{\mathcal{O}(\underline{\mathbf{D}})}{\mathcal{O}(\underline{\mathbf{R}})} \quad (\text{A7})$$

in which  $\mathcal{O}$  indicates an order of magnitude estimate. If  $\underline{\mathbf{F}}_{\perp}$  is small relative to  $\underline{\mathbf{F}}_{\parallel}$ , and if small causes give rise to small effects, we can replace  $\underline{\mathbf{F}}_{\perp}$  with  $\underline{\mathbf{F}}$  and Eq. (A6a) leads to the central force law given by Eq. (45). To develop the conditions that must be satisfied in order that  $\underline{\mathbf{F}}_{\perp}$  be negligible compared to  $\underline{\mathbf{F}}_{\parallel}$ , we consider the inequality given by

$$\underline{\mathbf{F}}_{\parallel} \gg \underline{\mathbf{F}}_{\perp} \quad (\text{A8})$$

In terms of the estimate given by Eq. (A7) this leads to

$$\underline{F}_= \gg \frac{O(\underline{D})}{O(\underline{R})} \quad (\text{A9})$$

and because of the constraint given by Eq. (A8) we can express this result as

$$\underline{F} \gg \frac{O(\underline{D})}{O(\underline{R})} \quad (\text{A10})$$

Making use of the definitions given by Eqs. (A2) this inequality can be arranged in the form

$$\frac{O\left[\int_{\mathcal{V}_1(t)} \tilde{\mathbf{r}}_1 \times \rho_1 \mathbf{b}_{12} dV + \int_{\mathcal{V}_2(t)} \tilde{\mathbf{r}}_2 \times \rho_2 \mathbf{b}_{21} dV\right]}{O(\underline{\mathbf{f}}_{12}) O\left[\left(\underline{\mathbf{r}}_{\text{CM}}\right)_1 - \left(\underline{\mathbf{r}}_{\text{CM}}\right)_2\right]} \ll 1 \quad (\text{A11})$$

On the basis of Eqs. (29) we obtain the two estimates

$$\int_{\mathcal{V}_1(t)} \tilde{\mathbf{r}}_1 \times \rho_1 \mathbf{b}_{12} dV = O(\tilde{\mathbf{r}}_1) \underline{\mathbf{f}}_{12}, \quad \int_{\mathcal{V}_2(t)} \tilde{\mathbf{r}}_2 \times \rho_2 \mathbf{b}_{21} dV = O(\tilde{\mathbf{r}}_2) \underline{\mathbf{f}}_{21} \quad (\text{A12})$$

and use of these [along with Eq. (31)] in Eq. (A11) leads to the constraint given by

$$\text{Constraint: } \frac{O(\tilde{\mathbf{r}}_1) + O(\tilde{\mathbf{r}}_2)}{O\left[\left(\underline{\mathbf{r}}_{\text{CM}}\right)_1 - \left(\underline{\mathbf{r}}_{\text{CM}}\right)_2\right]} \ll 1 \quad (\text{A13})$$

□

# NEW LABORATORY COURSE FOR SENIOR-LEVEL CHEMICAL ENGINEERING STUDENTS

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The career diversity for chemical engineers has changed dramatically over the last 30 years. For example, more than 75% of chemical engineering positions in 1975 were with companies involved in production of commodity fuels and chemicals.<sup>[1]</sup> By 2003, only 25% of the careers for chemical engineers were in these industries,<sup>[1]</sup> while biotech and electronics/materials industries employed approximately 15% and 10%, respectively, of chemical engineers.<sup>[2]</sup> These trends are expected to continue with a growing emphasis on the development and production of more complex materials including biologically active and nanostructured materials.<sup>[3]</sup>

The responsibilities of today's chemical engineer are evolving as a result of the changes in the industries that employ them. Chemical engineers are now more involved in the synthesis and development of new products and devices. Twenty-five years ago, only 15% of the graduating chemical engineers were in product development, whereas more than 50% of recent graduating chemical engineers are working in this area.<sup>[3]</sup> Also, the need for chemical engineers to be able to effectively interact with scientists from a range of disciplines such as materials science, biology, and medicine is increasing as a result of evolving employment opportunities.<sup>[4]</sup>

Even with the dramatic changes in career diversity and responsibilities for recent graduates, the chemical engineering curriculum has changed little over the last 40 years.<sup>[3, 5]</sup> Much of the focus remains with large-scale process equipment such as distillation towers and heat exchangers, and many of the examples used in courses continue to come from the petroleum refining and bulk chemical production industries. A growing number of leaders in chemical engineering believe that

chemical engineers need to be taught more about product and process synthesis rather than large-scale chemical engineering equipment.<sup>[1]</sup> Furthermore, it has been argued that more time needs to be spent in chemical engineering education on

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atomic- and molecular-scale phenomena, and on the translation of fundamental science to engineering principles.<sup>[6]</sup>

Because of these changes and needs, the Chemical Engineering Department at the University of Virginia (UVa) decided to overhaul its senior-level laboratory course to provide students with experiences and opportunities to learn concepts and develop skills required for success in today's changing world. The objectives of this paper are to communicate the overall concept of the new laboratory course, provide an overview of each experiment, and describe student feedback from the course. Details about each experiment can be obtained by corresponding with the author.

The objectives of the new 3-credit-hour laboratory course, based on a full course load of 15 to 18 credit hours per semester, are to:

- ▶ *Provide students with experiences that are more relevant to the contemporary chemical engineer.*
- ▶ *Engage students in*
  - *integration of process steps.*
  - *relationships between molecular structure and macroscopic properties.*
  - *translation of fundamental science to engineering principles.*
- ▶ *Provide students with an opportunity to develop teamwork skills in an environment similar to industry.*

These objectives were accomplished by first developing three 4-week-long experiments in Bioprocess Engineering (protein synthesis and purification), Catalysis and Energy Conversion (catalytic production of hydrogen coupled to fuel cells), and Polymer Synthesis and Characterization (structure/property relationships of advanced materials). A class structure was then developed to reflect a real-world chemical engineering environment. Sharing of information and ideas was accomplished by having small teams of students work together as part of a larger team on each experiment. Knowledge and experimental results were communicated between the smaller sub-teams using different types of written reports and an oral presentation.

The three experiments were set up in a new laboratory facility in Wilsdorf Hall that opened in the fall of 2006. This state-of-the-art laboratory, dedicated to undergraduate chemical engineering, has over 2,000 square feet of space, walk-in hoods, and abundant natural light (Figure 1). The major investment in the new laboratory space, and the equipment required for the three new experiments, represent a

high-level commitment to undergraduate chemical engineering at UVa.

This space also is used for the junior-year laboratory course for chemical engineering students at UVa during the prior semester. The emphasis of this laboratory course is on more traditional unit operations experiments with heat exchangers, a distillation column, a fluid flow demonstrator, and equipment for agitation and mixing.

Moving into a new laboratory facility made it easier to implement the new senior-level course in a single semester. This also provided the opportunity to benchmark the new course to the old course of more traditional unit operation experiments including a gas absorption column and a fixed-bed reactor.

## LABORATORY DESCRIPTION

Each of the three 4-week-long experiments is designed for division into three or four separate parts. Teams of six to eight students divide themselves into three or four sub-teams to work on the different parts of an experiment (two to three students per sub-team). A member of the teaching team is assigned to each experiment and is responsible for supervising the experiment and evaluating the students (teaching team consists of one faculty member and two graduate research assistants). Each teaching-team member spends 15-20 hours per week on the course, which includes two 4-hour lab periods/week, experiment preparation, grading, and office hours to answer questions.

The first week of each 4-week-long experiment is a planning period that is used by each teaching-team member to explain his or her experiment to a student team. The students also use this time to divide themselves into sub-teams and to become familiar with their part of the experiment. The final three weeks are used to run the experiments to accomplish the objectives of the experiment. The schedule of required



**Figure 1.** New 2,000-square-foot laboratory facility in Wilsdorf Hall for undergraduate chemical engineering at UVa.

reports and oral presentation for each experiment is shown in Table 1.

The total equipment cost for the three experiments was in excess of \$400,000. Major equipment costs for the Bioprocess Engineering experiment included the 5-liter fermenter (\$45,000), liquid chromatography workstation (\$62,000), and the ultra filtration apparatus (\$6,000). The major equipment costs for the Catalysis and Energy Conversion experiment were the plug flow reactor system (\$55,000), gas chromatograph (\$40,000), and fuel cell system (\$20,000). The two big expenditures for the Polymer Synthesis and Characterization experiment were for the dynamic mechanical analyzer (\$65,000) and the differential scanning calorimeter (\$55,000).

The summer prior to the first offering of the new laboratory course was spent by the instructor and five undergraduate students setting up equipment and working out the details of each experiment. Assistance was obtained during this time from other faculty members with expertise in the areas of the particular experiments. General course material, experimental procedures, and background information were prepared. Relevant journal articles and reference materials were placed on a Web site developed for the new course.

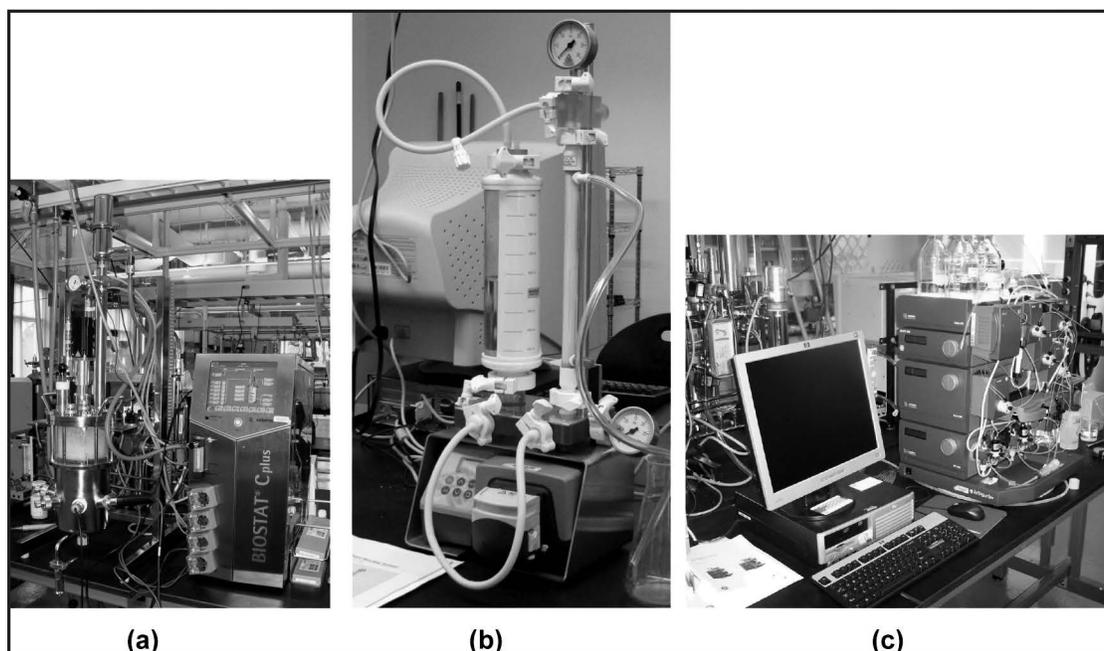
## BIOPROCESS ENGINEERING

The Bioprocess Engineering experiment involves the production of recombinant green fluorescent protein (GFP) from genetically transformed *E. coli* cells.<sup>[8]</sup> GFP is well-suited for use in this type of experiment for several reasons: its fluorescent nature allows students to detect its presence visually; the concentration of GFP can be measured in a protein mixture due to a unique absorbance peak at approximately 304 nm; and the extremely hydrophobic nature of GFP enables a straightforward purification strategy.<sup>[9]</sup> Because of this, laboratory experiments for undergraduate chemical engineering students have been developed for the production and purification of GFP.<sup>[10,11]</sup>

Information from published experiments with GFP has been used to develop an experiment that can be run in a 4-week time period with 4 hours/week of experimental time. A working cell bank of transformed cells, created by faculty and graduate students in preparation for this course, is used as inoculum. Students determine the effect of different process parameters on the growth of *E. coli* cells and protein expression using a 5-liter fermentation vessel (Figure 2a) in the upstream part of this experiment. Centrifugation, mechanical cell lyses, tangential flow ultra filtration (Figure 2b) and liquid chromatography (Figure 2c) are used in

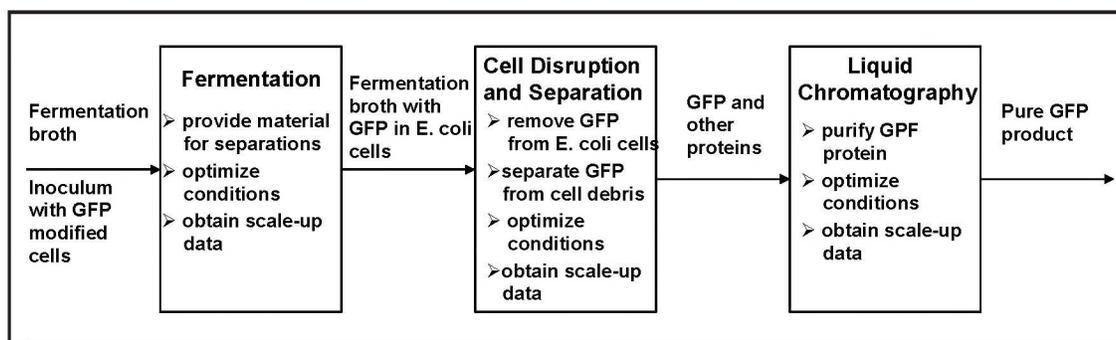
**TABLE 1**  
Schedule of required reports and oral presentation for each 4-week experiment.

End of Week	Required Report/Presentation	Comments
1	Planning Report	Team report with separate sub-team grades
2	Oral Presentation	Team presentation to teaching team member
3	Progress Report	Individually prepared report
4	Final Report	Team report that integrates work and results of each sub-team. A peer-evaluation process is used to adjust individual grades. <sup>[7]</sup>



**Figure 2.** Photographs of the major pieces of equipment in the Bioprocess Engineering experiment including (a) 5-liter Sartorius BIOSTAT CPlus® fermenter, (b) GE Healthcare QuixStand® benchtop ultra filtration apparatus, and (c) AKTA Purifier® liquid chromatography workstation.

**Figure 3.** Block diagram of the BioProcess Engineering experiment with the flow of materials outside each box and sub-team objectives listed inside each box.



the downstream part to recover and purify the GFP product.

A block diagram of the Bioprocess Engineering experiment (Figure 3) illustrates the flow of material through the experiment and highlights the objectives of each major part of the experiment.

The combination of fermentation, cell disruption and separation, and liquid chromatography enables students to evaluate and understand the overall process used to make a protein product. This helped the students develop an appreciation that a successful process-development team must work both cooperatively and independently to develop an optimized, multi-step manufacturing process.

Representative examples of student feedback from this experiment are:

- ▶ “This experiment fit in very well with biotech courses and tied them together.”
- ▶ “Enjoyed seeing the process from fermentation through downstream processing to final purified product.”
- ▶ “Enjoyed applying my coursework to actual experimentation.”
- ▶ “I liked this experiment because it introduced me to the field of biochemical engineering without having to take the biochemical engineering electives.”

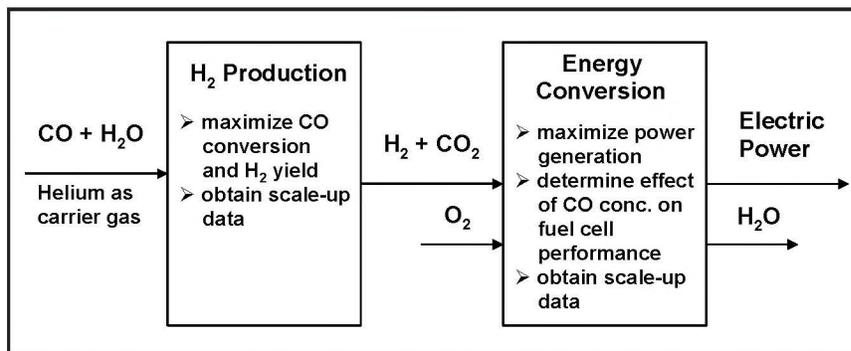
## CATALYSIS AND ENERGY CONVERSION

The Catalysis and Energy Conversion experiment is motivated by an interest in hydrogen as an alternative fuel source and the potential technical and environmental advantages of a fuel cell to convert hydrogen’s chemical energy into electrical energy.<sup>[12]</sup> The block diagram (Figure-4) shows the flow of material and the objectives of the major parts of this experiment.

Pure CO and H<sub>2</sub>O are converted to CO<sub>2</sub> and H<sub>2</sub> over a copper alumina catalyst (BASE, Selectra Shift 4P+<sup>[14]</sup>) in the reversible water-gas shift (WGS) reaction experiment shown in Eq (1).<sup>[13]</sup>



The reaction is conducted in a fixed-bed reactor located in a BTRS-Jr reactor system (Autoclave Engineers). Liquid water

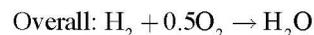
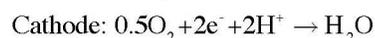
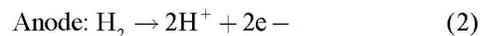


**Figure 4.** Block diagram of the Catalysis and Energy Conversion experiment with the flow of materials outside each box and sub-team objectives listed inside each box.

enters through an HPLC pump and is vaporized before being fed into the reactor. Helium is used as a carrier gas to minimize the temperature increase from the exothermic WGS reaction.

The concentration of CO and CO<sub>2</sub> in the reactor effluent is determined using an HP 6890 Series gas chromatograph. This information, along with the inlet flow rates to the reactor, is used by the students to determine the CO conversion and H<sub>2</sub> yield for a range of operating conditions. These data are used to identify the process conditions that result in the highest CO conversion and largest H<sub>2</sub> yield. Students also compare their experimental CO conversion values to their calculated equilibrium CO conversion values to determine whether the reaction is kinetically or thermodynamically limited.

A Nafion proton exchange membrane (PEM) fuel cell is used to convert the chemical energy in H<sub>2</sub> to electrical energy.<sup>[15]</sup> Fuel (H<sub>2</sub>) is fed into the anode side of a PEM fuel cell where it is converted into protons and electrons in the presence of the anode catalyst. The protons diffuse through the membrane and the electrons travel to the cathode through an external circuit. At the cathode catalyst, oxidant (O<sub>2</sub>, either from air or pure O<sub>2</sub> gas) reacts with the protons and the electrons to form H<sub>2</sub>O and heat. Eq. (2) is a summary of the reactions that occur on the anode and cathode sides of a PEM fuel cell.



The fuel cell part of this experiment is based on published laboratory experiments with PEM fuel cells.<sup>[16,17]</sup> The temperature of the fuel cell is varied from room temperature to 80 °C. Pure H<sub>2</sub> or H<sub>2</sub> mixed with a small amount of CO (<100 ppm) is passed through a heated humidifier before being fed to the anode side of the fuel cell. The moisture maintains a high proton conductivity of the electrolyte membrane. Likewise, pure O<sub>2</sub> or air as oxidant is passed through a humidifier before being fed to the cathode side of the fuel cell. The flow rates of both streams to the fuel cell are controlled by digital mass flow controllers (OMEGA, model FMA6500).

An Agilent Electronic Load (model 6060B) is connected between the anode and cathode sides of the fuel cell. This instrument is used to vary the external load on the fuel cell from 0 Ω to 1,000 Ω and to measure the voltage and current of the fuel cell.

Figure 5 is a plot of fuel cell voltage as a function of current density at three different fuel cell temperatures. Each curve in this figure, which is referred to as a polarization curve, was obtained by varying the external load on the fuel cell over the range of 0 Ω to 1,000 Ω.

Students are able to determine the optimum conditions for operating the fuel cell by examining fuel cell performance over a range of temperatures, pressures, and gas flow rates. Fuel cell efficiency, defined as the electric power generated divided by the product of the rate of reactant utilization and its Higher Heating Value, is calculated under the optimum conditions. This information is used by the students to scale-up their results from a single fuel cell data to a fuel cell “stack,” *i.e.*, fuel cells connected in series, which is capable of producing enough energy for an average-size home.

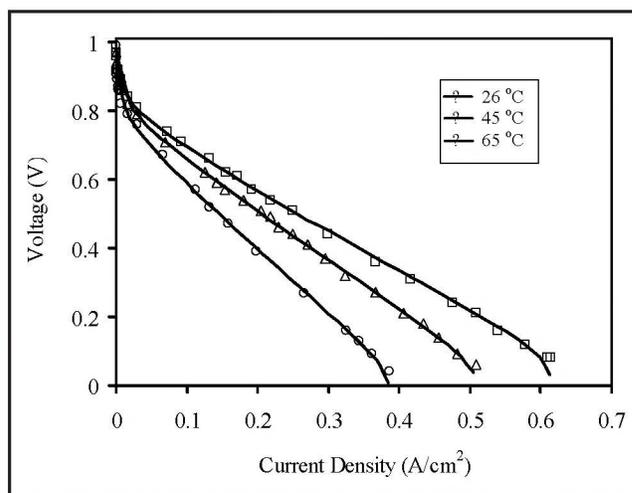
Students observe that a CO concentration in H<sub>2</sub> as low as 10 ppm can significantly affect the performance of a PEM fuel cell, which illustrates why it is important for the WGS reaction to be run with a very high CO conversion value. In addition, they appreciate why the H<sub>2</sub> produced in the upstream part of this experiment as currently configured cannot be fed directly to the PEM fuel cell since the lowest CO concentration in the reactant stream leaving the reactor is approximately 20,000 ppm. A new type of fuel cell made by BASF, that can tolerate a CO concentration as high as 30,000 ppm, is currently being evaluated for use in this experiment.<sup>[18]</sup>

Representative student comments from this experiment are:

- ▶ “I learned a great deal in this lab, having no previous experience with fuel cells.”
- ▶ “Enjoyed the real-life application with the fuel cell.”
- ▶ “I really liked the design problem.”
- ▶ “Enjoyed applying what we learned in class to real experimentation.”
- ▶ “Enjoyed learning about fuel cells and seeing the different factors that affect them.”
- ▶ “Reactor experiment was practical and related many of the basic chemical engineering concepts to practice.”

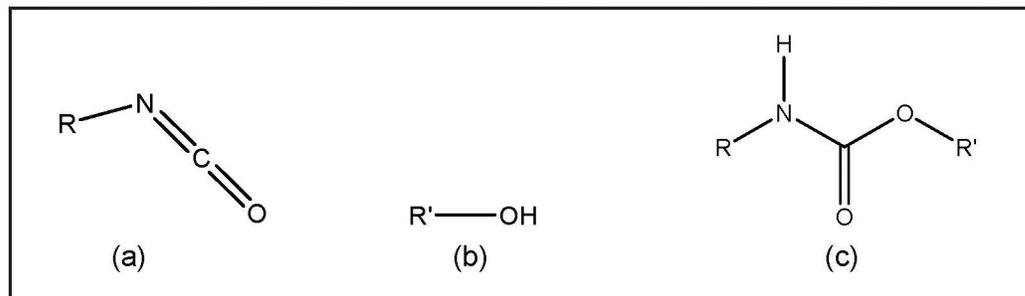
## POLYMER SYNTHESIS AND CHARACTERIZATION

Polyurethane is a polymer that contains urethane linkages formed by the reaction of a diisocyanate containing two or more isocyanate groups (NCO) with a glycol molecule or a low-molecular-weight diol containing two or more hydroxyl groups (OH).<sup>[19]</sup> Figure 6 includes structural representations of these different chemical groups where R and R' are two different carbon chains (R is usually aromatic, R' is usually aliphatic).



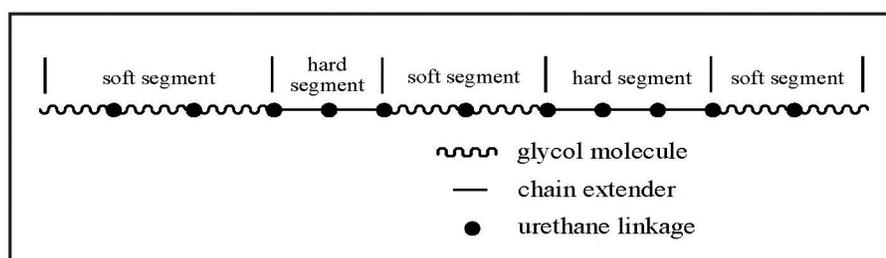
**Figure 5.** Effect of temperature on fuel cell performance. Experimental conditions: H<sub>2</sub> flow rate 30 ml/min, O<sub>2</sub> flow rate 30 ml/min, anode side pressure 10 psig, cathode side pressure 6 psig. Data obtained from student experimental measurements.

**Figure 6.** Structural representations of the (a) isocyanate and (b) hydroxyl reactive groups, and (c) urethane linkage.



Polyurethane polymer chains are composed of alternating “soft” segments and rigid “hard” segments. The soft segments are formed by the reaction of high-molecular glycol molecules with diisocyanate molecules. The number average molecular weight ( $M_n$ ) of the glycol molecules used to make a polyurethane polymer is usually between 1000 and 2000 (*i.e.*,  $M_n$  of  $R'$  is between 1000 and 2000). A typical soft segment of a polyurethane polymer contains between two and four glycol molecules that are joined together with urethane linkages.

The hard segments are formed from the reaction of diisocyanate molecules with a low molecular weight diol, such as 1,4 butanediol, that is typically referred to as the chain extender. The hard and soft segments are joined end-to-end with urethane linkages. For this reason, polyurethane polymers are usually classified as block copolymers. A schematic representation of a polyurethane polymer chain is shown in Figure 7.

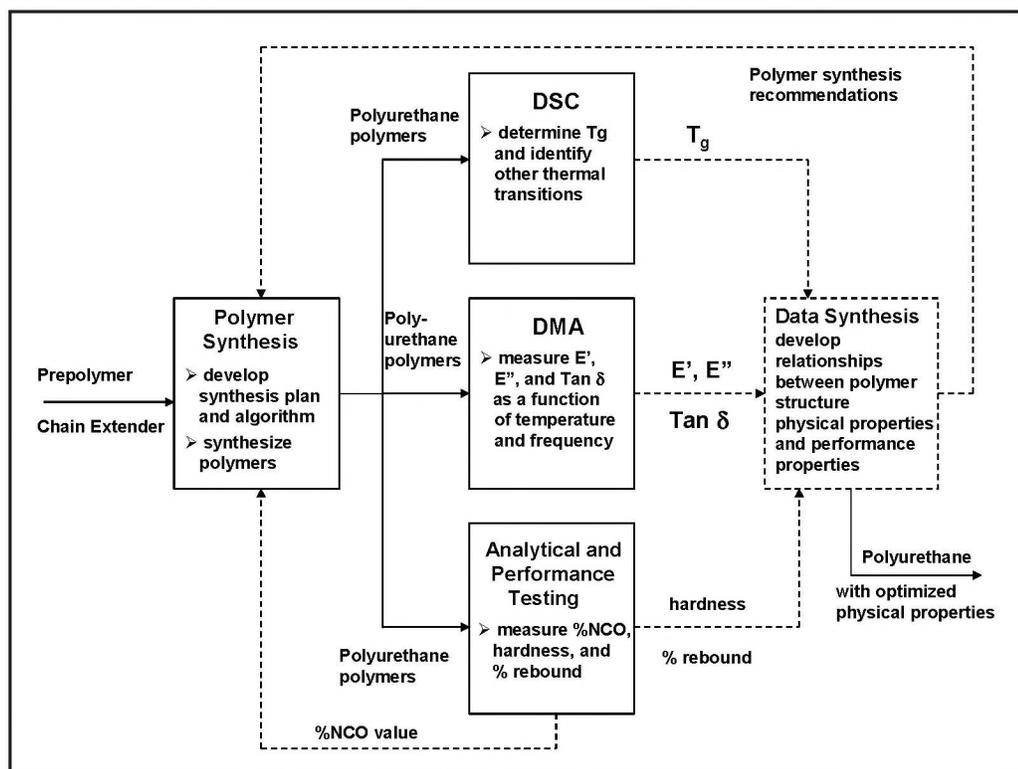


**Figure 7.** Schematic representation of a polyurethane polymer chain showing the soft segments (long chain glycol molecules connected with urethane groups) and hard segments (chain extender connected with urethane groups).

The students are given the assignment in the Polymer Synthesis and Characterization experiment to produce a soft, energy-absorbing polyurethane polymer for use in applications including the soles of shoes and personal protective equipment. This objective is accomplished by the students synthesizing polymers from several different prepolymers and chain extenders and then measuring the performance properties of the polymers. Figure 8 is a block diagram to illustrate the flow of materials and information through this experiment, and to summarize the objective of each of the four sub-teams.

The students synthesize polyurethane polymers by adding the appropriate amount of chain extender(s) to a prepolymer with a known mass and isocyanate concentration (%NCO) in a plastic cup. After mixing with a disposable stir-stick, the mixture is poured into heated sample molds and allowed to cure at 80 °C for 16 hours. The %NCO value of each prepolymer is measured by the students using a titration technique.

Four different polyurethane prepolymers are obtained from ITWC, Inc., for this experiment.<sup>[20]</sup> These prepolymers are prepared by reacting polyether- or polyester-based glycols with an excess of 4,4'-Diphenylmethane diisocyanate (MDI). An excess of MDI is used so that unreacted diisocyanate molecules remain after all the glycol hydroxyl groups have been consumed. The amount of excess diisocyanate is quantified with a parameter referred to as %NCO, which is simply the wt% of NCO in the prepolymer (prepolymers used in this experiment have NCO values between 6 and 12 wt%). Based on the %NCO, the amount of chain



**Figure 8.** Block diagram of the Polymer Synthesis and Characterization experiment to illustrate the flow of materials (solid lines) and information (dotted lines) through this experiment. The objectives of each of the four sub-teams are listed inside each box. Data synthesis is accomplished by the four sub-teams working together.

extender required to react all the isocyanate groups to form the final polymer can be determined.

Students use two different chain extenders (1,4 butanediol and diethylene glycol) to react the NCO groups of the prepolymer to form the final polyurethane polymers. Synthesizing polyurethane polymers with different types of soft and hard segments, and with different hard-segment concentrations, enables the students to test polymers with a wide range of rheological properties and thermal transitions and to observe a range of performance properties.

A Shore SRI Resilometer, commonly referred to as a Bayshore Resilometer, is used to measure the % rebound of the polyurethane polymers following ASTM procedure D2632. Polymer hardness is measured using hand-held durometers obtained following ASTM procedure D2240. “A” and “D” scale durometers are used so that polymers with a wide range of hardness values can be characterized.

A TA Instruments Q1000 differential scanning calorimeter (DSC) is used to determine the effect of polyurethane composition changes on the glass transition temperature ( $T_g$ ). DSC also is used to identify any other higher-temperature thermal transitions in these materials. The rheological properties of the polyurethane samples, including elastic ( $E'$ ) and viscous ( $E''$ ) modulus, are measured as a function of temperature and frequency using a dynamic mechanical analyzer (DMA) manufactured by TA Instruments (Model Q800). The energy damping coefficient,  $\tan \delta$ , which is the ratio of  $E''$  to  $E'$ , is calculated using the measured moduli values.

The students are challenged to use all of their measurements to develop an understanding of the relationships between molecular structure, rheological properties (*i.e.*,  $E'$  and  $\tan \delta$ ), and performance properties (*i.e.*, % rebound and hardness) of their polyurethane samples. They are then expected to communicate their understanding to the polymer synthesis team to help decide which prepolymer and chain extender(s) to use in their second batch of polymers to obtain a material with the best combination of energy absorbing and hardness properties for the stated end-use of the material.

Representative student comments from this experiment are:

- ▶ “This lab really allowed for all the sub-teams to come together, and I thought that that was very helpful.”
- ▶ “Learning about the challenges of polymer synthesis was very interesting.”
- ▶ “Enjoyed how the sub-teams relied on feedback from other sub-teams throughout the experiment.”
- ▶ “Learned a great deal including the application of techniques and end-use tests.”
- ▶ “This experiment really gave us a good idea of how polymers are made.”

## STUDENT FEEDBACK

Student feedback regarding the new laboratory course was obtained from the online course evaluation that is administered by the school and by a custom questionnaire that was administered at the end of the semester. The online course evaluation provided comparisons of student feedback from the old and new laboratory courses. The questionnaire provided an opportunity to obtain quantitative information about how well the objectives of the new laboratory course were met, how students enjoyed the organization of the new laboratory course, and how students felt about each of the three experiments that make up the new laboratory course.

The online course evaluation consists of 20 general questions about the course and the instructor. Students respond to each of the questions on a scale of 1 to 5 where 5 is the most favorable. Overall ratings for the course and instructor are calculated based on responses to the 20 questions by all the students. The overall course rating for the last two years of the old laboratory course was 4.03 and 4.05 (out of 5) indicating a good course rating. The overall course rating for the new laboratory course was 4.48 indicating a significant increase in course satisfaction by the students for the new course compared to the old course.

For the custom questionnaire, a response scale of 1 to 5 was provided for each statement, where 1 is strongly disagree and

**TABLE 2**  
Summary of student responses to the statements that they were provided on the custom questionnaire about how well the course objectives were met

Statement	Strongly Agree	Agree	Neutral or Disagree
1. Collectively, the three 4-week-long experiments provided me with educational opportunities that are relevant to today's practicing chemical engineer.	68%	32%	0%
2. The three 4-week-long experiments taught me about the:			
a. integration of process steps.	36%	56%	8%
b. relationship between molecular structure and macroscopic properties.	16%	60%	24%
c. translation of fundamental science to engineering principles.	28%	68%	4%
3. Dividing my lab team into smaller sub-teams provided an opportunity to develop teamwork skills in an environment similar to what I might experience working in industry.	48%	44%	8%

5 is strongly agree. Students were also encouraged to add individual comments about each statement. Included in Table 2 is a summary of student responses to the three statements about how well the course objectives were met.

Responses to the first statement clearly indicate that the students felt the new laboratory course taught them about technologies that are relevant to the modern chemical engineer. Individual comments indicated that the students enjoyed discussing the details of the experiments during job interviews.

Responses to the second statement indicate that the students learned something about the integration of process steps and how material learned in basic science classes can be applied to engineering-related problems. The connection between molecular structure and macroscopic properties was not made apparent to a number of students, however. Even so, individual comments indicated that the students appreciated the different learning opportunities they were provided during the course (“*Learned more in this course than any other course that I have taken here.*”). Most students felt that the team/sub-team structure was challenging, but felt that this experience helped prepare them for what they will experience working in industry based on responses to the third statement and on individual comments included with this statement. In particular, students commented that they enjoyed the opportunity to be part of smaller sub-teams that worked together to achieve a common goal.

Feedback from the students indicated that a successful multi-week experiment does not depend on whether or not the students had prior coursework related to the subject of the experiment. For example, students who had not taken any bioengineering electives appreciated the opportunity to learn about the field during the Bioprocess Engineering experiment, while students working toward a bioengineering concentration enjoyed being able to apply their classroom knowledge to hands-on experiences. Furthermore, although an elective course in polymers is currently not offered at UVa, students were able to learn enough about the subject, and the details of polymer rheology and thermal transitions, to have a productive and enjoyable laboratory experience in polymers.

An overall observation by the instructor is that students stayed much more focused and engaged with the new laboratory course throughout the semester compared to students during the old laboratory course. It is the instructor’s belief that the primary reason for the change in student attitude and interest is that the students find the three 4-week experiments that make up the new laboratory course more interesting and relevant to what they might do as chemical engineers after graduation than the traditional unit operations experiments that were used in the old laboratory course.

## ACKNOWLEDGMENTS

The authors gratefully acknowledge the financial support of Virginia’s Equipment Trust Fund that provided funds to purchase most of the equipment for the Bioprocess Engineering and Catalysis and Energy Conversion experiments. Also, the authors gratefully acknowledge the Office for Naval Research for funds that were used to purchase the major pieces of equipment for the Polymer Synthesis and Characterization experiment through its Defense University Research Instrumentation Program (DURIP), contract N00014-06-1-0853. Finally, the technical support of Steve Longacre from ITWC, Inc., throughout the development of the Polymer Synthesis and Characterization experiment is noted and gratefully acknowledged.

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## Random Thoughts . . .

# DOES YOUR DEPARTMENT CULTURE SUIT YOU?

RICHARD M. FELDER

North Carolina State University

If you are like most faculty members, your salary is paid by your university and you're subject to policies dictated by the Provost and Dean, but your department is your academic home. Cultures can vary dramatically from one department to another, and how much you look forward to coming to work every day can depend significantly on how well you are temperamentally suited to your department's culture. Just for the fun of it, fill out the questionnaire on the next page to gauge how you perceive that culture. For the questionnaire to be most useful, you should complete it before continuing to read. Go ahead—I'll wait.

\* \* \*

Finished? Look back at the bottom row. The more (a) answers you circled, the more your department can be characterized by words such as *collegial* and *supportive*; the more (b) answers, the more words like *individualistic* and *competitive* would apply. It's not that one type of department is good and the other is bad—they're just different. (I'm partial to collegial, but that's just me.)

Your comfort level at work depends on how compatible your personality is with the culture—collegial or individualistic—of your department. If you are strongly collegial, you'd probably be more comfortable in a collegial department than in an individualistic one; if you're strongly individualistic you might or might not be comfortable in a collegial department, but there is a good chance that your collegial colleagues would not be particularly comfortable with you. If either you or your department is somewhere near the balance point between collegial and individualistic, there's a reasonable chance that things will work out—and if they don't, it will likely be for reasons other than a culture incompatibility.

While I haven't attempted a rigorous validation of the questionnaire, to get a feeling for how it works I asked several of my friends on engineering faculties to complete it. Four of them in the same department—the department head, a full professor, an associate professor, and an assistant professor in his second year—respectively registered *a-b* scores of 14-3, 15-2, 14-3, and 15-2. In another department, the scores submitted by two professors (full and associate) were 12-5 and 9-8. Individual profiles from the other raters—all in different

departments—were 10-7, 11-6, 12-5, 12-5, and 0-17. In short, all but one department fell in a range from very collegial to fairly collegial, and that one showed up as virtually devoid of collegiality. I'm familiar with the departments in question and consider all of those ratings to be accurate.

If you are a department head and would like to increase your department's level of collegiality, have the faculty complete the questionnaire anonymously and use common (b) responses as prompts for change. If you see widely varying scores from different respondents, it could signal a problem such as the existence of cliques or the exclusion of women and minorities from full participation in department activities, and you should try to find out what's going on. If you are a faculty member, postdoctoral fellow, or graduate student looking for a new academic position, complete the questionnaire with your ideal department in mind before you go on your first interview trip. You should probably stop short of asking the search committee to fill out the questionnaire, but you might casually introduce some of the questions in your discussions with department faculty. The correspondence—or lack of it—between your responses and theirs could tell you a lot about how suitable the department is for you and vice versa.

## ACKNOWLEDGMENTS

My thanks go to Dave Clough of the University of Colorado, who gave me the idea for this column in a recent conversation, and to Rebecca Brent and other colleagues who completed early drafts of the questionnaire and offered excellent suggestions for improvement.

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### Academic Department Culture Assessment†

For each of the 17 questions, circle the letter next to the description that most closely matches your perception of your department.

1	a		Research collaborations among department faculty members are common and fluid (the collaborators are different from one project to another).
		b	Intradepartmental research collaborations are uncommon. When they exist, they usually involve the same faculty members year after year.
2	a		Most graduate students identify themselves first as belonging to their department, second as members of their advisor's research group.
		b	Most graduate students identify themselves first as members of their advisor's research group, second as belonging to their department.
3	a		Informal interactions between senior faculty and junior faculty are common.
		b	Informal interactions between senior faculty and junior faculty rarely occur.
4	a		Laboratory space and equipment are often shared by students working for different advisors.
		b	Sharing space and equipment across research groups is rare.
5	a		Groups of faculty members frequently go out for lunch together.
		b	Groups of faculty members rarely go out for lunch together.
6	a		Individual faculty achievements and honors are routinely acknowledged and celebrated.
		b	Faculty achievements and honors usually go without notice within the department.
7	a		Faculty members and their partners/families periodically socialize with one another.
		b	Social interactions among faculty members and partners/families almost never occur.
8	a		New faculty are routinely mentored in research and teaching by senior colleagues.
		b	Mentoring of new faculty does not routinely occur.
9	a		The whole faculty gathers regularly for refreshments and conversation.
		b	Gatherings of the faculty for refreshments and conversation rarely occur.
10	a		Graduate students are frequently co-advised by two or more department faculty members.
		b	Co-advising of graduate students within the department rarely occurs.
11	a		Relationships among faculty members are almost always cordial and cooperative.
		b	Relationships between many faculty members are often distant or competitive.
12	a		The department's teaching program quality is a source of pride or concern to the faculty.
		b	The department's teaching program is seldom a topic of conversation among the faculty.
13	a		Dissertation defenses are almost always amicable.
		b	Dissertation defenses often include hostile questions from members of other research groups.
14	a		Graduate students generally choose research advisors after they begin their graduate studies.
		b	Graduate students commonly commit to advisors before their first semester.
15	a		Faculty meetings are generally peaceful.
		b	Faculty meetings are often contentious.
16	a		The Department Head provides performance feedback to new faculty annually or more often.
		b	The Department Head does not regularly provide performance feedback to new faculty.
17	a		Retired faculty members regularly participate in department activities.
		b	Retired faculty members rarely participate in department activities.
<b>Sum*</b>			

\*Add the number of circled a's and b's in their respective columns.

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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.

# APPLICATIONS OF THE PENG-ROBINSON EQUATION OF STATE USING MATLAB

ZAKIA NASRI AND HOUSAM BINOUS

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The Peng-Robinson equation of state (PR EOS) was suggested in 1976<sup>[1]</sup> to satisfy the following objectives:

1. Parameters of this EOS should be defined in terms of the critical properties and the acentric factor.
2. Reasonable accuracy near the critical point, particularly for calculations of the compressibility factor and liquid density.
3. A single binary interaction parameter, which should be independent of temperature pressure and composition, is needed for the mixing rules.
4. PR EOS should be applicable in natural gas processes.

The PR EOS provided results similar to the Soave-Redlich-Kwong EOS, although it is generally superior in estimating the liquid densities of many materials, especially nonpolar ones.

The authors start by using the PR EOS to predict several pure-component properties, such as liquid and gas molar volumes for propane. The vapor-liquid isobaric diagram is then computed for a binary mixture composed of n-pentane and n-hexane at pressures of 2 and 8 bar. We compute the extent

of reaction in the case of the high-pressure ammonia synthesis in the next section. Finally, the adiabatic flash computation problem is presented and we conclude with several remarks concerning the use of MATLAB in chemical engineering.<sup>[2]</sup>

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## ESTIMATION OF PURE COMPONENT PROPERTIES

The Peng-Robinson equation of state<sup>[3-5]</sup> is

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

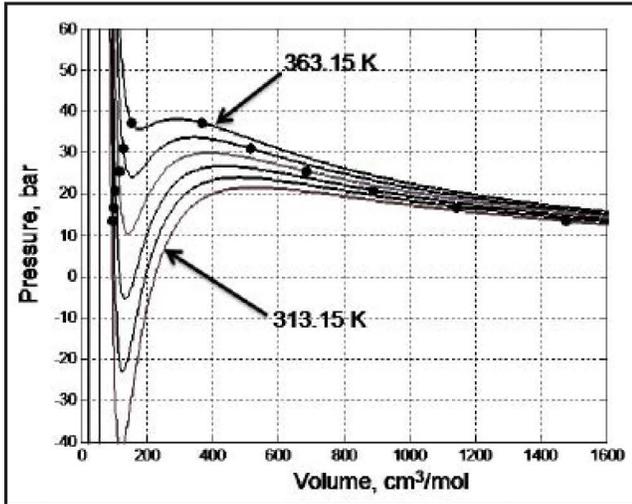


Figure 1. Isotherms for propane with spacing of 10 K.

where

$$b = 0.07780 \frac{RT_c}{P_c} \quad (2)$$

$$a = 0.45724 \frac{(RT_c)^2}{P_c} \left[ 1 + m \left( 1 - \sqrt{T_r} \right) \right]^2 \quad (3)$$

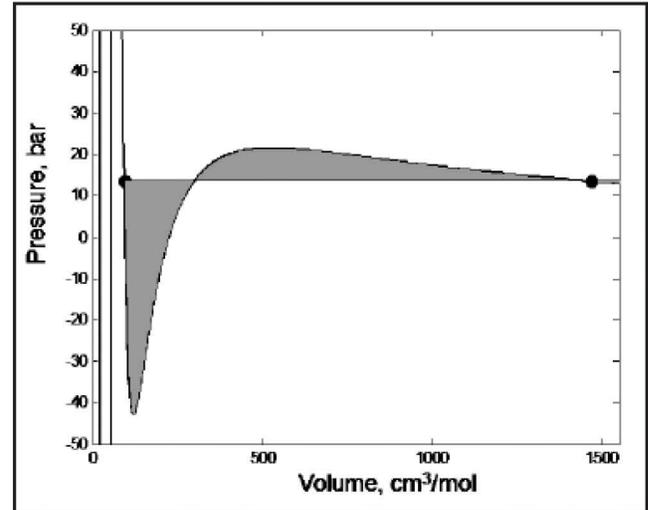


Figure 2. Isotherm at 313.15 K (shaded areas are equal)

TABLE 1

MATLAB Commands for Obtaining the Isotherms

```
% propane's critical temperature and pressure and acentric factor
Tc = 369.9;
Pc = 42.0;
Omega = 0.152;
% universal gas constant
R = 83.14;
% b and m for the PR EOS
b = 0.07780*R*Tc/Pc;
m = 0.37464 + 1.54226*Omega - 0.26992*Omega^2;
j=1;
for i=40:10:90
    % molar volume
    v=0.001:1:2500;
    % temperature
    T(i)=273.15+i;
    % reduced temperature
    Tre = T(i)/Tc;
    % a for the PR EOS
    a = 0.45724*(R*Tc)^2/Pc*(1 + m*(1 - sqrt(Tre)))^2;
    % PR EOS
    P=R*T(i)./(v - b) - a./(v.*(v + b)+b*(v-b));
    Pv=[Pv P'];
    % plotting isotherms for T varying from 313.15 to 363.15 K
    figure(2)
    h=plot(v,P);
    set(h,'color',rand(1,3),'linewidth',2);
    hold on
    axis([0 1600 -40 60])
    xlabel('Volume in cm3/mol')
    ylabel('pressure in bar')
    title('Isotherms for propane')
end
```

$$T_r = \frac{T}{T_c} \quad (4)$$

and

$$m = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad (5)$$

In Figure 1, we show isotherms (of the P/V relationship) obtained for propane at temperatures varying from 313.15 K to 363.15 K. Propane's critical temperature and pressure and acentric factor<sup>[5]</sup> are:

$$T_c=369.9 \text{ K}, P_c=42.0 \text{ bar and } \omega=0.152.$$

These isotherms are obtained using the MATLAB commands given in Table 1.

In Figure 2, one can read the vapor pressure as well as the liquid and gas molar volumes at different temperatures using the bold dots. These pure component properties are found by imposing that the two shaded areas in Figure 2 are equal; the MATLAB syntax for such an operation is given in Table 2.

The isotherm oscillates in a specific region and the PR EOS fails to describe real substances in this region. To fix this problem James Clerk Maxwell (1875) proposed to replace the isotherm in this region with a horizontal line positioned so that the areas of the two shaded regions are equal. The reason for

**TABLE 2**  
MATLAB Commands for Obtaining the Liquid and Gas Molar Volumes

```
function f=Pressure1(v,T)
% propane's critical temperature and pressure and acentric factor
Tc = 369.9;
Pc = 42.0;
Omega= 0.152;
% universal gas constant
R = 83.14;
% b and m for the PR EOS
b = 0.07780*R*Tc/Pc;
m = 0.37464 + 1.54226*Omega - 0.26992*Omega^2;
% reduced temperature
Tre = T/Tc;
% a for the PR EOS
a = 0.45724*(R*Tc)^2/Pc*(1 + m*(1 - sqrt(Tre)))^2;
% PR EOS
f=R*T./(v - b) - a./(v.*(v + b)+b*(v-b));
end

=====

function f=equations31(x,T)
% three algebraic equations, which solution gives the molar volumes
f(1)=-quad(@(v) Pressure1(v,T),x(1),x(2))+...
    feval(@(v) Pressure1(v,T),x(1))*(x(2)-x(1))...
    +quad(@(v) Pressure1(v,T),x(3),x(2))...
    -feval(@(v) Pressure1(v,T),x(2))*(x(2)-x(3));
f(2)=feval(@(v) Pressure1(v,T),x(1))-feval(@(v) Pressure1(v,T),x(3));
f(3)=feval(@(v) Pressure1(v,T),x(2))-feval(@(v) Pressure1(v,T),x(3));
end

=====

% using fsolve to get the molar volumes
5
X=fsolve(@(x) equations31(x,T(i)),[100 260 800])
% plot the bold dots in figure 2
h=plot(max(X),feval(@(v) Pressure1(v,T(i)),max(X)),'b.')
set(h,'markersize',20)
h=plot(min(X),feval(@(v) Pressure1(v,T(i)),min(X)),'b.')
set(h,'markersize',20)

where the solutions of this system of three non-linear algebraic equations, min(X) and max(X), are the
liquid and gas molar volumes. Once the vapor pressure and liquid and gas molar volumes are computed, it is
straightforward to get the bold dots using the following two lines of MATLAB® code:

h=plot(min(X),feval(@(v) Pressure1(v,T(i)),min(X)),'b.')
set(h,'markersize',20)
```

*Using the Maxwell equal area rule, one can get estimates for the vapor pressure as well as the liquid and gas molar volumes from the depicted isotherms.*

this equality is that the area in the P-V diagram corresponds to mechanical work and the change of free energy,  $\Delta A(T,V)$ , is equal to that work. This change of free energy is independent of the path because  $A(T,V)$  is a state function. Thus, this work should be equal if one takes the horizontal line drawn by Maxwell as a transformation path or the isotherm obtained using PR EOS as an alternative transformation path. The flat line portion of the isotherm now corresponds to liquid-vapor equilibrium. Using the Maxwell equal area rule, one can get estimates for the vapor pressure as well as the liquid and gas molar volumes from the depicted isotherms.

The values of the vapor pressure, calculated using the PR EOS, are then plotted vs. temperatures in Figure 3. These points agree with the curve calculated using the modified Antoine equation obtained from HYSYS 3.2, a major process simulator by Aspen Technology, Inc. (<<http://www.hyprotech.com>>), and given by

$$P^{\text{sat}} = \exp\left(52.3785 - \frac{3.4905510^3}{T} - 6.10875 \ln(T) + 1.11869 \cdot 10^{-5} T^2\right) / 100 \quad (6)$$

with T in Kelvin and  $P^{\text{sat}}$  in bar.

### VAPOR-LIQUID EQUILIBRIUM DIAGRAM FOR BINARY MIXTURES

The vapor-liquid isobaric equilibrium diagram for the binary mixture composed of n-pentane and n-hexane can be computed using the PR EOS. The liquid and vapor mole fractions are related by

$$y_i = K_i x_i \quad \text{with } i = 1 \text{ or } 2 \quad (7)$$

where  $K_i$  is the equilibrium constant.

The PR EOS is part of a family of equations called cubic because the compressibility factor, Z, is a solution of the following cubic equation written for a multicomponent mixture where we have used the mixing and combining rules,

$$Z^3 - (1 - B)Z^2 + (A - 3B^2 - 2B)Z + (-AB + B^2 + B^3) = 0 \quad (8)$$

where

$$A = \sum_{i=1}^c \sum_{j=1}^c y_i y_j A_{ij} \quad \text{or} \quad \sum_{i=1}^c \sum_{j=1}^c x_i x_j A_{ij} \quad (9)$$

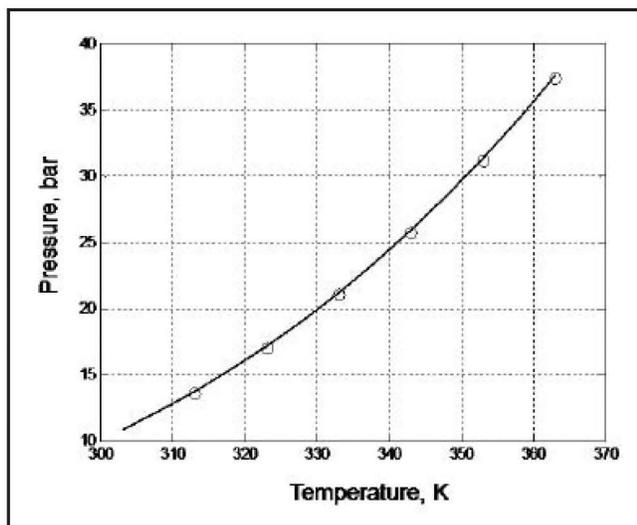


Figure 3. Vapor pressure vs. temperature for propane.

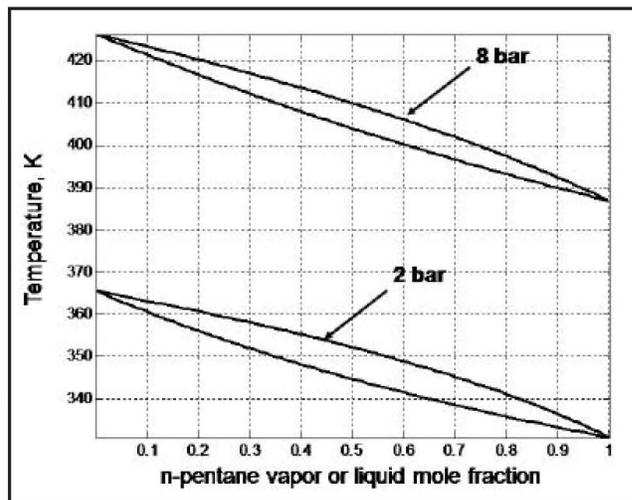


Figure 4. Isobaric VLE diagram for n-pentane/n-hexane mixture at 2 and 8 bar.

$$A_{ij} = (A_i A_j)^{0.5} (1 - k_{ij}) \quad (10)$$

$$B = \sum_{i=1}^C y_i B_i \text{ or } \sum_{i=1}^C x_i B_i \quad (11)$$

$$A_i = 0.45724 a_i \frac{P_r}{T_r^2} \text{ and } B_i = 0.07780 \frac{P_r}{T_r} \quad (12)$$

For each component, we define the reduced pressure and temperature by  $P_r = P/P_{c_i}$  and  $T_r = T/T_{c_i}$  and  $a_i$  is given by an equation similar to Eq. (3) for the pure component case. The binary interaction parameter,  $k_{ij}$ , is obtained from HYSYS 3.2 or assumed to be equal to zero if not available. The equilibrium constants are obtained using the  $\phi$ - $\phi$  method as follows,

$$K_i = \frac{\phi_{l_i}}{\phi_{v_i}} \text{ for } i = 1 \text{ to } C \quad (13)$$

where

$$\phi_{v_i} = \exp \left[ \left( Z_v - 1 \right) \frac{B_i}{B} - \ln \left( Z_v - B \right) - \frac{A}{2\sqrt{2}B} \left( \frac{2 \sum_j y_j A_{ij}}{A} - \frac{B_i}{B} \right) \ln \left( \frac{Z_v + (1 + \sqrt{2})B}{Z_v + (1 - \sqrt{2})B} \right) \right] \quad (14)$$

A similar expression is obtained for the liquid phase fugacity coefficient,  $\phi_{l_i}$ , by replacing the gas phase compressibility factor,  $Z_{v_i}$  with its liquid phase counterpart,  $Z_{l_i}$ . These two compressibility factors are the largest and smallest roots of Eq. (8), respectively. We perform several flash calculations to obtain both the bubble-point and the dew-point curves using the famous Rachford and Rice equation given by:

$$\sum_{i=1}^C \frac{z_i (K_i - 1)}{1 + \phi (K_i - 1)} = 0 \quad (15)$$

where  $z_i$  is the mole fraction of component  $i$  in the feed. The MATLAB commands for the VLE data determination are given in Table 3 (next page).

Figure 4 is obtained for pressures of 2 and 8 bar. These results agree with those given by DISTIL by Hyprotech Ltd. One advantage of the PR EOS is that one can compute VLE data for low, moderate, and high pressures with the same code. According to Figure 4, one could assume that the binary mixture is ideal at low pressures since both n-hexane and n-pentane are nonpolar molecules.

## HIGH-PRESSURE CHEMICAL EQUILIBRIUM COMPUTATION

Nitrogen and hydrogen react to form ammonia,  $N_2 + 3H_2 \rightleftharpoons NH_3$ . This reaction is favored by low temperatures and high pressures. Kinetic considerations, however, oblige us to use high temperatures. Thus, reactors are operated at very high pressures to get a reasonably high conversion of reactants. High gas-phase pressures imply significant deviation from ideality and the need to take into account the fugacity coefficients.<sup>[5]</sup> In fact, the equilibrium constant depends on  $K_v$  as follows:

$$K_a = \prod_{i=1}^C a_i^{v_i} = \frac{y_{NH_3}}{y_{N_2}^{0.5} y_{H_2}^{1.5}} \frac{1}{P} K_v = \frac{X(2-X)}{\left[ \frac{1-X}{2} \right]^{0.5} \left[ \frac{3(1-X)}{2} \right]^{1.5}} \frac{1}{P} K_v \quad (16)$$

***Nitrogen and hydrogen react to form ammonia. This reaction is favored by low temperatures and high pressures. Kinetic considerations, however, oblige us to use high temperatures. Thus, reactors are operated at very high pressures to get a reasonably high conversion of reactants.***

**TABLE 3**

MATLAB Commands for Obtaining the VLE Data

```
function f=flash(x)
global z
phi=0;
% critical temperature and pressure and
acentric factor
% for n-pentane and n-hexane
Pc=[33.75 30.32];
Tc=[196.45+273.15 234.748+273.15];
w=[0.25389 0.3000];
% pressure is set equal to 2 bars
P=2;
% reduced temperature and pressure
Tre=x(5)./Tc;
Pre=P./Pc;
% m, a, Ai, Bi, Aij, A, B for the PR EOS
m=0.37464 + 1.54226.*w-0.26992.*w.^2;
for i=1:2
    for j=1:2
        Ab(i,j)=(Ap(i)*Ap(j))^0.5;
    end
end
Av=0;
for i=1:2
    for j=1:2
        Av=Av+x(i+2)*x(j+2)*Ab(i,j);
    end
end
Bv=0;
for i=1:2
    Bv=Bv+x(i+2)*Bp(i);
end
Bl=0;
for i=1:2
    Bl=Bl+x(i)*Bp(i);
end
Al=0;
for i=1:2
    for j=1:2
        Al=Al+x(i)*x(j)*Ab(i,j);
    end
end
Alsum=[0 0];
for i=1:2
    for j=1:2
        Alsum(i)=Alsum(i)+x(j)*Ab(i,j);
    end
end
Avsum=[0 0];
for i=1:2
    for j=1:2
        Avsum(i)=Avsum(i)+x(j+2)*Ab(i,j);
    end
end
% liquid and gas phase compressibility factors
Zv=max(roots([1 -1+Bv Av-3*Bv^2-2*Bv -
```

*continued next column*

**TABLE 3, continued**

```
Av*Bv+Bv^2+Bv^3])); Zl=min(roots([1 -1+Bl
Al-3*Bl^2-2*Bl -Al*Bl+Bl^2+Bl^3]));
% coefficients phiiv=exp((Zv-1).*Bp/Bv-log(Zv-
Bv)...
-Av/
(2*sqrt(2)*Bv)*log((Zv+(1+sqrt(2))*Bv)/
(Zv+(1-sqrt(2))*Bv)).*...
(2.*Avsum./Av-Bp./Bv));
phil=exp((Zl-1).*Bp/Bl-log(Zl-Bl)...
-Al/
(2*sqrt(2)*Bl)*log((Zl+(1+sqrt(2))*Bl)/
(Zl+(1-sqrt(2))*Bl)).*...
(2.*Alsum./Al-Bp./Bl));
% equilibrium constant
K=phil./phiiv;
% the system of five algebraic equations
for i=1:2
    f(i)=x(i+2)-K(i)*x(i);
end
for i=1:2
    f(i+2)=x(i)-z(i)/(1+phi*(K(i)-1));
end f(5)=0;
for i=1:2
    f(5)=f(5)+z(i)*(K(i)-1)/(1+phi*(K(i)-
1));
end
=====
clc
global z
clear sol
% flash calculation using fsolve and a zero-
order collocation method
z=[0.0001 0.9999];
options = optimset('Display','off');
[X]=fsolve(@PT1,[0.01 0.9 0.01 0.9 360],op-
tions); x0=X;
sol(1,1)=X(1);
sol(2,1)=X(3);
sol(3,1)=X(5);
for i=1:100
    z=[0.01*i 1-0.01*i];
    [X]=fsolve(@PT1,x0,options);
    x0=X;
    sol(1,i+1)=X(1);
    sol(2,i+1)=X(3);
    sol(3,i+1)=X(5);
end
% plotting bubble curve
h=plot(sol(1,:),sol(3,:),'b')
set(h,'linewidth',2)
hold on
% plotting dew curve
h=plot(sol(2,:),sol(3,:),'r')
9
set(h,'linewidth',2)
axis tight
xlabel('vapor or liquid mole fraction')
ylabel('temperature in K')
grid on
```

**TABLE 4**

**MATLAB Commands for Ammonia Synthesis Problem**

```
function f=ammonia(x,T,P)
Y(1)=x(1);
Y(2)=x(2);
Y(3)=x(3);
Zv=x(5);
% critical pressure for hydrogen, nitrogen
and ammonia
Pc=[13.16 33.94 112.77];
% critical temperature for hydrogen, nitro-
gen and ammonia
Tc=[33.44 126.19 405.55];
% acentric factor for hydrogen, nitrogen and
ammonia
w=[0.0 0.0206 0.2582];
% reduced temperature
Tre=T./Tc;
% reduced pressure
Pre=P./Pc;
% Parameters for the Soave-Redlich-Kwong
Equation of State
% m, a, Ap, Bp Av, Bv, B1, A1
m=0.480+1.574.*w-0.176.*w.^2;
a=(1+m.*(1-Tre.^0.5)).^2;
Ap=0.42747.*a.*Pre./Tre.^2;
Bp=0.08664.*Pre./Tre;
for i=1:3
    for j=1:3
        Ab(i,j)=(Ap(i)*Ap(j))^0.5;
    end
end
Av=0;
for i=1:3
    for j=1:3
        Av=Av+y(i)*y(j)*Ab(i,j);
    end
end
Bv=0;
for i=1:3
    Bv=Bv+y(i)*Bp(i);
end
% Equilibrium constant versus temperature
Ka298 = exp(16.5*1000/(8.314*298.15));
a = 24.619 - 0.5*27.318 - 1.5*26.879;
b = (3.75 - 0.5*(0.623) - 1.5*(0.435))*10^-
2;
c = (-0.138 + 0.5*(0.095) + 1.5*(0.033))*10^-
5;
d = (0.5*(2.871) + 1.5*(0.87))*10^-9;
K=Ka298*exp(a/8.314*log(T/298.15) +
b/(2*8.314)*(T-298.15) ...
+ c/(6*8.314)*(T^2-298.15^2) +
d/(12*8.314)*(T^3 - 298.15^3) + ...
1/8.314*(46100 + (298.15)*a +
b/2*(298.15^2) + ...
c/3*(298.15^3) + d/4*(298.15^4))*(1/T-
```

*continued next column*

**TABLE 4, continued**

```
1/298.15));
% fugacity coefficients for vapor phase
phiv=exp((Zv-1).*Bp/Bv-log(Zv-Bv)...
-Av/Bv*log((Zv+Bv)/Zv)).*(2.*Ap.^0.5./
Av^0.5-Bp./Bv));
% system of algebraic equations
f(1)=1-x(1)-x(2)-x(3);f(2)=x(1)*(2-x(4))-
1.5*(1-x(4));
f(3)=x(2)*(2-x(4))-0.5*(1-x(4));
f(4)=K*(0.5*(1-x(4)))^0.5*(1.5*(1-x(4)))^1.5
*phiv(1)^1.5*phiv(2)^0.5...
-x(4)*(2-x(4))/P*phiv(3);
f(5)=x(5)^3-x(5)^2+(Av-Bv-Bv^2)*x(5)-Av*Bv;
f(6)=x(6)-phiv(3)/(phiv(1)^1.5*phiv(2)^0.5);
end
=====
=clc
% temperature is 800 K
T=800;
% calculation using fsolve and a zero-order
collocation method
options=optimset('Display','off');
i=1;
X0=[0.2 0.1 0.4 0.9 0.9 0.9];
for P=10:100:1600
    if(i==1) X=fsolve(@(x) ammonia(x,T,P),X0
,options);
    else X=fsolve(@(x) ammonia(x,T,P),[y1(i-
1) y2(i-1) y3(i-1) Xe(i-1)...
Z(i-1) Kv(i-1)],options);
    end;
    y1(i)=X(1);
    y2(i)=X(2);
    y3(i)=X(3);
    Xe(i)=X(4);
    Z(i)=X(5);
    Kv(i)=X(6);
    Pp(i)=P;
    i=i+1;
end
% plotting the extent of reaction versus
pressure at 800 K
figure(1)
plot(Pp,Xe,'r')
axis tight
xlabel('Pressure in bars')
ylabel('Extent of reaction at T=800K')
% plotting the correction coefficient, Kv,
versus pressure at 800 K
figure(2)
plot(Pp,Kv,'b')
axis tight
xlabel('Pressure in bars')
ylabel('Kv at T=800K')
```

where  $K_v$  is given by:

$$K_v = \frac{\phi_{\text{NH}_3}}{\phi_{\text{N}_2}^{0.5} \phi_{\text{H}_2}^{1.5}} \quad (17)$$

$$a_i = \phi_i y_i P \quad (18)$$

The extent of reaction,  $X$ , is defined by the following equation:  $N_i = N_{i,0} + v_i X$  where  $N_i$  and  $N_{i,0}$  are the number of moles of species  $i$  at time  $t$  and initially, respectively, and  $v_i$  is the stoichiometric coefficient. The unknowns in this type of problems are five: the mole fraction in the gas phase, the extent of reaction, and the gas-phase compressibility factor. Once again, the calculation uses the built-in function *fsolve* to solve five nonlinear algebraic equations simultaneously. The MATLAB commands, which allow the determination of the five unknowns, are given in Table 4 (previous page).

In Figure 5, we plot  $K_v$  vs. pressure at a temperature of 800 K. Values of  $K_v$  are significantly different from unity, which means that this factor must be taken into account at high pressures. The extent of reaction at equilibrium versus pressure, for the same temperature, is represented in Figure 6. The extent of reaction approaches unity at high pressures, in agreement with LeChatelier's rule.

### ADIABATIC FLASH CALCULATIONS FOR MULTI-COMPONENT MIXTURES

A quaternary mixture, at 33.016 bar and 37.778 °C, is composed of 0.41% hydrogen, 5.71% methane, 70.97% benzene, and 22.91% toluene. This mixture is sent to a stabilizer to remove hydrogen and methane. The feed pressure is decreased adiabatically from 33.016 bar to 11.232 bar by valve and pipeline pressure drop. To find the vapor-phase fraction, the temperature, and other relevant variables, one needs the following expression for the departure function from ideality for the enthalpy in order to compute enthalpy<sup>[5]</sup>:

$$H^D = RT(Z-1) + \frac{1}{2\sqrt{2}B} \frac{RT}{P} \text{Log} \left[ \frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right] \left[ T \frac{d}{dT} \left( A \frac{(RT)^2}{P} \right) - A \frac{(RT)^2}{P} \right] \quad (19)$$

This problem has been solved using a tedious iterative technique.<sup>[6]</sup> The unknowns in this problem are the mole fractions in the two phases, the temperature, the vapor phase fraction as well as the compressibility factors. We have 12 nonlinear algebraic equations to solve simultaneously. These equations are three equilibrium relations, three component mass balances, two summation rules, two cubic equations of the compressibility factors, the enthalpy balance,  $H_{\text{feed}} = \phi H_v + (1-\phi)H_L$ , and the Rachford and Rice equation. The MATLAB commands, which allow the determination of the 12 unknowns, are based on the optimization toolbox function *fsolve*. The code is similar to the one presented in the previous section except for the code for the calculation of the enthalpy. This code is presented in Table 5 and uses the symbolic computation capability of MATLAB to compute the temperature derivative term in Eq. (19).

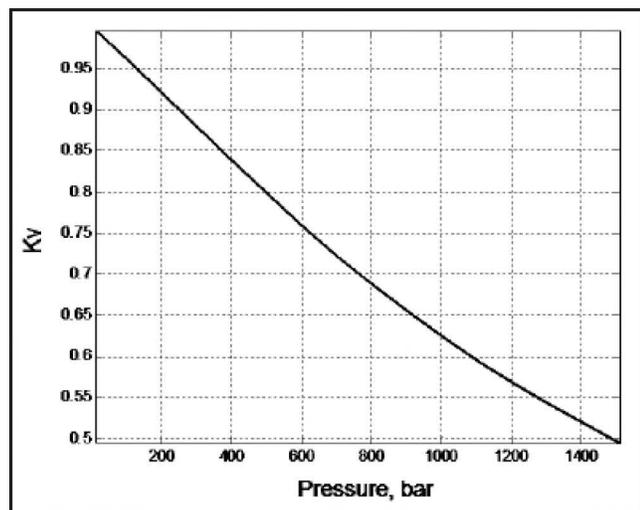


Figure 5.  $K_v$  for the ammonia synthesis reaction at 800 K.

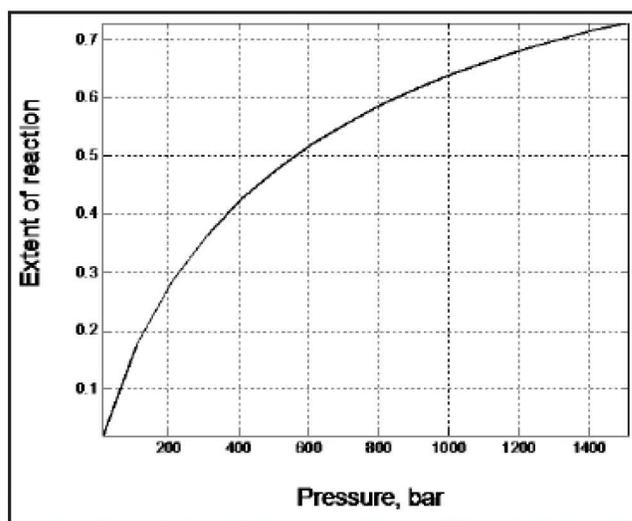


Figure 6. Extent of reaction for the ammonia synthesis reaction at 800 K.

TABLE 5

MATLAB Commands for Obtaining the Feed Enthalpy

```

clc
% defining symbolic variables
syms TF af AP Abf BP ZF
% critical pressure and temperature (in psi
and °R) and acentric factor
% for hydrogen, methane, benzene and toluene
Pc(1) = 190.8; Tc(1) = 59.7; w(1) = 0.0;
Pc(2) = 673.1; Tc(2) = 343.9; w(2) = 0.0;
Pc(3) = 714.2; Tc(3) = 1012.7; w(3) = 0.2116;
Pc(4) = 587.8; Tc(4) = 1069.1; w(4) = 0.2415;
% feed pressure in psi
P=485;
% feed composition
z(1)= 0.0041; z(2) = 0.0571; z(3) = 0.7097;
z(4) = 0.2291;
% various terms of the Peng-Robinson EOS
for i=1:4
m(i)=0.37464+1.54226*w(i)-0.26992*w(i)^2;
end
13
for i=1:4
af(i)=(1+m(i)*(1-(TF/Tc(i))^0.5))^2;
end
for i=1:4
AP(i)=0.45724*af(i)*(P/Pc(i))/(TF/Tc(i))^2;
end
% binary interaction parameters obtained from
HYSYS
k(1, 1) = 0; k(2, 2) = 0; k(3, 3) = 0; k(4,
4) = 0;
k(2, 1) = k(1, 2); k(3, 1) = k(1, 3); k(4, 1)
= k(1, 4);
k(2, 3) = k(3, 2); k(3, 4) = k(4, 3); k(2, 4)
= k(4, 2);
k(1, 2) = 0.20200; k(1, 3) = 0.2851;
k(1, 4) = 0.28510; k(3, 2) = 3.9999*10^-2;
k(4, 2) = 6.4900*10^-2; k(4, 3) =
9.51910*10^-4;
for i=1:4
for j=1:4
Abf(i,j)=(AP(i)*AP(j))^0.5*(1-k(i,j));
end
end
for i=1:4
BP(i)=0.07780*(P/Pc(i))/(TF/Tc(i));
end
AF=0;
for i=1:4
for j=1:4
AF=AF+z(i)*z(j)*Abf(i,j);
end
end
end
BF=0;
for i=1:4
BF=BF+z(i)*BP(i);
end
% computing enthalpy
TFK=310.9278;
TOK=298.15;

Ac(1, 1) = 29.088; Ac(2, 1) = -0.192*10^-2;
Ac(3, 1) = 0.4*10^-5;

```

continued next column

TABLE 5, continued

```

Ac(4, 1) = -0.87*10^-9;
Ac(1, 2) = 19.875 ; Ac(2, 2) = 5.021*10^-2;
Ac(3, 2) = 1.268*10^-5;
Ac(4, 2) = -11.004*10^-9;
Ac(1, 3) = -36.193; Ac(2, 3) = 48.444*10^-2;
Ac(3, 3) = -31.548*10^-5;
Ac(4, 3) = 77.573*10^-9;
Ac(1, 4) = -34.364; Ac(2, 4) = 55.887*10^-2;
Ac(3, 4) = -34.435*10^-5;
Ac(4, 4) = 80.335*10^-9;
HF1=0;
for i=1:4
HF1=HF1+(Ac(1,i)*TFK*z(i)+Ac(2,i)*TFK^2/
2*z(i)...
+Ac(3,i)*TFK^3/3*z(i)+Ac(4,i)*TFK^4/
4*z(i)...
-(Ac(1,i)*TOK*z(i)+Ac(2,i)*TOK^2/
2*z(i)...
+Ac(3,i)*TOK^3/3*z(i)+Ac(4,i)*TOK^4/
4*z(i)));
end
R=1.987;
X=diff(AF*(R*TF)^2/P);
TF=100+459.67;
ZF=0.116934;
HF2=subs(1.987*TF*(ZF-1)+1/(2*sqrt(2)*BF*1.98
7*TF/P)*...
log((ZF+BF*(1+sqrt(2)))/(ZF+BF*(1-
sqrt(2)))))...
*(TF*X-AF*(1.987*TF)^2/P),TF)/(9.486e-
4)/453.593;
HF=HF1+HF2

```

We find a feed enthalpy equal to  $-29913$  kJ/kmol. The vapor-phase fraction and temperature are  $0.0367$  and  $38.126$  °C, respectively.

## MATLAB: A SOFTWARE FOR TEACHING CHEMICAL ENGINEERING

It is the authors' experience that teaching and understanding applied thermodynamics can be very tedious and abstract if the lectures do not show how results of a flash distillation or vapor-liquid diagrams can be obtained. The study of such problems usually involves solving nonlinear algebraic equations, which is readily performed by the MATLAB function, *fsolve*. Little programming skill is required by the student, who gets acquainted with the basic MATLAB commands in a few days.<sup>[7]</sup> MATLAB can be used in other chemical engineering problems such as process dynamics and control, fluid mechanics, heat transfer, and chemical reaction engineering. With his student Zakia Nasri, Dr Binous has also performed similar computations using Mathematica.<sup>[8]</sup>

## CONCLUSION

We have shown through simple examples how one can take advantage of the numerical and graphical capabilities of MATLAB to perform properties estimation for pure com-

ponents and VLE calculations for binary mixtures. In addition, we have performed high-pressure chemical-equilibrium calculations. An example of an adiabatic flash computation was also presented. Similar computations were performed by the author using Mathematica.<sup>[9]</sup> These classic problems are junior- and senior-level study material at the National Institute of Applied Sciences in Tunis. The students excel in these types of problems despite the fact that they do not have prior knowledge of MATLAB and Mathematica.

## NOMENCLATURE

$a_i$	activity of species $i$ [bar]
$c$	number of components
$H^D$	departure from ideal enthalpy [cal/mol]
$k_{ij}$	binary interaction parameter
$K_i$	equilibrium constant
$P_{c,i}$	critical pressure [bar]
$P_{r,i}$	reduced pressure
$P^{\text{sat}}$	vapor pressure [bar]
$R$	universal gas constant [cal/(mol. K)]
$T_{c,i}$	critical temperature [K]
$T_{r,i}$	reduced temperature
$x$	liquid mole fraction
$y$	vapor mole fraction
$Z$	compressibility factor

$z$	mole fraction in the feed
$v_i$	stoichiometric coefficient
$\phi$	vapor phase fraction
$\phi_i, \phi_v$	fugacity coefficients
$\omega$	acentric factor

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# IDEAS FOR CREATING AND OVERCOMING STUDENT SILENCES

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**F**ifty minutes of teacher talk with passive student listening is relatively ineffective in developing student learning. By creating silences, teachers can encourage productive, active, student learning. Likewise, by overcoming silences, students can change from passive listeners to active talkers/discussers of their learning.

In this paper we consider creating and overcoming silences. Ideas are given for creating silences for individual active activities and creating silences, via wait times, to provoke facilitated class discussion. Then suggestions are given on how to overcome student silence via peer discussion and on overcoming the silence between teacher and students. But first consider the research upon which these ideas are based.

## 1. RESEARCH BASIS FOR CREATING AND OVERCOMING SILENCES

The fundamental research for creating and overcoming silences is extensive and is related to Chickering and Gamson's<sup>[1]</sup> summary of seven features to improve learning, Ramsden's<sup>[2]</sup> research on developing deep learning, and the concept of 20-minute student attention spans.<sup>[4-7, 9-12]</sup>

Chickering and Gamson<sup>[1]</sup> suggest that the seven ideas to improve student learning are: 1) prefer active to passive; 2) prefer cooperation to competition; 3) use clear time-on-task; 4) expect success; 5) have good teacher-student interaction;

6) provide prompt feedback; and 7) account for individual student-learning preferences. Ramsden's<sup>[2]</sup> research suggests that deep learning is promoted by good teaching, clear goals and standards of assessment, an emphasis on student independence, a social climate fostering good relationships among the students, openness to students, and vocational relevance, while negative impact results from a heavy workload and a large amount of formal lecturing without freedom for individual or group study. Hake's<sup>[3]</sup> research—comparing the performance on standardized, validated tests of 6,000 first-

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year physics students, some of whom received interactive engagement activities in class vs. some that received traditional lecture—showed that students who received interactive-engagement learned twice as much as those receiving traditional lectures.

After 20 minutes of teacher talk, boredom sets in, and student recall of information presented after 20 minutes is greatly reduced.<sup>[4-7, 9-12]</sup> Indeed, Liebman<sup>[13]</sup> suggests that the attention span is as low as 8 to 10 minutes. McKeachie<sup>[14]</sup> reports that immediately after 50 minutes of straight teacher talk, students can recall about 70% of the content presented in the first 10 minutes but only 20% of the content in the last 10 minutes. To overcome this and to improve student learning, after 10 to 20 minutes of teacher talk, instructors can introduce activities to engage students actively in the learning process. Prince<sup>[15]</sup> reviews such options. Two ideas for active learning that are the focus in this paper are, 1) to use silence for individual student activity related to their learning; and 2) for the teacher to remain silent and allow wait time and then facilitate class discussion. Such activities also apply some of the Chickering-Gamson<sup>[1]</sup> principles to improve learning: using active instead of passive, using cooperation instead of competition, providing prompt feedback, and providing clear time-on-task.

Ramsden's<sup>[2]</sup> research has shown the importance of the social climate in the class on the development of deep learning. Ideas presented in this paper address how to develop a strong social climate in class and how to improve the quality of teacher-student interaction.

In section 2, we consider how to create silences for individual work. In section 3, we explore creating silences, or wait times, as a prelude to full class discussion. Then in section 4, ideas are given for overcoming student silences via peer activities and, in section 5, overcoming silences between teacher and students. Finally, in section 6, a measure of the effectiveness of these approaches is given. Each is considered in turn.

## 2. CREATING SILENCES FOR INDIVIDUAL WORK

After 20 minutes of teacher talk, instructors can create silences by asking students to do individual work such as writing reflections (section 2.1), solving a problem (section 2.2), or answering a test question (section 2.3).

### 2.1 Writing reflections

A **reflection** is a comment about what has been experienced in the past: knowledge, attitudes, feelings, or reactions to what was done or felt. The reflection could be free writing, prompted free writing, or perhaps a structured checklist. Here are some example details about the format and the timing.

Format: For prompted free writing, provide lined worksheets that have a title and a place for name and date. Table 1 is an example. This may include a prompt that can be given verbally or can be written on the form. Example prompts include:

*“I discovered...”*, *“The most important idea was . . .”*, *“The most interesting idea was . . .”*, *“Now I realize that . . .”*. The prompts could stimulate: a comparison of the present experience to past experience (corresponding to revised Bloom's cognitive taxonomy level 2 understand)<sup>[15, 16]</sup>; an evaluation of the experience (revised Bloom's level 5); a creation of something new based on the integration of past and present experience (revised Bloom's level 6<sup>[16]</sup>); or attitudinal comments and change (Krathwohl's attitudinal taxonomy level 4<sup>[17]</sup>). As a side note, for the cognitive domain, Bloom, *et al.*,<sup>[15]</sup> published a taxonomy or structured list representing increasing level of difficulty in learning in the cognitive domain. This has been revised by Anderson, *et al.*<sup>[16]</sup> Such a classification is extremely helpful in analyzing the degree of difficulty expected in a task. For example, on an exam students should be given a chance to demonstrate an ability to do tasks of varying levels, rather than assigning only tasks at Bloom's level 6. Similarly, students can use such a taxonomy to monitor their growth. For the affective domain, a similar taxonomy has been developed.<sup>[17]</sup>

A further example of a prompted format, applying Bloom's level 5 evaluate, is a listing of the topics plus a rating for each. An example is given in Table 2.

Another example of a prompted format (that combines Bloom's levels 2, 3, and 4—understand, apply, and analyze) is Larkin's checklist format in the context of physics.<sup>[18]</sup> In this example, the reflective tasks

TABLE 1 Example Reflections		
Reflection	Name _____	Date _____
<i>“Now I realize that . . . I need to study the text before I come to class. I thought I could pick up most of the ideas from lectures but in this course I need to come to class prepared.”</i>		
Reflection	Name _____	Date _____
<i>“I discovered that . . . you can't push on a rope. This sounds simple, but I now realize this really helps me to solve pulley problems.”</i>		

are to write down an equation, and then, for each symbol, identify its kind (number, vector, tensor), the sign and direction, the units, the typical magnitude, and the meaning in words. Students are also asked to compare each concept with other similar quantities with which it might be confused.

Timing: two to three minutes; be specific:

*“Please take out the reflection worksheet and write reflections for the next two minutes. For this reflection, please use the prompt ‘I discovered.’ Any questions? OK, time is running. Quiet please.”*

### 2.2 Individual problem solving

Individuals are asked to solve a simplified problem. Usually we design the problem to test the student’s comprehension of the most challenging parts of a concept. An example might be to plot, on log-probability paper, some particle-size data and determine the geometric average and geometric standard deviation. Instead of giving the students 50 data points, however, only two data points are given so that the task can be done within the allowed two minutes. The timing and instruction details are the same as for reflections, described above.

### 2.3 Individual response to test questions

An example of this approach is used by Mazur.<sup>[11]</sup> Instead of formally talking at the beginning of class time, Mazur posts reading that the students are expected to do before class. In the first activity each student is silently to solve multiple-choice questions. The time allowed is one minute. The test can be projected onto a screen.

All of the three examples listed require that the student silently does the task alone. What options are available to provide closure for this individual activity, or, is closure needed?

In our experience, closure is indeed needed. After any of these silent activities, three actions can be used.

A first action is to share the experience. Whenever students are given an individual task, we have found that most want to tell someone about the activity. Two options include: a) a leader summary where the teacher asks for feedback from the students and records ideas from students, which usually takes about 10 minutes of class time for a class of 30 because most students want to ensure that their ideas are noted by the instructor; b) ask students to *“Turn to a neighbor and say ‘That was an interesting activity because . . .’ and talk to your neighbor for the next 90 seconds. You need not share what you wrote. You may be more comfortable talking about the ease with which you did the task. Any questions? OK, noise level up.”* For the problem-solving or test activity, the prompt might be *“Convince your neighbor that your answer is correct.”* This provides prompt feedback to each because the instructor can a) provide the correct answer and then have further peer dialogue; b) collect responses to the questions (via clickers, or a show of hands) and then elaborate on the correct answer and the reasons why one might mistakenly select the other answers. In collecting the responses, do not stop after the “correct” answer has been received. Rather, continue with a prompt such as *“OK, we are collecting answers, what other answers are there to this?”* Or *“Are you sure we have all the possible answers here?”*

A second action is to follow this activity with applause. Applause helps to close the activity; applause suggests that this is a desired classroom activity, and encourages students to come prepared for class, and to do the individual activity

Rate the ideas	Already do this	Would work	Might work	Not my style
Create silences for individual reflections				
Create silences for individual activities				
Create wait times after posing questions				
Overcome silences for diad “Turn to a neighbor..”				
Overcome silences for diad TAPPS				
Overcome silences with small group activity				
Use ombudspersons				
Use written feedback at the end of each class				
Ask them to reflect in class				
Know the names of your students				
Overcome silences between you and students				
Other _____				
What conclusions do you draw from your responses?				

***Instruction is a two-way street.  
Teachers should seek feedback  
throughout the semester about the  
quality of the teaching/learning.***

---

to the best of their ability. Applause nurtures even the wrong answers being presented.

A third activity is to collect, mark, and return the written responses to the students or to ask them to use this as evidence in a weekly reflective journal in which they self-assess their learning journey. Suggestions about self assessment via reflective journals are given by Woods and Sheardown.<sup>[19]</sup>

Creating silent times for individual student activity is an excellent “active” addition to the classroom.

### **3. CREATING SILENCE TO NURTURE FACILITATED FULL-CLASS DISCUSSION**

An approach to encourage active learning in the classroom is for the instructor to pose a question and solicit student response and a “lively discussion” from a “full class” of about 30 students. (If the class is larger than 30, then a large class—of say 200—can be divided into groups of about 30 so the instructor engages in discussion with one particular group at a time.)<sup>[20, 21]</sup> When an instructor poses a question to prompt classroom discussion, inevitably the students know that if they are silent, the instructor will answer his/her own question. To combat this, after a question has been posed, allow a silent wait time. How long is a wait time? The research evidence is not clear. Rowe’s research<sup>[22, 23]</sup> identified a wait time of 1 second. Whitman and Schwenk<sup>[24]</sup> discuss using a wait time of 3 to 5 seconds. Woods, *et al.*,<sup>[9]</sup> talk of a wait time of 30 seconds. Gedalof<sup>[20]</sup> suggests 7 to 10 seconds. Huntsberger<sup>[25]</sup> distinguishes between a 3- to 7-second wait time (if the question is addressed to an individual) and a wait time of “several minutes” (if the question is asked to a group in general). Rogers<sup>[26]</sup> notes that an average wait time faculty allow is 2-3 seconds. Increasing wait times will significantly increase the number of student responses and Rogers says that the literature actually suggests 17 seconds as the optimal wait time. Rasmussen<sup>[21]</sup> recommends a wait time of 10 to 15 seconds. Whether the wait time is 1 or 30 seconds is not the issue. The importance is to recognize and cope effectively with the phenomena “as a question poser.” Here are some options. Explain that often when a question is asked that the students know if they are silent that the teacher will rephrase the question or answer the question. One might say “*I really want you to think about and answer the questions I pose. There will be a silent wait time to give you a chance to create a response to the question. I really want to gather ideas from you.*” Then, when an answer or response comes in, acknowledge it by writing it down and with applause. Continue gathering ideas beyond

the right answer. Do not criticize the ideas when they come in. Gather the student’s ideas. If no student response is given after a wait time of 20 to 30 seconds, then invoke “*Turn to a neighbor and say ‘How would you respond to this question?’ Noise level up for 2 minutes.*” Then at the end of two minutes say “*Please share with us what you talked about.*”

### **4. OVERCOMING STUDENT SILENCES TO USE STUDENT/STUDENT INTERACTION**

An effective learning environment engages students actively in the learning, uses cooperation not competition, provides prompt feedback, and creates a good social climate. After 20 minutes of teacher talk or when the students seem confused or their eyes glaze over, ask pairs of students or small groups to talk. The talking should be on task. For diads a useful prompt is “*Turn to your neighbor and say . . .*”

- ‘*Did you understand that?’*”
- ‘*Summarize what’s happened so far.’*”
- ‘*Do you believe that?’*”
- ‘*The key point so far is . . .*’”
- ‘*A practical application of this stuff is . . .*’”
- ‘*Let’s compare lecture notes that we have taken so far . . .*’”
- ‘*So what’s that all about?’*”
- ‘*Please explain that to me in simple terms.’*”

Instead of using diads, a small group of three to five students could be used. The size is dictated mainly by the classroom configuration. If the students are unfamiliar with group discussion, the talking-stick approach can be used. An object, such as a stick, pen, or paper, is given to the speaker, who talks briefly and then passes the stick to the right so that, in turn, all have a chance to talk. If one prefers not to talk, they can pass. The ground rule is that only the person holding the stick can talk at a time.

Diads could also solve problems using the Whimbey Talk Aloud Pairs Problem Solving, or TAPPS. Here each person has a specific role. One person plays the role of the talker/problem solver: Verbalize thoughts, focus on being accurate (instead of rush! rush! time pressures), have clear communication so that others can follow and understand—this is the role of the talker/problem solver when given a written problem statement. The other person plays the role of the listener; his/her role is not to solve the problem, but to encourage verbalization, to encourage a focus on checking and double checking, and to ensure that he/she comprehends the other’s approach. The listener is not to correct or make value judgments about the other’s efforts. Typically this activity would last 5 to 15 minutes. Then, each should write out reflections about what he/she discovered. Brief diad discussion of the process is useful. Then, the people reverse roles. Feedback forms can be used to help each see how the roles are being played. More is given by Woods.<sup>[27]</sup>

## 5. OVERCOMING SILENCE BETWEEN INSTRUCTOR AND STUDENTS

Two basic ideas are given: how to break the silence to get feedback about the learning and how to establish connections with students to improve the social climate.

### 5.1 Overcoming silences to monitor the quality of the teaching and learning

Instruction is a two-way street. Teachers should seek feedback throughout the semester about the quality of the teaching/learning. Some options include the use of class ombudspersons, clickers, red cards, half-minute papers, and a wide variety of ideas given by Angelo and Cross.<sup>[28]</sup> Ombudspersons are a team of volunteers from the class who provide feedback to the instructor throughout the year about the quality of the teaching and learning. Clickers refers to a method to receive anonymous response to questions via audience response systems, referred to as clickers.<sup>[29]</sup> In red cards, each student is given a display card that they can hold up whenever they are confused. A half-minute paper asks students to anonymously respond to such questions as "What was the muddiest point in this class? What was the most important point?" The papers are then collected to provide feedback to the teacher about that particular class.

### 5.2 Overcoming silence between students and instructor to improve the social atmosphere

Here are ideas on how to improve the social atmosphere and to have quantity and quality time between faculty and students: know and call students by name; celebrate their successes; help them network with visitors to the department, including seminar speakers; critique their resumes; build trust and be willing to confidentially hear about their concerns and personal problems; personalize feedback on assignments; come early to class and stay late; take time to chat in the hall; walk with them between classes; attend events that they think are important and where you are comfortable (such as convocation and the iron ring ceremony for engineering students); create special events (such as a Christmas carol sing-song with a class band); invite them to your home; and be willing to share personal experiences, attitudes, and values. Invest time in explaining your role and their role in the teaching and learning process. This includes explanations in the course syllabus/outline and time spent in class explaining your choice of learning environment. Here is an example from a course syllabus:

*The process of teaching and learning is a two-way street. I want you to do well and succeed in the course and in your career. Here is what you can expect from me: clear indication of the objectives, support and encouragement, sharing of experience, prompt feedback, respect and trust, response to your suggestions, and a caring environment in class. Here is what I expect from you: participation and success in all activities, feedback on how best I can help you, helping to create a caring environment in class, and respect and*

*trust in me and your colleagues. In this class I use ombudspersons to provide input about how best I can create the best learning environment for you.*

In another example, there was a dramatic improvement in student performance in problem-based learning when up-front explanation and preparation time for this new learning environment was increased from two hours to six hours.<sup>[30]</sup>

In summary, many simple things can be done to break the silences between students and teacher.

## 6. EFFECTIVENESS OF THESE APPROACHES

We have used these approaches in our classes for the past 15 years. One measure of effectiveness is to compare the student response to the Course Perceptions Questionnaire (developed and validated by Ramsden<sup>[2]</sup>) for straight lecture-style courses vs. student response to our courses that use silences as described in this paper. For straight lecture-style courses the responses were 18 to 20 whereas for our courses the responses were 28 to 32. A larger number is desired.

## 7. SUMMARY

Silences can be created to allow individual students to actively engage in reflection and adaptation of new ideas. Silences, or wait times, should be created after a teacher poses a question to the class. Such wait times encourage students to participate in discussion instead of waiting for the teacher to answer his/her own question.

Silence between students can be overcome by using a variety of diad and small-group activities in class to actively engage students in the learning process. Ideas are given on how to overcome the silence between students and faculty.

Research evidence supporting these suggestions is given.

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# USE OF ENGINEERING DESIGN COMPETITIONS

## *for Undergraduate and Capstone Projects*

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Providing high-quality undergraduate education is the goal of any engineering school. As part of this, the use of final-year design projects or capstone projects is a useful tool to engage students and enhance the undergraduate experience. At the University of Waterloo Department of Chemical Engineering many engineering students choose to do design projects and capstone projects as part of their involvement with various technical competition teams. Recently, many team entries have included hydrogen fuel cell technology such as “Challenge X—Crossover to Sustainable Mobility,” a competition sponsored by GM, the USDOE, and Natural Resources Canada, in which students designed and built a full-size hydrogen fuel cell vehicle. Students have also entered into the H2U Hydrogen Facility Design Competition sponsored by the U.S. National Hydrogen Association as well as others. Although all of these design competitions are multidisciplinary and involve members from all departments and other faculties, chemical engineering students have typically held leadership roles because of the applicability of the competition subject matter. Further, faculty advisors have also come from the Department of Chemical Engineering.

Undergraduate design projects and upper-year capstone projects offer many valuable benefits to students. As well as being an opportunity for applying concepts learned during

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a student's previous classes, these projects are also used by many schools to help the students develop "soft skills" such as leadership, communication, and project management.<sup>[1-2]</sup> Studies of undergraduate research, which shares many similarities with design work, found that students were able to develop professionally by acquiring research and other technical skills. They were also able to gain a greater sense of what science and engineering research work entailed, which changed their attitudes toward such work and helped clarify career plans. A separate survey study by Kardash<sup>[3]</sup> echoes some of the above points. This study was able to further detail the skills gained by undergraduate researchers, finding that the ability to understand concepts in one's field, observe and collect data, and write a research paper all improved after the research experience. Making design projects available to first-year engineering students is thought to lead to lower attrition rates since students can see the applicability of course material which they may otherwise characterize as "boring."<sup>[4]</sup>

Technical competitions can also provide the framework for design projects. Competitions, such as the Chem-E-Car competition, involve a significant design and analysis component<sup>[5]</sup> and can be complemented with presentations and reporting to also encourage development of communication skills. A study by Padgett<sup>[6]</sup> found that when a design competition is used, student motivation can be very high and it is believed that undergraduate education may improve through a better retention of course concepts. Further, students learn team-building skills<sup>[2]</sup> and younger students have been observed to develop an interest in undergraduate research after participation.<sup>[7, 8]</sup>

There are also benefits to participating professors and graduate students. Faculty and graduate students who serve as supervisors for undergraduate researchers gain valuable mentoring experience that can be later translated to other jobs.<sup>[9]</sup> Some of the challenges with undergraduate research include extra start-up time and effort required. Also, since students come from a variety of different backgrounds their abilities can be varied. Undergraduate schedules tend to be variable as they attempt to balance lab work as well as social lives, schoolwork, and exams. Thus, work output and motivation can be variable.<sup>[3]</sup> Further, graduate students involved as mentors will have less time to focus on their own thesis work.

This paper will examine the benefits and challenges of using competitions for undergraduate design projects and upper-year capstone projects through the use of a case study of students participating in the Hydrogen Ambassador Competition. Experiences as they relate to undergraduate and graduate students, as well as faculty advisors and the department and faculty as a whole, will be explored from the perspective of the authors—one of whom participated as a graduate student and the other as a faculty advisor—as well as from surveying undergraduate student participants. The aim is to show that the use of competitions can benefit all parties and is worth the extra effort.

## CASE STUDY BACKGROUND—HYDROGEN FUEL CELL UNDERWATER DIVER PROPULSION

In 2005 a Hydrogen Ambassador Competition was announced as part of the Hydrogen and Fuel Cells Exhibit at the Hanover Fair, one of the largest trade shows in Germany. The goal of the competition was to develop an idea for the commercial use of fuel cells in an application that could be developed and marketed today. If accepted, the idea and any prototypes could be shown at the 2006 Hanover Fair. The project began with three students—two graduate students from the Department of Chemical Engineering and a 4th-year student from the Department of Electrical Engineering who was going to use the competition submission as a capstone project. These students formed the core of the team and together they developed the idea of entering a fuel cell-powered diver propulsion vehicle. A diver propulsion vehicle is any kind of external propulsion aid for an underwater diver. Over the course of the project a number of other ChE undergraduates were added to the team to complete the project, which also extended to other events beyond the Hanover Fair.

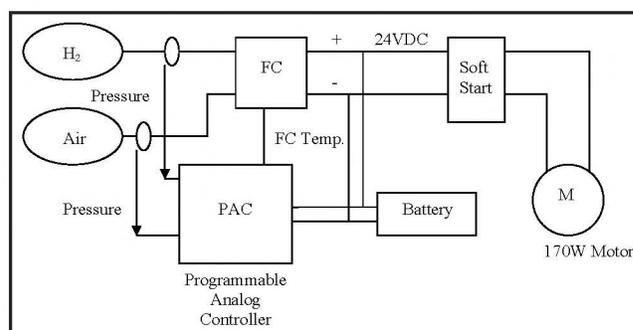


Figure 1. Overall fuel cell DPV system.



Figure 2. Completed prototype of the fuel cell-powered diver propulsion vehicle.

The design of a fuel cell-powered diver propulsion vehicle (DPV) involved many technical challenges for the students participating. The main thrust of the project was to take an existing battery-powered DPV and replace the battery with a fuel cell while keeping the same size and basic functionality of the unit. A fuel cell is an electrochemical device similar to a battery. Unlike a battery, which contains a finite amount of reactants, a fuel cell can be continuously supplied with reactants and therefore theoretically generate electricity for as long as a user may want. The benefit of using a fuel cell in the DPV is that it would have near-instantaneous refilling times as compared to the 8-hour recharge times of the battery, and offer longer range. Some of the impediments are that the weight is higher and the cost is significantly higher at the current stage of fuel cell technology development. Nevertheless, such a product would certainly be accessible for wealthy diving enthusiasts or military interests.

To acquire the necessary materials to develop a prototype, team members contacted manufacturers of stock DPVs and fuel cells. A DPV was obtained from DAKA corporation and a fuel cell stack from Hydrogenics corporation. The fuel cell was sized to meet the requirements of the DPV motor. To fund the rest of the project, and to assist in travel funding, group members submitted proposals to an undergraduate engineering endowment fund (Waterloo Engineering Endowment Fund — WEEF), and sought financial support from the Department of Chemical Engineering, Department of Electrical Engineering, and the Dean of Engineering's office. Materials, fittings, and other equipment were also used from the faculty advisor's research lab, and the faculty advisor also provided funding for smaller components.

Figure 1 is a schematic of the fuel cell system that needed to be designed. It includes features such as compressed-air and hydrogen reactants, pressure sensors, DC/DC converters, an electrical control system, temperature management, and safety features, as well as other auxiliary systems. Component selection and packaging was possibly the most challenging aspect of the project since components needed to not only be suitable for the demands of the fuel cell system but also fit into the same space occupied by the battery in the DPV. This involved extensive design work and the fabrication of several frames and mounts. The design of the control system was also a challenge since functionality of the system and safety considerations were of importance. Finally, the testing work was centered around evaluating the fuel cell stack received from Hydrogenics as well as creating testing apparatuses for the fuel cell system at different levels of development. Although this task was not as challenging technically, it required many practical electrical, mechanical, and workshop skills as well as experience with compressed gasses, specifically hydrogen.

Ultimately, the final prototype shown in Figure 2 was exhibited at the fuel cell exhibit at the Hanover fair. This included a small booth in the same area as other hydrogen ambassador

***When surveyed, undergraduate competition participants highlighted the hard and soft skills gained through participation as part of the positive benefits. Technical skills such as programming and building hardware as well as gaining experience with new technology were specifically mentioned as were soft skills such as project management and oral communication skills.***

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competitors and fuel cell companies as well as a live interview on the main stage. While at the fair, government officials also toured the booth for the DPV and the project was also featured on a number of fuel cell and hydrogen-related news Web sites. The project was also presented as a poster at the Toronto Green Energy Fair at the University of Toronto and was featured in a University of Waterloo Faculty of Engineering *Annual Report*, which is read by alumni.

## **BENEFITS AND CHALLENGES**

### **Undergraduate Experience**

The hydrogen fuel cell DPV project for the Hydrogen Ambassador's Competition had many of the characteristics essential to creating a positive undergraduate design experience for both younger undergraduate and final-year capstone project participants. It should be noted here that undergraduates receive no extra credits for participating in the competition and students doing capstone projects within the competition are only marked on their selected design project and not on any extra work that they may also do.

Over 35 participants from several competitions including the Hydrogen Ambassador Competition were surveyed. They were asked to reflect on the perceived benefits and challenges of working on a project centered on a competition as well as to give their opinions on how the project work for a competition differed from project work done for credit. A list of the questions and typical responses is provided in Table 1 (next page).

First, the organizational structure of the team was particularly well suited to meeting the needs of all the undergraduate participants. The graduate students at the core of the team were able to supervise the overall project and day-to-day lab activities, and to divide tasks among all the students. This provided necessary control for safety aspects, as well as the ability to teach necessary technical skills to the undergraduates. Furthermore, the tasks themselves could be divided to

**TABLE 1**  
Survey Questions and Typical Responses

Question	Typical Responses
Were the projects that you did with the team technical in nature? Did you apply concepts learned in courses?	Projects were mostly technical in nature and related to the design and building of components. Tasks also extended to economic analysis and public outreach. In all technical and economic cases, course concepts were applied.
Were team projects organized and did they have clear objectives? Could projects be completed in a school semester?	Due to the structure of the competitions there were clear objectives that each team was required to meet that enhanced the organization of tasks. Since the teams themselves designed the tasks to meet the objectives, they could usually be completed in the required time frame.
List some of the main benefits of participating on a project team for competition.	Respondents benefited from experience with new technologies, job opportunities, development of new skills, and the acquisition of real-world experience.
List some of the main drawbacks of participating on a project team for competition?	All respondents unanimously identified the large time commitment involved as a drawback since it takes away from time needed to spend on classwork.
Is participating on a project for a competition different from other noncompetition projects?	Survey respondents all thought that competitions were different. They generally thought that projects for competitions had more stringent deadlines, real consequences to failure, and that the idea of winning was highly motivational and lacking in other class-based projects.
What skills have you gained from your experiences?	Technical skills: CAD, fuel cell system design, mechanical design, electrical design, system controls, computer programming. Nontechnical skills: time and project management, teamwork, marketing, oral and written skills.
Did you receive any academic credit?	The majority of respondents received no academic credit, 14% participated as part of a capstone project.
Did participation increase your appreciation for engineering?	All respondents agreed that their appreciation for engineering had increased.

meet the needs and interests of the individual students. Undergraduate participants generally wanted more experience with hands-on aspects of the project, and had a great desire to actually work with the fuel cell technology. Undergraduate could therefore be given “mini” projects such as the design and fabrication of tank mounts, hydrogen management components, the sizing and selection of components, or the testing of the system. These projects had a very narrow scope and could be done in the allotted time and around the undergraduates’ other commitments. When surveyed, undergraduate competition participants highlighted the hard and soft skills gained through participation as part of the positive benefits. Technical skills such as programming and building hardware as well as gaining experience with new technology were specifically mentioned as were soft skills such as project management and oral communication skills. Finally respondents also described being exposed to a multidisciplinary team as a positive benefit.

Undergraduates using the project as the basis of their capstone project also had a positive experience. As a requirement, capstone projects had to be broader and more complicated than the projects given to younger, undergraduate participants; this was easily accommodated. One such project was performed by a core team member who focused on the design and setup

of the DPV control system. This applied skills in detail control system development as well as hardware selection and integration. Other capstone projects included the design and construction of a hydrogen management and water knockout system, and testing of the fuel cell systems. All students were also involved in the overall project design, sponsorship recruiting, and testing. Once the initial events associated with the project were complete, other projects such as further design iterations of the control software were initiated. These projects were also of sufficient size and scope to be used as capstone projects for students even after the completion of the original competition.

There were certain benefits that were unique to the use of a competition for undergraduate design projects apart from the obvious travel to the Hanover Fair—although the potential for travel to an international conference was certainly a very strong motivator for participants in this competition. Through the fund-raising activities students had an opportunity to interact with members of undergraduate funding organizations, departments, and the Faculty of Engineering and thus develop communication and project-management skills, as well an introduction in dealing with media organizations. The experience of being part of a competition with real awards and recognition was also a much more satisfying experience than

capstone projects which only lead to academic credit. This was primarily because of the unique experience of teambuilding and camaraderie that comes from competing and winning as a group. The competition aspect also adds more “flair” to the project, and creates a better and more memorable experience. Survey respondents described these real rewards, the desire to win, and tangible consequences for failure as a positive motivating force that was not present in other design projects for credit. Many students desire exposure to new and innovative technologies, and in this case being able to work with a hydrogen fuel cell stack provided this experience. Therefore students generally applied themselves more and hence were able to gain more from the academic experience.

Despite the many benefits of the project there were several challenges when applying this particular contest to undergraduates. Only a certain type of student is capable of carrying out the projects. As indicated by Smith,<sup>[10]</sup> the participants must be more driven and resourceful and be able to work in a diverse team with more of an organizational structure as compared to smaller group work. Since the scope of the project as a whole was large, the most successful students were those who could work independently *and* on a team, simultaneously. From the perspective of undergraduate participants, the most common challenge was that time spent on the competition project meant less time spent studying as well as challenges when transferring work from one participant to another. The timeline of the competition was also a concern in this case study, as initial proposals for the Hydrogen Ambassador Competition were required before the official start of capstone projects (this was one reason why graduate students initiated entry into the competition). Also, undergraduates were challenged by missing a week of classes to attend the conference during the school term.

### **Graduate Experience**

The graduate experience in the project was also unique. Since the project was initiated with a team that included graduate students, there were ample opportunities to develop leadership and project-management skills. Also, some of the tasks required increased focus and skill that normally only a graduate student with more experience would possess. One of the challenges of participation was that the competition was not an extension of a specific student’s research project, but was instead a side project with limited prospects for academic credit or recognition in the realm of research. As such, many of the benefits from the participation depended on the value that the students attributed to them. For the graduate students involved in the DPV project the extra work created by the project was offset by the travel opportunity to Germany and participation in an industry-focused international conference in the fuel cell field. The graduate students also benefited from increased exposure to the department and faculty, which eventually lead to participation in the *Engineering Annual*

*Report*. Most importantly, the graduate students benefited from having a separate experience from their thesis work, which added value to their resumes and increased their marketability in the workplace. In this case participation in a system-integration project provided a broader understanding of fuel cell engineering and the challenges associated with fuel cell engineering.

### **Faculty Advisor and Departmental Experience**

From a faculty perspective it can be difficult to see the benefits to supporting students in a competition of this nature, especially graduate students since there is little value added to specific publishable research. Undergraduate design projects can sometimes assist specific research projects in the lab simply by providing extra labor. With projects based on competitions, however, the goals of the design are often separate from the research interests of the advisor. As such, one challenge is the time commitment needed to help manage the project as there is little recognition in merit reviews and no teaching relief to the advisor. Nevertheless there are many reasons to participate.

If the professional development and education of both undergraduates and graduate students is valued then participation in the Hydrogen Ambassador Competition had many benefits. The most important one was that the educational experience of the student team members was enhanced. A project of this nature excites undergraduates and thus assists in graduate recruitment and placement of graduates in the industry. Of the students involved with the DPV, two were already graduate students with fuel cell-related research; one went on to work in the fuel cell industry, a second went on to graduate studies in fuel cell research, and another continued graduate studies in the green energy field (other members are still continuing their undergraduate education). Another benefit was that the prize of going to the fuel cell exhibit within the Hanover Fair placed the lab in a high-profile industry event that allowed for increased exposure of the lab and its research aims to potential industry partners. A final benefit is that the DPV platform can be used for future capstone projects. This is important because often there is little budget to support capstone projects and thus project with high equipment costs are generally not feasible. Ultimately it becomes a decision based on what values faculty advisors have and what role they feel they play in the education of their students.

At the departmental and faculty level the main benefits for financially supporting the participants of this project is the increased international exposure of the institution. For this project in particular, the exposure was at a trade show where potential student co-operative education employers would be present, and thus able to see the quality of work by students at the university. To this end the participants also distributed information about the Waterloo engineering program and co-operative education program at a display booth. New students

to both the graduate and undergraduate program often comment that their university decision was based on exposure to one of the student team projects at some event.

## CONCLUSIONS

This paper has shown that engineering design competitions can be effectively used as an educational tool to give undergraduate students project design opportunities as well as used for capstone projects. The use of competitions meets all the requirements of a good project, and provides a valuable interdisciplinary experience. For the DPV, the projects had focused topics with clear objectives and gave students experience with an exciting technology. The project had a large-enough breadth to accommodate a number of students, adequate possibilities for true partnership among all the participants, and potential for completion within a reasonable time frame. There were also many benefits for graduate-student involvement including the development of leadership skills and a wider exposure to the technology. For the faculty advisor, department, and faculty, support of this design competition provided a strong educational opportunity for a number of students as well as good exposure for the institution.

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# CHALLENGES IN TEACHING 'COLLOID AND SURFACE CHEMISTRY'

## *A Danish Experience*

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Seven years ago we were asked, as one of our first teaching duties at the Technical University of Denmark (DTU), to teach a 5-ECTS-point course entitled Colloid and Surface Chemistry. The topic is both exciting and demanding, largely due to its multidisciplinary nature. Several “local” requirements posed additional challenges. The course is part of the international program of the university, typically at the start of the M.Sc. studies (7th-8th semester) and can be taken by students of different M.Sc. programs (advanced and applied chemistry, chemical engineering, or petroleum engineering). B.Sc. students toward the end of their studies can also take the course. Also, due to the multidisciplinary nature of the course topic, a wide variety of industries in Denmark has shown interest in the course, which has led to development of a separate industry course.

In this article we report on our experience from the first years of teaching the course and how teaching methods and course material have been adapted to meet the aforementioned challenges, as well as feedback and course evaluation from students. First, we present the learning objectives of the course followed by a discussion of the teaching methods used over the years. The most challenging topics covered in our course are highlighted as well as a discussion of the textbooks employed. Supplementary initiatives (*e.g.*, link to a laboratory course) are briefly presented followed by our assessment of the current status and some suggestions.

### COURSE NATURE, CONTEXT, AND LEARNING OBJECTIVES

The time allocated for a typical 5-ECTS-point course at DTU is one four-hour block a week during a 13-week semester, followed by an examination. We have been during the last three years using the textbook of Pashley and Karaman<sup>[1]</sup> as part of the course material. Self notes from the teachers are

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also used; they are available to the students via the intranet system at DTU, called Campusnet. We have found it particularly difficult to find a suitable textbook that could fulfill the course requirements and be appealing to different audiences and the increasing number of students (Figure 1), and a discussion of the three textbooks used in the lifetime of this course is provided in Table 1. Further discussion on textbooks and teaching in Colloid and Surface Chemistry has been provided by Woods and Wasan.<sup>[11]</sup> The comments shown in Table 1 are based on the opinions of both the students and the teachers. We have, however, considered other textbooks as well,<sup>[4-10]</sup> but we have not found them suitable for our course.

The course is evaluated with a four-hour written “open book” exam (*i.e.*, all material available).

From the beginning of the academic year 2007-8, DTU adopted learning objectives as a standard part of all course descriptions in the course catalogue. The overall target of the course is to present to the students the most important principles and phenomena related to colloid systems and surface chemistry. These areas have important and extensive applications in the understanding and design of processes such as adhesion, lubrication, cleaning, enhanced oil recovery, and waste-water and air purification, as well in the understanding and design of products such as detergents, cosmetics, pharmaceuticals, polymer-containing items, and food. There are also numerous applications in nature, *e.g.*, fog, water droplets, and capillary phenomena.

The specific learning objectives of the course are for students to be able to:

- Calculate surface and liquid-liquid interfacial tensions with various theories
- Use different theories for estimating the solid-liquid and solid-solid interfacial tensions and employ them in wetting and adhesion studies
- Recognize the various mechanisms of adhesion and use various methods (Zisman’s plots, theories) for its assessment
- Describe the most important theories in surface chemistry
- Use the Gibbs equation for adsorption calculations

- Explain the creation of micelles (CMC) from surfactants and tell how CMC can be measured and how it depends on salt, temperature, and chain length
- Relate the adsorption in gas-solid and solid-liquid surfaces and use the Langmuir and BET theories for adsorption calculations
- Calculate the molecular weight and shape of colloidal particles
- Describe the most important (van der Waals and double-layer) forces between colloidal particles and their differences in relation to the intermolecular forces
- Explain the most important parameters in colloid force-theories (zeta potential, Debye thickness, Hamaker constant) and perform calculations with those
- Describe the DLVO theory for the stability of colloidal particles as well as compare the various mechanisms for steric stabilization
- Describe the stabilization mechanisms in emulsions (and foams) and design emulsions using various semi-empirical tools (HLB, Bancroft rule, etc.)

These learning objectives, which are presented using active verbs, focus on the abilities or competencies the students must possess after they have completed the course.

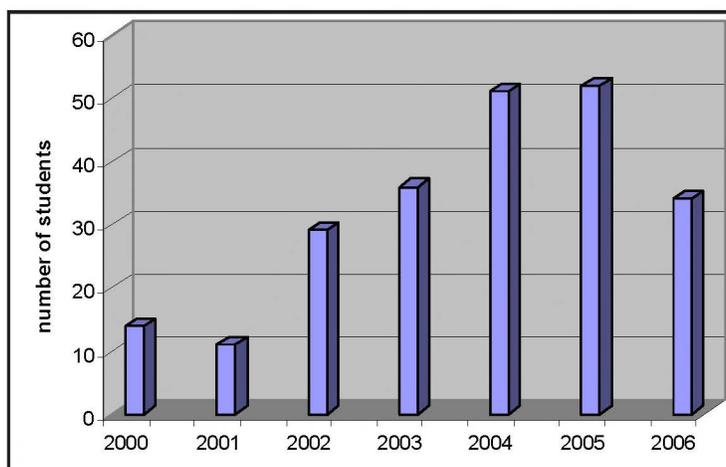


Figure 1. Students in the course over the years.

Book	Used in period	Comments by students	Comments by teachers
Shaw <sup>[2]</sup>	2000–2003	Detailed presentations. Boring layout. No applications.	Extensive presentation of numerous topics. Includes exercises—not worked-out problems. No presentation of modern theories for interfacial tensions.
Goodwin <sup>[1]</sup>	2004	Too condensed. Too high-level.	Advanced textbook, requires previous knowledge of colloids and interfaces.
Pashley and Karaman <sup>[1]</sup>	2005–2006	Somewhat too brief, no details; easy to read, though.	Very interesting industrial case stories and worked-out laboratory exercises. Does not include chapter on colloid particles characterization.

## CENTRAL TECHNICAL AND SCIENTIFIC TOPICS

Due to the multidisciplinary nature of the subject as well as the varying interests of the students, among other reasons, we have found it necessary from the start of the course to emphasize:

- (i) The applications of colloid and surface chemistry in various fields—especially chemical industry—including paints, adhesives and detergents, petroleum industry (especially the surface phenomena), materials with emphasis on polymers, cosmetics, agrochemicals, and food colloids (Figure 2)
- (ii) The links between the most important topics and concepts as well as their interrelations

One of the positive features of the currently used textbook<sup>[1]</sup> is the large number of “industrial stories” presented. The book, however, includes numerous applications “hidden” throughout the text and we felt it necessary to summarize those applications for the students.

We have found that presentations of key concepts and tools are extremely helpful in promoting understanding of the coursework as well as in assisting in practical applications. Equally useful is a summary of the key equations, considering the variety of topics covered.

The key concepts of broad importance covered in the course are:

1. The estimation methods for surface and interfacial tensions, especially theories for the latter based on intermolecular forces and their applications to wetting and adhesion

2. Distinguishing between “general” laws and concepts and theories-specific equations, but also a demonstration of the major applications of the general laws especially of surface chemistry
3. The equivalency interrelation of the Gibbs adsorption equation with the adsorption theories and two-dimensional equation of state (surface pressure-area plots)
4. The structure-property relationships in surfactants and the complexity of the various factors affecting micellization and the value at CMC
5. The similarities/differences (both in terms of physics and equations) of the adsorptions at various interfaces: gas-liquid, liquid-liquid, liquid-solid, solid-gas, and how information from one type of interface, e.g., solid-gas, can be used in analyzing data in liquid-solid/liquid interfaces
6. The complexity of adsorption on solids—differences between gas, surfactant, and polymers
7. The complexity of solid surfaces and cautiousness needed in the interpretation of wetting-adhesion phenomena
8. How a variety of properties/measurements for colloidal particles (kinetic, optical, rheological) can yield important information for the particles—especially their molecular weight and shape
9. The similarities but also important differences between intermolecular and interparticle/surface forces
10. The essential concepts of the electrical and van der Waals forces between colloid particles—especially zeta potential, double-layer thickness, and Hamaker constants
11. The DLVO theory for colloidal stability, how

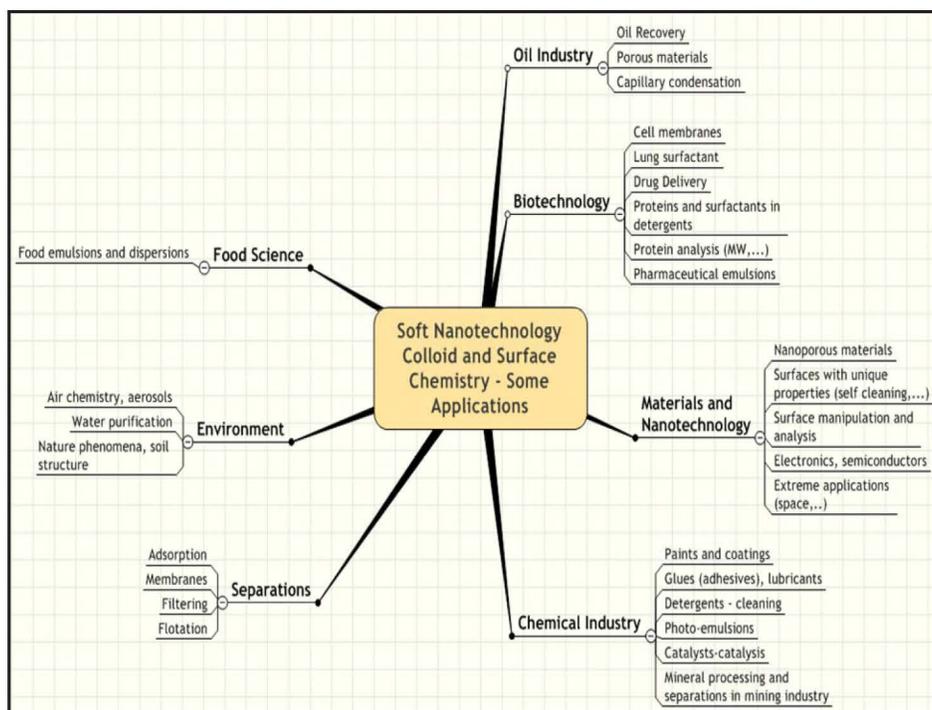


Figure 2. Selected applications of Colloid and Surface Chemistry.

stability can be modified (qualitatively), and the “other” non-DLVO stabilization mechanisms due to hydration and steric forces; a bit on kinetics of aggregation

12. Basic tools for studying emulsion stability and link to DLVO

In addition, in a short course with emphasis on applications we have found it difficult to include lengthy derivations such as those in surface thermodynamics (for the Gibbs adsorption equation) and those related to charged interfaces. The final results were, of course, thoroughly discussed also via numerical examples exercises, both in the classroom and homework problems. Table 2 shows the various types of exercises used, fulfilling different goals, covering aspects from very simple, straightforward demonstrations all the way to more complex synthetic problems—including a few inspired from industrial applications and projects.

## TEACHING METHODS

The weekly 4-hour segments for a 5-ECTS-point course at DTU present a challenge but also a gift for planning the learning activities. Obviously it is impossible to give a straight 4-hour lecture. On the other hand, the sessions offer the opportunity to spend time with students and incorporate more dialogue and interactive learning activities, where the students will become active participants and not simply passive listeners (as in a traditional lecture). We have experimented with different teaching methods in this environment and have arrived at the conclusion that variation and mixture of various methods can give a positive learning environment. It is very important, however, to explain to students what to expect, because unnecessary roadblocks to learning occur when student expectation is not met. In the following section we discuss various elements which have been tested in our teaching of this course.

**TABLE 2**  
Different Categories of Exercises Used in Class or Homework Problems

Exercise Category	Some Examples
1. Simple calculations; Demonstrations based on few experimental data	Adsorption from solution—role of solvent • Competitive adsorption of surfactants on solids • Vapor pressure of droplets via the Kelvin equation • Estimating surface tension via capillary rise • Avogadro number from Brownian motion data • Free energy, enthalpy, and entropy changes in micellization from CMC-temperature data • Debye lengths of single and mixed salts (for aqueous colloids) • Zeta potential via electrophoresis and Huckel/Smoluckowski equations • Hamaker constants for colloidal particles in various media • Heat of adsorption from adsorption data • Spreading of liquids and works of adhesion and cohesion • Molecular weight (MW) of proteins from sedimentation (equilibrium or velocity) data
2. Derivations	Molecular weight equation from gravity or centrifugal measurements • Stokes-Einstein equation and Brownian distance • The maximum of the work of adhesion from Zisman plot • Link of critical and solid surface tensions from interfacial theories • Contact angle via combining Young equation and interfacial theories • CPP (critical packing parameter) of spherical micelles, and the aggregation number of SDS (Sodium Dodecyl Sulphate) • From adsorption theories to surface tension/concentration equations and vice versa—derivation of the two-dimensions ideal law • The general equation for the Debye length as a function of valency, temperature, and medium and specific cases for aqueous solutions at 25 °C • CCC (Critical Coagulation Concentration) via the DLVO theory and surface potential at CCC
3. Group contribution (GC) methods; Estimations via theories	Surface and interfacial tensions of liquid-liquid interfaces, <i>e.g.</i> , water-alkanes (aliphatics and aromatics), glycol-alkanes, mercury-water, or hydrocarbons via the Fowkes, Girifalco-Good, and Hansen theories • Estimation of the dispersion part of the surface tension of water • Surface tensions via Parachor and corresponding states methods • Surface tensions via Hamaker constants • Resistance of adhesive points in presence of liquids via the Owens-Wendt theory • Solid surface tensions via contact angle data and a theory, <i>e.g.</i> , Owens-Wendt • HLB (Hydrophilic-Lipophilic Balance) of surfactants for use in emulsions via the GC method of Davies-Rideal
4. Inspired from industrial problems	Adhesion in silicon-epoxy coatings via the van Oss-Good theory • Stability of Alumina particles in various media using Hamaker constants alone • Composite and individual adsorptions of solid pigments in paints via Langmuir's equation • Kinetics and creaming of emulsions • Stability (electric vs. steric) of latex paints and kinetics of destabilization
5. Requiring graphical solutions and extrapolations	MW of biomolecules (proteins) via surface pressure-area data • Kinetics of aggregation via particle-time data • MW of polymers from osmotic pressures • MW of colloid particles via sedimentation coefficients • Adsorption, area/molecule, and CMC from surfactant solutions from surface tension-concentration data • Adsorption of gas on solids from volume-pressure data using Langmuir and BET → calculation of specific area of solid • Adsorption of compounds from solution on solids from adsorption-concentration data → calculation of area of adsorbed compound
6. Combined and general	Characterization and wetting of polymer surfaces, <i>e.g.</i> , nylon, PET, and Teflon (critical surface tension, Zisman, contact angle, theories, work of adhesion) • Stability of colloids (potential-distance, potential energy-distance curves, Debye length, zeta potential, Schulze-Hardy rule, and CCC • Kinetics of aggregation of (hydro)sols (half-life time, Phase Inversion Temperature for emulsions, stability ratio)

A central component in the course is the variety of teaching methods/approaches employed. Such variety has been considered necessary both for enhancing understanding and for making best use of time within the 4-hour modules used at DTU. The teaching methods we use include:

- Traditional elements such as lectures and problems
- Active individual and group work
- Special features to raise interest of students
  - (i) Traditional elements: short lectures with exercises solved by the individual student, with an appropriate choice/balance between exercises suitable for in-class work and homework.
  - (ii) Active individual work or group work on selected topics (see later). Active discussion during the exercise section is absolutely necessary and we find it necessary that both the teacher and teaching assistant are present.
  - (iii) Special features designed to spur and raise the student interest in the topic: these include “the question of the day” (Table 3), guest lecturers and company visits (e.g., a visit to Novozymes for surfactant-enzyme-based detergents or a guest lecture related to the link of fuel cells with colloid stability). The question of the day was an initiative

*aimed at putting one simple and relevant question to which all students could more or less directly relate, as a headline for each 4-hour session.*

For the group-work sessions, suitable topics have been chosen, e.g., electrokinetical phenomena, electric double layer, and colloid stability. In small groups the students are encouraged to read short parts of the textbook and slides and then discuss the topic among themselves, answering well-defined but general questions given in advance. A discussion in plenum would follow. For example, in the case of “electrokinetical phenomena as used in colloid chemistry,” these questions “to inspire the group work” can be:

- What are they?
- How do they work?
- Which of them is the most important in your opinion?
- What do they measure?
- What do they tell us and how are they used in practice?
- What are the limitations?

We soon realized that a 5-ECTS-point course cannot cover both the theoretical and the experimental aspects of Colloids and Interfaces and thus a laboratory exercise course, which runs during January (duration: three full weeks) following the theory course, has been established. Despite the fact that one might have expected a laboratory course to have been as popular (if not more so!) than a theory course, in practice we have observed the opposite, for reasons not entirely clear to us. To make the laboratory course more attractive to students, we have tried to illustrate the “evident” links between theory and laboratory courses as well as a clear illustration of how, in colloid and surface science, theory and experiments go hand-in-hand and little can be said and done without well-defined and planned experiments. Theories and concepts are, of course, useful in this planning and in understanding the results. Table 4 (next page) summarizes these links.

## STUDENT EVALUATION, CONCLUDING REMARKS, AND SOME SUGGESTIONS

Student satisfaction with the course has been high despite the difficulties associated with finding an appropriate textbook for our needs. Greater satisfaction with the course material evident in recent years could be attributed to the availability of extensive slides from the lecturers in the form of PowerPoint presentations with Notes. Our experience from teaching Colloid and Surface Chemistry in a mixed student audience with different expectations, interests, and directions has been presented. We have discussed curriculum, textbooks, and learning objectives emphasizing the “unifying concepts” that can enhance understanding. Despite the numerous textbooks available, we feel that only a few cover both topics in substantial detail and at a level suitable for undergraduate students.

**TABLE 3**  
“The question of the day” (Autumn 2003)

Day	Question
1	How can mosquitos walk on water?
2	Do detergent companies cheat us?
3	What is common for the leaves of lotus and wings of butterflies?
4	Why is it so difficult to paint Teflon?
5	How do you make good bread—or, what is gluten?
6	Why were PEG (polyethylene glycol) solutions used for the conservation of the wooden VASA ship in Stockholm, Sweden?
7	Why is the sky blue but the sunset red?
8	What do milk, mayonnaise, and shampoos have in common?
9	Why—where—what about enzymes?
10	In which three ways can you measure the molar mass of colloids?
11	When is a colloidal suspension stable—above or below the critical coagulation concentration?
12	What is the most important thing you have learned about colloidal and surface chemistry, and how is it relevant to you in practice ?
13	Why do plastic paint buckets always have dusty lids?
14	Why does the bathroom mirror always steam up?
15	What makes a no-stick frying pan no-stick?

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**TABLE 4**  
What can/should be measured and what can be calculated in "Colloid and Surface Chemistry"?

Property	Can we measure it? How?	Can we estimate it? How?	Comments/Importance
Surface tension of pure liquids and liquid solutions	X (Du Nouy, Pendant Drop, Wilhelmy plate, capillary rise)	X (Parachor, solubility parameters, corresponding states)	Wetting, adhesion, lubrication, . . .
Interfacial tension of liquid-liquid interfaces	X (Du Nouy)	X (many methods, e.g., Fowkes, Hansen, Girifalco-Good)	Surfactants, . . .
Surface tension of solids		X (Zisman plot, extrapolation from liquid data, solubility parameters, parachor)	Wetting, adhesion, . . .
Interfacial tension of solid-liquid and solid-solid interfaces		X (many methods, e.g., Fowkes, Hansen, van Oss-Good)	Wetting, adhesion, characterization and modification of surfaces, . . . (paints, glues, . . .)
Contact angle between liquid and solid	X (many goniometers and other methods)	X (combination of Young equation with a theory for solid-liquid interfaces)	Wetting, adhesion, characterization and modification of surfaces, . . .
Critical micelle concentration of surfactants	X (change of surface tension or other properties with concentration)		Detergency, . . .
Surface or zeta potential of particles	X (micro electrophoresis)		Stability of colloidal dispersions
Adsorption of gases/liquids on solids	X (many methods)	X (many theories, e.g., Langmuir, BET, Freudlich)	Stability, surface analysis
Topography of a surface	X (AFM, STM)		Surface analysis and modification
HLB (Hydrophilic-Lipophilic Balance)		X (group contribution methods, solubility parameters)	Design of emulsions including stability of emulsions and determining the emulsion type
Work of adhesion	X (JKR, AFM)	X (the ideal one via Young-Dupre and similar equations)	Adhesion, detergency
Interparticle forces and colloid stability	X (surface force apparatus, AFM, and other methods for stability, e.g., Turbiscan)	X (DLVO theory)	Stability of all types of colloids (paints, food colloids, . . .)
Molecular weight of polymers and proteins	X (many methods, e.g., ultracentrifuge and osmotic pressure)		Characterization of high-molecular-weight molecules
Creaming and sedimentation of suspensions and emulsions	X (Turbiscan)	X (Stokes equation for dilute dispersions)	Stability of colloids
Critical Coagulation Concentration	X (series of experiments adding salts in colloidal dispersions until coagulation occurs)	X (DLVO theory)	Stability of colloids
Determining emulsion type		X (HLB and Bancroft rule)	Emulsion design

# THE CHEMICAL ENGINEER'S TOOLBOX

## *A Glass Box Approach to Numerical Problem Solving*

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An introductory computer programming course has been a permanent staple of the undergraduate engineering curriculum ever since the appearance of mainframe computers. While the principal programming language that is taught has changed over the years, much remains the same. The course is typically taken during the freshman year, well before any of the core engineering courses. Students wonder why they have to take the class when they're in it, and this viewpoint is unfortunately reinforced in retrospect as they are rarely if ever called upon to apply their programming skills. When they are asked to solve numerical problems, a commercial software package is typically used in a "black box" fashion, thus perpetuating the notion that their computer programming course was a waste of time.

Hardware and software advances and curricular adjustments have improved this situation. Laptop computers are used in the classroom to a greater extent. Access to computing facilities, in general, is less of an issue than ever before. In addition, the availability of programming languages such as Matlab<sup>[1]</sup> that come equipped with built-in solvers and graphics makes it easier to apply computer programs to solve engineering problems. The use of such software, however, is only effective if one can broker a departmental or institutional arrangement where a common numerical software package is used in related engineering courses. Another consideration is that many commercial numerical software packages are designed to be used in a "black box" mode. This can foster their use in a way that does not require the user to understand the underlying numerical algorithms. In an academic setting, this may not meet all of the intended educational objectives.

Another approach taken to promote numerical problem solving in the undergraduate engineering curriculum has been to have the individual engineering departments teach computer programming rather than farming out this task to the computer science department. This arrangement offers the advantage of being able to offer discipline-specific instruction and example applications. Nonetheless, the impact of a more enlightened experience in the introductory computer programming course quickly fades if the students do not regularly apply their computer application skills in problem solving. As the saying goes, "use it or lose it."



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## COMPUTER PROGRAMMING IN RHIT'S CHEMICAL ENGINEERING DEPARTMENT

The Department of Chemical Engineering at Rose-Hulman Institute of Technology has made similar modifications to its curriculum to address the issues outlined above. Since 1996, all undergraduate students at Rose-Hulman have been equipped with a laptop at the start of their freshman year. In 2002, the department inherited from its computer science colleagues the task of teaching introductory programming to students enrolled in chemical engineering. This two-credit-hour course, Programming and Computation for Chemical Engineers, is taken in the spring quarter of the students' freshman year.<sup>[2]</sup> It has included instruction on Microsoft Excel<sup>[3]</sup> (~1/3) as well as computer programming (~2/3). Excel's integrated Macro language, Visual Basic for Applications (VBA), has been used as a medium for teaching programming concepts to the students.

The decision to use VBA was motivated by several factors. First, the convenience and efficiency of using a single software package for the entire course reduced the instructional overhead. Since VBA is integrated with Excel, this also lessened the students' anxiety due to their familiarity with this application. Assuming that the use of VBA would continue into their chemical engineering courses, it circumvented the

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*After several years of teaching the students how to program in VBA, it was recognized that their programming skills were still largely abandoned after the freshman year.*

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need for faculty in the department to embrace an unfamiliar software package. For example, Matlab was used in an earlier version of this course, and ~1/2 of the faculty had rarely or never used it before. Other important factors included the results of a comprehensive survey conducted by CACHE<sup>[4]</sup> that suggested Excel was the most widely used software by practicing chemical engineers. Lastly, it was recognized that the programming elements in VBA (*e.g.*, loops, decision constructs) were sufficiently similar to those in other common programming languages. As such, it would not be too difficult for students to subsequently learn how to program in a different language if required.

After several years of teaching the students how to program in VBA, it was recognized that their programming skills were still largely abandoned after the freshman year. It is believed that much of this is due to the relatively large investment in resurrecting their VBA course material and programs for application

in subsequent coursework. This inevitably involves relearning some aspects of VBA, especially if more than a quarter or two has passed since they took their programming course. Most students are reluctant to do so, thus creating an obstacle to the objective of teaching them how to apply their programming skills to chemical engineering problem solving.

The principal pedagogical challenge that remains is twofold. First, we simply need to increase the opportunities for students to apply their computer application skills to numerical problem solving while minimizing the instructional overhead. The use of a common numerical software package throughout the curriculum is a key part of a solution to this issue. Additionally, to be most effective, the software must be used by students in a manner that increases their understanding of the numerical algorithms while minimizing the actual programming effort.

## THE CHEMICAL ENGINEER'S TOOLBOX

A novel approach to address this challenge is being evaluated with the students who have recently completed the Programming and Computation for Chemical Engineers course. The central idea is to compile the general-purpose programs that the students developed in this course into an Excel Add-In. This addresses the need to increase the numerical problem-solving opportunities by making the programs more accessible. The programs appear as functions built into their Excel application. This approach also addresses the need for the students to understand the underlying numerical algorithms. They will use their own programs in a transparent software environment. One may refer to this as a "glass box" approach to numerical problem solving, in contrast with the more familiar "black box" approach. The Excel Add-In can also be continuously populated with more complicated programs and numerical algorithms as the students move up the curriculum. This Add-In, hereafter referred to as the Chemical Engineer's Toolbox, is distributed to sophomore-level students at the start of the fall quarter for use in their introductory Material and Energy Balances course.

We envision that the students will use the Toolbox in a couple of different ways that serve to improve their learning of chemical engineering principles. For relatively routine computing tasks such as interpolation or numerical integration, the availability of Excel functions that streamline these calculations will enable them to spend more time learning the fundamentals of the problem and less time setting up a spreadsheet. In addition, as the students move up the curriculum, the relatively simple programs that they developed as freshmen can serve as templates or starting points for more sophisticated numerical problem solving. For example, a program that computes the specific volume using a simple pure component equation of state may be modified to account for nonideality or multiple components as an assignment in a thermodynamics course.

## PROGRAMMING IN VBA

Before describing the Chemical Engineer's Toolbox, we offer a summary description of the VBA programming environment and language. The VBA programs are developed using the Visual Basic Editor, a graphical computer programming package that is seamlessly integrated with Excel. It consists of a multiple-pane window as shown in Figure 1. The two panes on the left are the Project Explorer and the Properties Window. The Project Explorer includes a listing of all open workbooks and installed Add-Ins, both of which are referred to as projects in VBA. Each project includes any associated objects (*e.g.*, worksheets), forms, and modules. A form is a customized graphical user interface, or GUI, that is created in the Visual Basic Editor and can be used to conveniently facilitate input and output for a VBA program. A module is simply a sheet onto which related VBA procedures are typed and stored. The code contained in a module appears in the pane

to the right of the Project Explorer. The Properties Window can be seen below the Project Explorer pane. This window is used to specify the properties associated with objects contained in a VBA project.

The VBA programming language contains all of the traditional structured programming constructs (loops, decisions, etc.) and some aspects of object-oriented programming as well. A detailed description of the VBA programming language may be found in several recently published books.<sup>[5-7]</sup> VBA programs are referred to as procedures. There are several different types of VBA procedures, and methods to execute them. In Excel, the simplest approach is to use VBA function procedures since the protocol for calling one is identical to that of any of Excel's built-in functions (*e.g.*, SUM, SQRT, MINVERSE). For this reason, the collection of VBA programs in the Toolbox is comprised exclusively of function procedures.

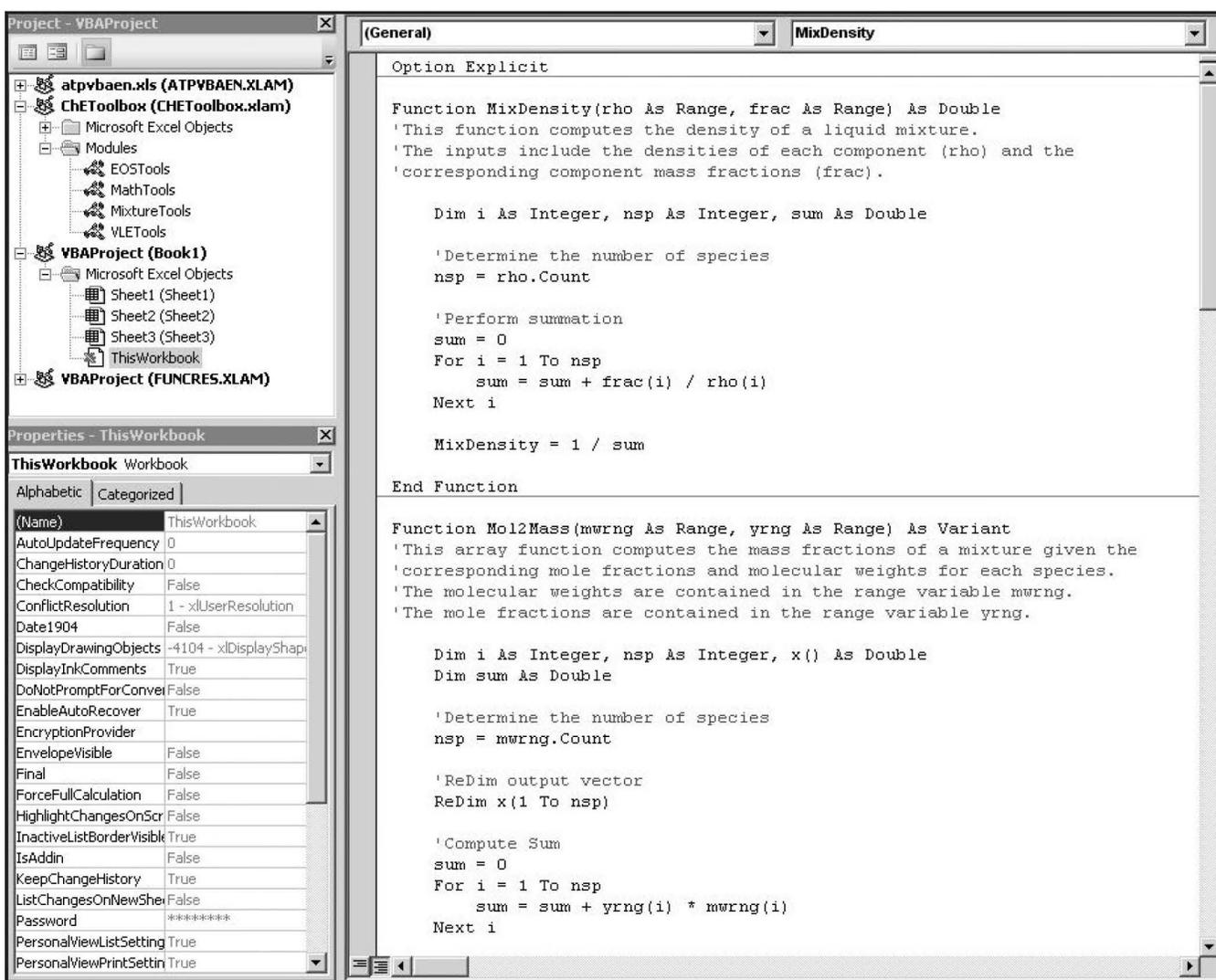


Figure 1. Visual Basic Editor used to create VBA programs in Excel.

## A CLOSER LOOK AT THE CHEMICAL ENGINEER'S TOOLBOX

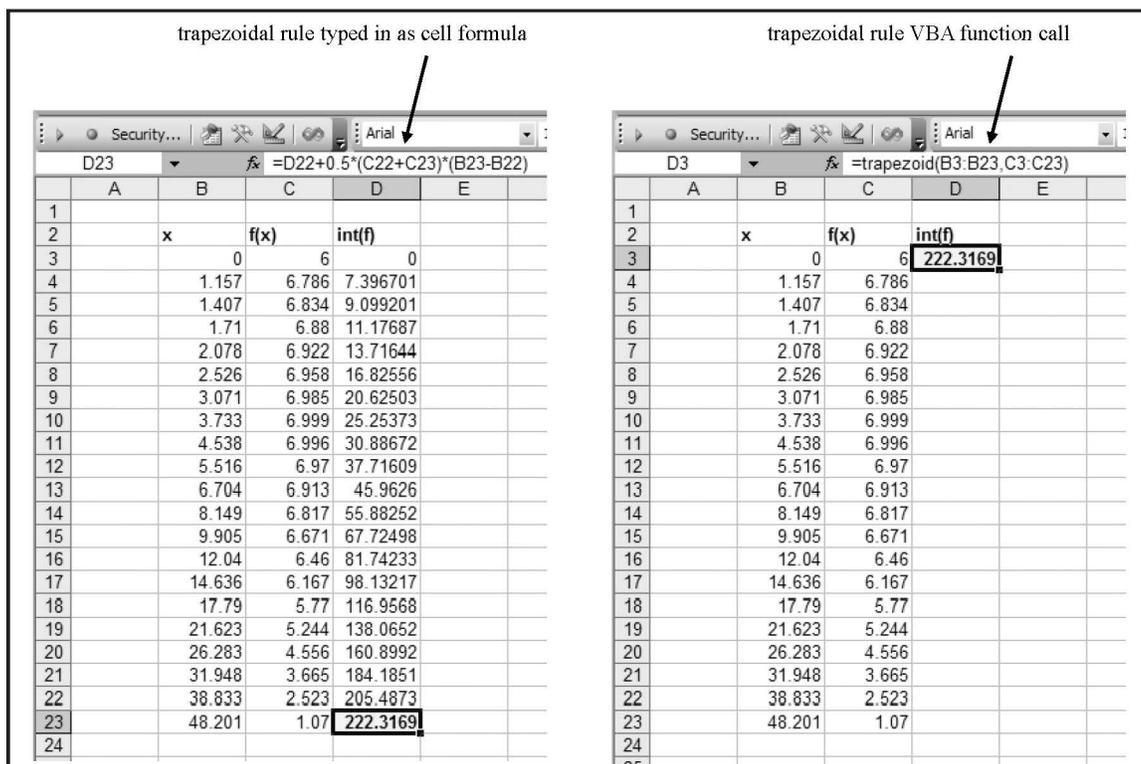
The initial version of the Toolbox is tailored to chemical engineering students beginning their sophomore year of instruction. It contains a collection of Excel functions that includes general math tools as well as tools designed to solve problems specific to their introductory Material and Energy Balances course. A list of the Toolbox functions can be found in Table 1.

It is seen that some of the functions do not require specification of a system of units (e.g., Trapezoid, LinearSys), while others do (e.g., Pvpap, BubbleT). For the units-dependent

functions, the Toolbox uses the SI system. This simplifies the coding of the VBA programs, but also requires the user to ensure that the function inputs are in SI units, and to convert the function output units if necessary. Note that the interested student could easily modify their VBA programs to accommodate additional systems of units. This type of creative enhancement of their Toolbox functions is encouraged.

We next consider a specific Toolbox function to demonstrate how it is applied to solve a problem and to illustrate some important characteristics of the underlying VBA code. A VBA function procedure that performs numerical integration using the trapezoidal rule [see Eq. (1) below] is developed by the

**Figure 2.** Comparison of a trapezoidal rule numerical integration using a spreadsheet with that using a Chemical Engineer's Toolbox VBA function.



```
Function trapezoid(xrng As Range, frng As Range) As Double
'This function performs a numerical integration using the trapezoidal rule.
'The independent variable is contained in the xrng object variable.
'The integrand is contained in the frng object variable.

Dim npts As Integer 'Number of discrete points
Dim i As Integer 'Loop index

'Determine the number of discrete points
npts = xrng.Count

'Initialize summation variable
trapezoid = 0

'Sum up areas of trapezoids representing integral
For i = 1 To npts - 1
trapezoid = trapezoid + 0.5 * (frng(i) + frng(i + 1)) * (xrng(i + 1) - xrng(i))
Next i

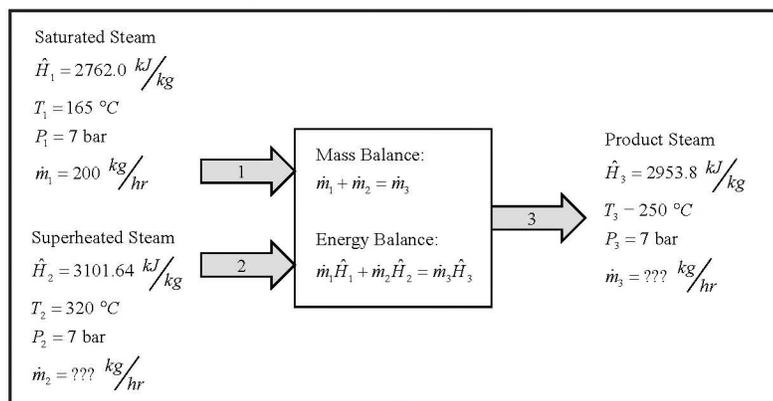
End Function
```

**Figure 3.** VBA code for the trapezoidal rule function.

students in their Programming and Computation for Chemical Engineers course.

$$\int_{x_0}^{x_f} f(x) dx \approx \sum_{i=1}^{n-1} \frac{(f(x_i) + f(x_{i+1})))}{2} \times (x_{i+1} - x_i) \quad (1)$$

This simple computational task can be accomplished using only a spreadsheet. In fact, the students are required to do so during the first part of the course. This serves to reinforce the value of having a customized function available for this purpose—it streamlines the calculation and eliminates the possibility of incorrectly implementing the trapezoidal rule formula once it has been programmed correctly. This is shown in Figure 2, where an



**Figure 4.** Schematic illustration of the steam-mixing problem based on problem 7.35b in Felder and Rousseau.<sup>[8]</sup>

example numerical integration is performed using a spreadsheet-only implementation and again using the Toolbox function.

The corresponding VBA code for the trapezoidal rule function is seen in Figure 3. The students are taught to create computer programs that are reusable, *i.e.*, not specific to a given problem. For example, the trapezoidal rule function can be used to integrate using any number of discrete independent variable points that are equally or unequally spaced. In addition, the students are encouraged to write programs that can be easily modified if necessary. An example would be to expand the trapezoidal rule function so that it can perform numerical integration using Simpson's 1/3 rule, as well. If the code includes sensibly named variables and is sufficiently commented, this task is more easily accomplished.

In the following section, we provide a couple of example applications of the Chemical Engineer's Toolbox. These are taken from Felder and Rousseau's textbook *Elementary Principles of Chemical Processes*<sup>[8]</sup> to demonstrate how the Toolbox may be used for problem solving in an introductory Material and Energy Balances course.

## EXAMPLE APPLICATIONS OF THE CHEMICAL ENGINEER'S TOOLBOX

The first example problem involves the adiabatic mixing of two streams containing saturated and superheated steam as shown in Figure 4. This corresponds to problem 7.35b in Felder and Rousseau,<sup>[8]</sup>

**TABLE 1**  
Functions in the Sophomore Version of the Chemical Engineer's Toolbox

Function Name	Description
Trapezoid	Performs numerical integration using the trapezoidal rule.
LinearSys	Solves a system of linear equations.
Interp_1	Performs linear or cubic interpolation in one dimension.
Interp_2	Performs linear or cubic interpolation in two dimensions.
NewtonRaphson	Solves a single nonlinear algebraic equation using the Newton-Raphson method.
ModEuler	Solves an initial value ODE using the modified Euler method.
Mol2Mass	Converts mole fractions to mass fractions.
Mass2Mol	Converts mass fractions to mole fractions.
MW_mix	Computes the average molecular weight of a mixture.
Density_mix	Computes the density of a liquid mixture.
V_VDW	Computes the specific volume of a gas using the van der Waals EOS.
V_Virial	Computes the specific volume of a gas using the virial EOS.
V_RK	Computes the specific volume of a gas using the Redlich-Kwong EOS.
Pvap	Computes the vapor pressure of a pure component using the Antoine equation.
BubbleP	Computes the bubble point pressure and corresponding vapor composition using Raoult's law and the Antoine equation.
BubbleT	Computes the bubble point temperature and corresponding vapor composition using Raoult's law and the Antoine equation.
DewP	Computes the dew point pressure and corresponding liquid composition using Raoult's law and the Antoine equation.
DewT	Computes the dew point temperature and corresponding vapor composition using Raoult's law and the Antoine equation.

with some of the pressures and temperatures modified to underscore the use of the Toolbox functions. The problem requires the students to simultaneously solve material and energy balances around the system by making use of saturated and superheated steam tables.

C19		fx = Interp_2(320,7,D15:E15,C16:C17,D16:E17)						
	A	B	C	D	E	F	G	H
1								
2								
3	Enthalpy of Stream 3							
4								
5		T, °C	P, bar	H, kJ/kg				
6		250	5	2961				
7		250	10	2943				
8								
9		H <sub>3</sub> =	2953.80					
10								
11								
12	Enthalpy of Stream 2							
13								
14				T, °C				
15				300	350			
16				5	3065	3168		
17		P, bar		10	3052	3159		
18								
19		H <sub>2</sub> =	3101.64					
20								
21								
22	Solution of Mass and Energy Balances (Ax = b)							
23								
24			A Matrix	b Vector				
25	Mass		1	-1	-200			
26	Energy		3101.64	-2953.8	-552400			
27								
28	m <sub>2</sub> =	259.47						
29	m <sub>3</sub> =	459.47						
30								

Figure 5. Toolbox-assisted solution to problem 7.35b in Felder and Rousseau.<sup>[8]</sup>

H3		fx (=bubblet(760,B3:B5,C3:C5,D3:D5,E3:E5))						
	A	B	C	D	E	F	G	H
1								
2		x <sub>i</sub>	A	B	C			
3	Benzene	0.226	6.89272	1203.531	219.888	T <sub>bp</sub>	108.0936	
4	Ethylbenzene	0.443	6.9565	1423.543	213.091	x <sub>B</sub>	0.497173	
5	Toluene	0.331	6.95805	1346.773	219.693	x <sub>E</sub>	0.194951	
6						x <sub>T</sub>	0.307876	
7								
8								
9		x <sub>i</sub>	A	B	C			
10	Benzene	0.443	6.89272	1203.531	219.888	T <sub>bp</sub>	96.48083	
11	Ethylbenzene	0.226	6.9565	1423.543	213.091	x <sub>B</sub>	0.714674	
12	Toluene	0.331	6.95805	1346.773	219.693	x <sub>E</sub>	0.067822	
13						x <sub>T</sub>	0.217504	
14								
15								
16								
17		x <sub>i</sub>	A	B	C			
18	Benzene	0.226	6.89272	1203.531	219.888	T <sub>bp</sub>	104.4884	
19	Ethylbenzene	0.226	6.9565	1423.543	213.091	x <sub>B</sub>	0.45261	
20	Toluene	0.548	6.95805	1346.773	219.693	x <sub>E</sub>	0.088576	
21						x <sub>T</sub>	0.458814	
22								

Figure 6. Toolbox-assisted solution to problem 6.58b in Felder and Rousseau.

This problem is particularly well-suited for application of the Chemical Engineer's Toolbox since it requires repetition of many routine calculations. For example, the steam enthalpies for streams 2 and 3 ( $\hat{H}_2$  and  $\hat{H}_3$  in Figure 4) must be determined by two- and one-dimensional interpolation, respectively, using the values available in the steam tables. The interpolation tasks are conveniently performed using the Interp\_2 and Interp\_1 functions. In addition, the solution of the material and energy balance equations are obtained using the LinearSys function. The Toolbox-assisted solution to this problem is illustrated in Figure 5. Clearly, the solution could have been obtained without the Toolbox, but having the functions available minimizes the time spent performing rote calculations and provides more time for the students to learn the fundamental steps that lead to the solution. Additionally, the underlying code that comprises the functions is fully accessible to the students.

The second example application of the Toolbox makes use of the bubble point temperature function, BubbleT. Problem 6.58b in Felder and Rousseau<sup>[8]</sup> involves the calculation of the bubble point temperature of an ideal mixture of benzene, ethylbenzene, and toluene. The students are asked to compute the bubble point temperature at atmospheric pressure for three different liquid mixture compositions by using Raoult's Law and the Antoine equation.

$$\sum_i y_i P = \sum_i x_i P_i^{\text{sat}} \quad (2)$$

$$\log_{10} P_i^{\text{sat}} = A_i - \frac{B_i}{T + C_i} \quad (3)$$

This numerical problem consists of solving a single nonlinear algebraic equation where the unknown variable is the temperature, T. Excel's Goal Seek utility is recommended in the problem statement.

This problem represents an example where the Toolbox may be used in a manner that expands the students' learning opportunities beyond the original problem statement. For example, the students can be asked to create a Txy diagram by using the BubbleT and DewT functions since they return the temperature and phase composition. In this example, the BubbleT function was applied to solve for the bubble point temperatures of three ternary mixtures specified in the problem statement. BubbleT is an array function (*i.e.*, returns an array of numbers) that computes not only the bubble point temperature but also the corresponding vapor composition. The required inputs include the total pressure, liquid phase mole frac-

tions, and the Antoine equation coefficients for each species. The Toolbox-assisted solution to problem 6.58b is shown in Figure 6. The additional function output consisting of the vapor phase composition enriches the students' learning associated with the problem. Unlike the "black box" Goal Seek approach, the students can also see the underlying numerical algorithm (Regula-Falsi method as described in Appendix A of Felder and Rousseau) implemented in the BubbleT function, providing them with a more fundamental understanding of the solution technique. In addition, the BubbleT function can serve as a basis for incorporating non-ideal effects when the students learn more about vapor-liquid equilibrium in a subsequent thermodynamics course.

## SUMMARY AND CONCLUDING REMARKS

The Chemical Engineer's Toolbox was developed as a proactive approach to improve students' computer application skills in the undergraduate chemical engineering curriculum. The primary benefits of the Toolbox that enhance student learning are its convenient access as an Excel Add-In and the transparent "glass box" environment in which the

programs are created and stored. The students are provided with the Toolbox at the start of their sophomore year for use in their introductory material and energy balances course. It is anticipated that additional VBA program modules will be defined and created by faculty and students alike in courses to follow in fluid mechanics, heat transfer, thermodynamics, mass transfer, and reactor engineering.

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# 'OLD DEAD GUYS'

## Using Activity Breaks to Teach History

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Teaching students in the classroom on a regular basis quickly reveals the importance of activity breaks. Activity breaks can be used for active learning exercises such as in-class teams, think-pair-share, or minute papers.<sup>[1]</sup> The core elements of all active-learning methods are student activity and engagement in the learning process. These methods have been shown to have a positive effect on student learning.<sup>[2]</sup>

An alternative focus of this active-learning activity break can be to educate students about the history and personalities of chemical engineering. Almost every lecture in a chemical engineering class contains references to the people and their accomplishments that form the foundation for today's students: Antoine equation, Gibbs' free energy, Arrhenius equation, Reynolds number, McCabe-Thiele plot, Bode plot. Why are these figures famous today? Because they came up with solutions to important problems. While many of these historical figures are at least vaguely familiar to us as instruc-

tors, the students are usually completely unfamiliar with them. By focusing on the history and personalities, chemical engineering comes alive and the students become familiar with the human side of our profession. These examples can also be used to demonstrate to students the reasons why these problems were so important and how their solutions led to practical developments and applications. Since there is often at least one historical figure mentioned in every class lecture, they provide an opportunity to re-engage the students and re-focus on the topic through the use of a historically focused activity break.

### APPROACH

When a historical figure is encountered during a class period, it is often part of a derivation, and student attention is waning. This provides an ideal opportunity for a historically focused activity break. This break serves as a way to put an exclamation point on a concept and to connect the person to this concept. The students are first asked to guess when the historical figure lived and did the work that bears his or her name. As expected, a few wildly inaccurate guesses usually result. Next, the students are shown a picture/portrait of the historical figure. Slightly more accurate guesses are then given. The guesses serve as a way to encourage participation. Since no one is likely to know the answer, a wrong guess does not demonstrate a lack of technical knowledge to their peers. Finally, the students are shown a picture together with biographical information about the historical figure. This information typically includes birth and death dates, institutions attended, degrees earned and dates, major accomplishments,



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Svante Arrhenius	Edward Teller
Cato Guldberg	Paul Emmet
Peter Waage	Irving Langmuir
Maud Menten	Thomas Sherwood
Leonor Michaelis	Alan Colburn
Hans Lineweaver	Ernest Thiele
Dean Burk	Gerhard Damköhler

and awards earned (Figure 1 and Figure 2). The degree and institution data show students that people from many fields have contributed knowledge important to chemical engineering. It also exposes students to the importance of advanced degrees in science and engineering but also that some historical figures had no more than a bachelor's degree. Major accomplishments other than the one of current interest are also listed. In this way, the versatility of these historical figures is demonstrated as well as the fact that people often succeed and contribute to fields outside their area of study. The break is concluded with a short discussion of why the accomplishment occurred at that time, the historical context in which it occurred, what other historical events influenced it, and other broad societal influences (intended and unintended).

## RESULTS AND DISCUSSION

The historically focused activity breaks have been used over the last five years in two separate courses (a junior-level required course in Kinetics and Reaction Engineering and a senior-level elective in Industrial Chemical Production). For the Kinetics and Reaction Engineering class, 14 biographies have been developed (Table 1). Six biographies have been developed for the Industrial Chemical Production class.

From the instructor perspective, what appears to draw the students into the presentations is when they include controversy. For example, Thomas Midgley was responsible for two of the most important inventions of the 20th century: tetra-ethyl lead gasoline additive and chlorofluorocarbon refrigerants. These inventions lead to the tremendous success of the automobile and allowed large population growth in the American south and southwest. As a result of these inventions he won numerous awards. Before the century was over, however, the side effects of these inventions were well known and both substances were tightly regulated. Similarly, Fritz Haber and Carl Bosch developed catalysts to produce ammonia from nitrogen and hydrogen. This allowed Germany to make explosives for its war efforts after it lost access to conventional nitrogen sources. On the positive side, subsequent ammonia production and use as a fertilizer has also allowed a worldwide expansion of agriculture production. Examples such as the two above help our students understand the impact

	Thomas Midgley, Jr.
	b. 1889 d. 1944
	Ph.D. Cornell
	1922 Discovered tetraethyl lead as anti-knock additive to gasoline.
	1928 Discovered chlorofluorocarbons were essentially "inert" and could be used as refrigerants.
	Nichols Medal 1922 Perkins Medal 1937 Priestly Medal 1941 (ACS) William Gibbs Medal 1942

Image used by permission of Thomas Midgley IV.

*Figure 1. Thomas Midgley picture and biography for classroom use.*

	Wilhelm Ostwald
	b. 1853, Riga, Latvia d. 1932, Leipzig, Germany
	Univ. of Tartu 1875 (Estonia) Univ. of Tartu 1878, Ph.D.
	1877: Prof. of Physical Chemistry at Leipzig University. Students included: Arrhenius (Nobel Prize 1903) Van't Hoff (Nobel Prize 1901) Nernst (Nobel Prize 1920)
	Received Nobel Prize in Chemistry in 1909 for "Work on catalysis, chemical equilibria, and reaction velocities."

*Figure 2. Wilhelm Ostwald picture and biography for classroom use.*

of engineering in a global and societal context and contribute directly to desired outcome (h) of Criterion 3 in ABET.

Students can also be educated about the practice of science and engineering through these historical biographies. For example, most faculties are aware of the mentor/mentee relationships between professors and graduate students. If the historical biography lists an individual's advisor and students, the students can see how one generation of scientists educates/trains the next generation. An ideal example of this is Ostwald, who mentored three Nobel laureates (Figure 2).

Whenever possible, women and minorities should be featured as historical figures (*e.g.*, Maud Menten of Michaelis-Menten kinetics). There is an ongoing effort by the NSF and other organizations to encourage the participation of women and minorities in science and engineering. By highlighting the contributions of these groups, our own students can be encouraged. It should also be noted that many historical women and minorities succeeded in spite of the roadblocks placed by society. This can be used to show students that anyone can succeed

despite whatever roadblocks they face. Resources focused on information specifically about women and minorities in science may be used to prepare these biographies.<sup>[3-5]</sup>

The use of historical biographies also allows the opportunity to expose undergraduate students to the scientific literature. Show the students a copy of the paper where Thiele investigated the relationship between catalytic activity and particle size<sup>[6]</sup> (which led to the Thiele modulus) or when Michaelis and Menten published their understanding of enzyme kinetics.<sup>[7]</sup> By showing students the original papers, they can begin to understand the process whereby a problem evolves into a research project, becomes published in a research journal, is accepted by the researchers in the field, and graduates to textbook fundamentals.

Information and images for these biographies can come from a wide variety of sources. For historical figures in transport phenomena, Bird has presented an extensive list of microbiographies.<sup>[8]</sup> Similarly, for historical figures in catalysis, more in-depth information is available from Davis.<sup>[9]</sup> Additional published sources include the *Dictionary of Scientific Biography*,<sup>[10]</sup> the *Bibliographical Memoirs by the National Academy of Sciences*,<sup>[11]</sup> and the *Memorial Tributes* series by the National Academy of Engineering.<sup>[12]</sup> Finally, the American Institute of Chemical Engineers is currently celebrating its centennial; as part of this celebration, a number of sessions at the fall 2008 meeting were devoted to the history of chemical engineering. Thus, the meeting proceedings may provide another resource.

Many online information sources are quite useful. The International Center for Heat and Mass Transfer has a Web page with biographies of historical figures with dimensionless parameters named after them.<sup>[13]</sup> If the figures come from a medicine/biology background, the <whomanedit.com> Web site provides biographical information.<sup>[14]</sup> Finally, Wikipedia provides an ever expanding source of information.<sup>[15]</sup> For images, useful Web sites include the ChemTeam Photo Gallery<sup>[16]</sup> and Pictures of Physicists.<sup>[17]</sup> Again, if all else fails, both Google and Google-image searches can cast a very wide net.

## STUDENT FEEDBACK

Student response has been very positive and in fact they are responsible for coining the term “Old Dead Guys.” After a few of these biographies were presented, the students started to expect them, often asking before class if there will be any “Old Dead Guys” today. Additionally, the students have pointed out instances where I have missed opportunities to present more of these biographies. In several cases where it was difficult to locate an image of the historical figure, individual students have instigated their own successful Web searches to find an image. All of these responses indicate that the students are taking ownership of the concept.

The most recent class went a step further. They spontaneously decided to determine which member of our department most resembled the historical figure. Due to the preponderance of beards on 19th-century scientists, the two members of our department with beards were frequent winners. Subsequently, this class incorporated this idea into their own classroom presentation. Approximately 75 percent of the student presentations included a biography of a historically relevant figure. Several students also noted to me how hard they worked to find biographical data and images of the historical figure. Additionally, as part of these presentations, the students competed informally to see who could incorporate the oldest historical figure into their presentation.

## CONCLUSIONS

Historically focused activity breaks provide an excellent way to incorporate history into the classroom. By connecting the historical figure with a solution to an important problem, the students gain a better understanding of the subject matter. These history lessons also serve to put a human face on chemical engineering while providing an opportunity to educate students about the broader societal impact of science and engineering.

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# NUMERICAL PROBLEMS AND AGENT-BASED MODELS

## *For a Mass Transfer Course*

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In the traditional undergraduate chemical engineering curriculum, the mathematical formulations of engineering problems are solved almost exclusively by analytical methods. A prototypical example is the analytical solution of differential equations in transport. Many interesting—and not particularly exotic—problems cannot be solved analytically, however. In the past, limiting cases and approximations might have been used to circumvent this problem. But with the availability of fast computers and user-friendly software for numerical computation, we risk becoming irrelevant if we do not equip our students to use these new tools. Other disciplines are also concerned about this problem. For example, concerns about whether undergraduates are equipped to tackle problems of increasing complexity recently led the Mathematical Association of America to convene a working group of chemists to examine the connections between the undergraduate mathematics and chemistry curricula.<sup>[1]</sup>

The mass transfer course is an ideal one for including numerical solution methods for chemical engineers, because the students have already seen the same mathematical methods in their fluid mechanics and heat transfer courses. At Northwestern University, momentum, heat, and mass transport are taught separately in successive quarters in the third (junior) year. Fluid mechanics is taught first, along with the requisite vector analysis, followed by heat transfer. By the time mass transfer is encountered, the analogies to fluid and heat transfer can be used to speed the coverage of the core material, leaving more time for exploration of other topics, such as numerical methods or short group projects.

At Northwestern University's McCormick School of Engineering and Applied Science, the computer solution of numerical problems is introduced to first-year students through the Engineering First program using MATLAB.<sup>[2]</sup> While FORTRAN 77 was often taught to chemical engineering students in the past, MATLAB now seems to be a favored

introductory programming language in the United States. It has the advantage of incorporating a graphical user interface and good graphing capabilities. In addition, MATLAB boasts a range of ODE and PDE solvers that are of particular use for transport problems. With the widespread availability of such tools built into the software and on the Internet, it is no longer necessary to make students write their own code to solve these types of problems. Researchers in industry also typically operate by using numerical codes written and published by experts in the relevant area of numerical computation. The researcher is thus able to devote more time to solving problems in his or her own field of expertise. Therefore the ability to understand and use existing pieces of high-level code is of great practical importance.

Discrete particle- or agent-based simulations are rarely taught to undergraduates, but they are becoming increasingly commonplace in fields as diverse as materials science, transportation, and sociology.<sup>[3]</sup> One could argue that such skills are of more use to a chemical engineering graduate entering the

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workforce today than the knowledge of rigorous distillation column design. Stochastic simulation has become an integral part of the computational chemist's or biologist's toolbox, with a number of practitioners calling for its inclusion in the undergraduate curriculum.<sup>[4]</sup> As chemical engineers have also embraced molecular simulation in their research, some chemical engineering departments have added undergraduate courses in molecular simulation and theory, covering topics such as the estimation of thermochemical and reaction rate data and the prediction of phase equilibria and transport properties by molecular simulation.<sup>[5]</sup>

Solving problems numerically forces students to think about mathematics in a different light, in that it is no longer possible to simply learn the analytical solution. Some element of programming is invariably involved in solving equations numerically, forcing students to break the solution down into the simplest steps possible, which can in turn lead to a more concrete understanding of the mathematical relationships. For students to become comfortable with solving problems numerically, such problems must be incorporated throughout the curriculum. In this paper, we give examples of problems we posed to expose students to numerical solutions and simulations in the context of mass transfer. The following sequence of problems was assigned to increase the students' familiarity with the solution of ODEs using MATLAB. We started off with a diffusion problem that could be solved analytically and had the students compare the analytical solution to the numerical solution generated by a boundary value solver intrinsic to MATLAB. We also encouraged them to experiment with different values of the parameters fed to the boundary-value solver to see whether the quality of the numerical solution or the time taken to reach it were affected. We then posed a problem with reaction and diffusion that had no analytical solution. Students were asked to vary the reaction rate constant until the concentration profiles in the system began to resemble those for the limiting case of reaction being much faster than diffusion. Finally, we presented students with a lattice simulation of cells invading a polymer tissue engineering scaffold and had them experiment with the different parameters controlling the rate of cellular invasion and the concentration profile of the invading cells in the polymer matrix.

All of the problems discussed in this paper can be found at the Web site <<http://zeolites.cqe.northwestern.edu/Publications/SupportingInfo/Download.html>>.

Instructors can obtain MATLAB solutions by sending e-mail to [snurr@northwestern.edu](mailto:snurr@northwestern.edu).

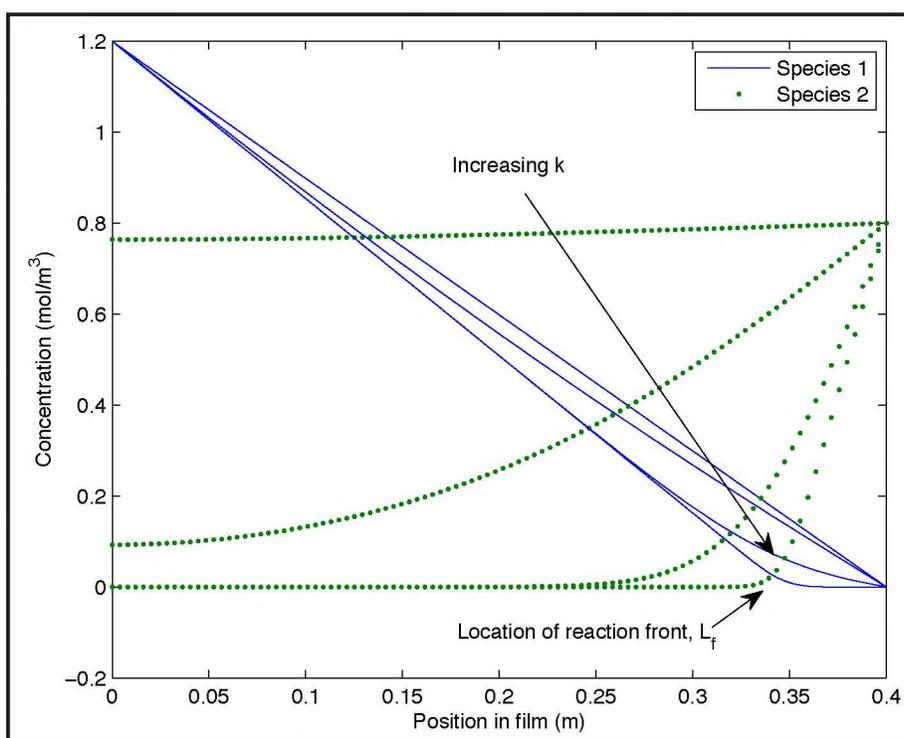
## AN INTRODUCTORY ODE PROBLEM WITH AN ANALYTICAL SOLUTION

To provide a fairly gentle reintroduction to MATLAB, we first asked students to determine the concentration profile and flux of a liquid, A, slowly evaporating into a gaseous mixture of A and B from a reservoir of pure A located at the bottom of a cylindrical tube. Since the evaporation of the liquid is slow, one may assume that the surface of the liquid is stationary. This example is covered in many texts and an analytical solution is straightforward. We used the text by Middleman,<sup>[6]</sup> where this problem is solved as Example 2.1.1. We asked the students to generate a numerical solution using MATLAB and compare this with the analytical solution. The steady-state equations to be solved are

$$\frac{dx}{dz} = \frac{-(1-x)N}{CD} \quad (1)$$

$$\frac{dN}{dz} = 0$$

where  $x$  is the mole fraction of A in the gas phase,  $N$  is the



**Figure 1.** Binary diffusion and second-order reaction in a stagnant film. The concentration profiles of each species are shown for four different values of the reaction rate constant, with the diffusivity of each species held constant. If reaction is much faster than diffusion, almost all the reaction takes place at the reaction front, marked on the figure as  $L_f$ .

flux of A,  $C$  is the total concentration in the gas phase, and  $D$  is the diffusivity of gaseous A in B. The boundary conditions are that at  $z = 0$ ,  $x = x_0$  (determined from the vapor pressure of A at the liquid/gas interface), and at  $z = L$  (end of the tube),  $x = x_1$ , the mole fraction of x in the gas mixture flowing past the tube.

MATLAB incorporates a two-point boundary value problem solver called `bvp4c`, which is useful in solving this problem. The `bvp4c` solver requires as input an initial guess to the solution in a data structure that consists of the initial mesh points in the domain of the solution and the values of the initial guess for each mesh point. This data structure can be formed by another function intrinsic to MATLAB called `bvpinit`. The other inputs to `bvp4c` are the functions describing the system of ODEs and the boundary conditions. Our ODE function consisted of just the first of the above equations, with  $N$  as a parameter to be determined. Since most students had only encountered initial-value ODE problems, we first discussed the differences between initial value and boundary value problems in class, pointing out that the latter can have no solutions or an infinite number of solutions. A hands-on introduction to MATLAB covered the use of file input and output, functions, function handles, data structures, and graphing. This was followed by fairly explicit guidance in the use of the boundary value solver functions. Students were also encouraged to try different initial guesses for the solution and the unknown parameter and to examine the effects on the validity of the solution and the time taken to reach it. Increasing the number of initial mesh points from 10 to 10,000 resulted in an increase in computation time from a few seconds to over a minute but did not affect the quality of the solution for this simple problem. Certain initial guesses for the concentration profile, however, resulted in numerical disasters — with the result that no solution could be found. The solution was completely insensitive to the initial guess for the unknown parameter,  $N$ . Finding that this parameter was in exact agreement with the analytical solution strengthened the students' confidence in their ability to obtain correct numerical solutions.

## A MORE CHALLENGING BOUNDARY VALUE PROBLEM

We followed by posing a problem without an analytical solution, in this case Middleman's Example 3.2.9. This example consists of steady-state binary diffusion through a stagnant liquid film in which a second-order reaction is taking place. The equations to solve are

$$\begin{aligned} D_1 \frac{d^2 C_1}{dz^2} - k C_1 C_2 &= 0 \\ D_2 \frac{d^2 C_2}{dz^2} - k C_1 C_2 &= 0 \end{aligned} \quad (2)$$

At  $z = 0$ ,  $C_1$  is maintained at a constant value of  $C_{10}$ , and component 2 is not allowed to cross the plane, *i.e.*,  $dC_2/dz = 0$ . At  $z = L$ ,

$C_2$  is maintained at a constant value of  $C_{2L}$ , and all of component 1 is required to react within the film so that  $C_1 = 0$ .

The concentration profiles in the film for different rate constants are plotted in Figure 1. While no analytical solution is possible, an approximation in the limit of fast reaction is possible. If the reaction is sufficiently fast and there is no excess of either species, the concentration of each species becomes essentially zero upon crossing a small zone known as the reaction front, in which almost all the reaction takes place. This behavior can be seen in the concentration profiles in Figure 1 corresponding to the highest values of the reaction rate constant,  $k$ . The location of the reaction front,  $L_f$ , can be found from the realization that, due to the stoichiometry of the reaction, the fluxes of the two components must be equal. Then

$$L_f = L \left/ \left( 1 + \frac{C_{2L} D_2}{C_{10} D_1} \right) \right. \quad (3)$$

Since the `bvp4c` solver can only be used to solve systems of first-order equations, the above system of equations and boundary conditions must be rewritten as such via the substitution  $y_i = dC_i/dz$ , which results in a system of four first-order equations to go with the four boundary conditions. The students were expected to arrive at this realization on their own. They were asked to calculate the concentration profiles of the components in the film and find the value of the rate constant at which the reaction front approximation becomes valid. This exercise was repeated with different diffusivity values to emphasize that the behavior of the system is governed by the ratio of reaction rate constant to diffusivity, essentially the Thiele modulus.

## FURTHER NUMERICAL PROJECTS

The tools that students gained in the problems above could be readily extended to explore multicomponent diffusion, a topic that is often completely ignored even in graduate transport courses. For example, consider binary diffusion of species  $i$  and  $j$  through a zeolite membrane. The membrane can be considered a third, nondiffusing component. The fluxes of the two species with respect to the stationary membrane frame of reference can be written as<sup>[7]</sup>

$$\begin{aligned} J_i &= -D_{ii} \nabla C_i - D_{ij} \nabla C_j \\ J_j &= -D_{ji} \nabla C_i - D_{jj} \nabla C_j \end{aligned} \quad (4)$$

where  $J_i$  is the flux of component  $i$ ,  $D_{ii}$  is its main-term diffusivity, and  $D_{ij}$  is its cross-term diffusivity. In general  $D_{ij} \neq D_{ji}$ , and for guest molecules in zeolites all of the diffusion coefficients may depend on the concentrations of both species. Sanborn and Snurr have reported the concentration-dependent diffusion coefficients for mixtures of methane and  $CF_4$  in the zeolite faujasite, calculated from equilibrium molecular dynamics simulations and fitted to simple analytical functions of the concentrations.<sup>[8]</sup> They used MATLAB to solve Eqs. (4) for

several interesting sets of boundary conditions. For “co-diffusion” boundary conditions, both species have a higher concentration on one side of the membrane. For “counter-diffusion” boundary conditions, species *i* has a higher concentration on one side but species *j* has a higher concentration on the other side of the membrane. Normally, one would expect species *i* and *j* then to diffuse in opposite directions (counter-diffusion). Depending on the magnitudes of the main- vs. cross-term diffusivities, however, it is possible that both species will diffuse in the same direction.<sup>[8]</sup> This illustrates that for molecules in tightly confined spaces, such as zeolite pores, the seemingly esoteric cross terms may, in fact, be important. As an interesting question, one may ask the students if this violates the laws of thermodynamics. (It does not, as both species still diffuse downhill in chemical potential, illustrating that chemical potential and not concentration is the real driving force for diffusion.)

Multicomponent diffusion is often ignored in courses because of the lack of access to the needed diffusion coefficients and because numerical solutions of the differential equations are usually required. This example shows that modern molecular simulations may provide access to difficult-to-measure multicomponent diffusivities. It also shows that the numerical solution of the differential equations is easily undertaken with widely available software such as MATLAB.

## AGENT-BASED MODELING

Certain types of problems may be more easily modeled as computer algorithms than as differential equations. While this type of modeling is now commonplace, competing with and sometimes replacing equation-based approaches, chemical engineering students tend to be almost entirely unacquainted with it by the end of their undergraduate careers.<sup>[3]</sup> An intriguing and intuitive example of this type of modeling is a simulation of ants foraging for food,<sup>[9]</sup> which can be found at the Web site of Northwestern University’s Center for Connected Learning and Computer-Based Modeling, <<http://ccl.northwestern.edu/netlogo/models/Ants>>.

This simulation concerns the manner in which a colony of ants finds food and transports it back to their anthill. It could easily be used as an in-class demonstration of a different mechanism for mass transfer, albeit one that would be extremely difficult to describe by differential equations.

In this simulation, each ant encountering a large piece of food deposits a chemical trail as it transports some of that food back to the nest. The chemical trail evaporates and diffuses over time. Ants can sniff out the chemical trail and follow its gradient uphill. A similar mechanism using a “nest scent” is used to return to the nest once food has been found. The chemical trails are reinforced by repeated traversal, which induces more ants to chip away at the food source until it is completely consumed. Once this occurs, the chemical trail begins to dissipate and the colony consequently forages else-

where. The colony generally exploits food sources closest to the nest before foraging further afield since the evaporation and diffusion of the chemical retards the formation of stable chemical trails to more distant food sources.

The ant simulation described above is an example of agent-based modeling based on the cellular automaton paradigm. Cellular automaton simulations are used to model complex systems comprised of interacting autonomous agents. Agent behaviors are modeled explicitly, using a range of behavioral models and representation schemes at appropriate levels of detail. The crux of agent-based modeling and simulation is that agents only interact and exchange locally available information with other agents in their immediate vicinity. What constitutes an agent’s “immediate vicinity” varies depending on the type of system being simulated. For example, neighbors may be spatially close for a simulation in continuous space, occupying adjacent grid cells in a lattice simulation, or connected nodes in a simulation of a network. Generally, an agent’s set of neighbors changes rapidly as a simulation proceeds. The problem of identifying an agent’s neighbors can dominate the computational expense of such a simulation, particularly as the number of agents increases. Different algorithms for neighbor-searching vary dramatically in performance depending on the topology of the neighbor interaction, the language used to program the search, and the platform on which the calculation is run.<sup>[10]</sup> For example, Mathematica, with its high-level list-processing functions and cellular automata package, can run these simulations extremely efficiently. There is a substantially steeper learning curve to programming in Mathematica, however, due to the variety of programming paradigms it supports, and since our students already had acquaintance with MATLAB, we decided to implement an agent-based simulation project in MATLAB.

We developed an agent-based simulation project relevant to chemical engineering based on the cellular automaton simulations of Shea and Pasquini<sup>[11]</sup> of cells invading a polymer tissue engineering scaffold representative of those implanted in a wound or regenerating tissue. The scaffold, which serves to maintain a space conducive to tissue formation, contains an interconnected open-pore structure that can either be seeded with progenitor cells or be infiltrated by such cells from the surrounding tissue. The progenitor cells within the scaffold migrate, proliferate, and differentiate to form a functional tissue that must eventually be integrated with the host. Although tissue engineering is currently a very active area of academic and industrial research, this was our students’ first encounter with the field.

The scaffold consists of impermeable polymer walls that define a pore structure. These walls are modeled as evenly spaced planes in the *x*, *y*, and *z* directions, which form cubic cavities called macropores. There are randomly placed holes called micropores in the macropore walls. Cells move between macropores through these micropores. (Note that the terms “macropore” and “micropore” as used in tissue engineering do not correspond to the standard IUPAC definitions.)

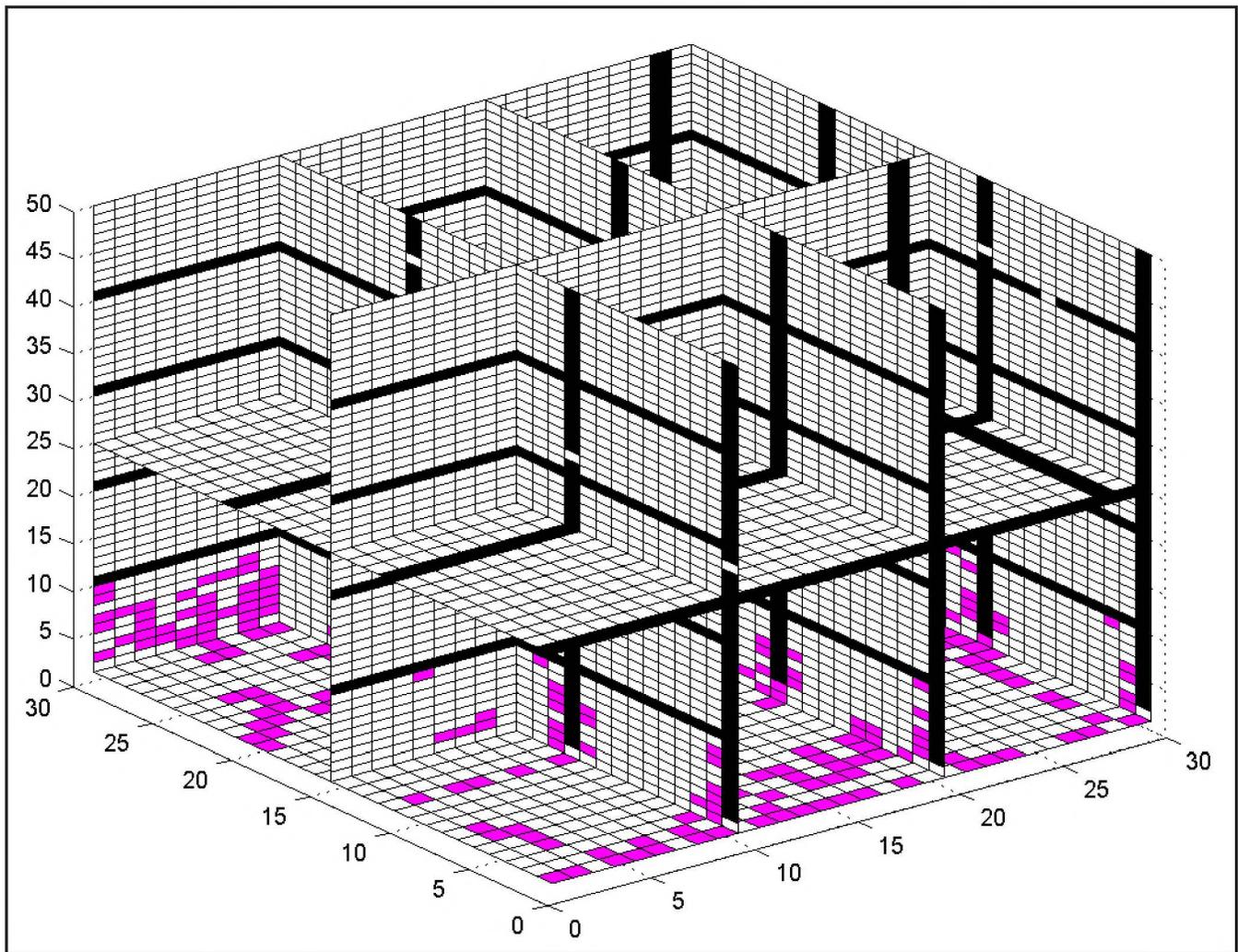
A lattice model is used to simulate the motion of cells in this scaffold, with the lattice spacing being equal to the cell size. Thus each lattice site can only be occupied by a single cell. The macropore walls are several tens of lattice spacings apart and a single lattice spacing in thickness, and the micropores in our simulations are a single lattice spacing in size. Cells can occupy vacant sites in this model pore network and migrate or reproduce if space is available. Each cell must, however, remain in some physical contact with the solid support of the walls, either directly or through adhesion to other cells that are in contact with the walls. This model is used to examine how cells penetrate from the external surface of the scaffold to its interior, ultimately filling the void space as they reproduce.

We used a simulation cell consisting of three macropores in the x and y directions and five macropores in the z direction. The cells are initially placed at the bottom x-y plane, with periodic boundary conditions being used in the x and y directions. The z direction points inward into the scaffold, with the cells initially filling the z = 0 plane and migrating in the positive z direction. Several two-dimensional slices of this three-dimensional lattice are shown together in Figure 2.

The mean square displacement for cellular migration is given by

$$\langle d^2 \rangle = nS^2Pt \quad (5)$$

where  $\langle d^2 \rangle$  is the mean square displacement, n is the number



**Figure 2.** 2-D slices of a 3-D polymeric tissue-engineering scaffold. The scaffold is placed within some healing tissue and serves to maintain a space conducive to the growth of new tissue from progenitor cells. The polymeric walls form macropores that are connected by randomly placed micropores. The scaffold is shown divided into lattice sites. Empty lattice sites in the scaffold are white, sites occupied by polymer walls are black, and sites occupied by cells are purple (gray).

The micropores can be seen as holes in the black macropore walls. In this simulation the progenitor cells are initially present at the bottom of the scaffold (z = 0 plane) and migrate vertically into it, in the positive z-direction. A selection of horizontal and vertical slices through the scaffold is shown.

of dimensions,  $S$  is the root mean square speed, and  $t$  is the time.  $P$  is the persistence time, *i.e.*, the time for which the direction of the moving cell remains constant. Variations in  $P$  have been shown to have little impact on system behavior.<sup>[12]</sup>  $P$  was chosen to be the same as the simulation time step. Setting the displacement,  $d$ , equal to the lattice spacing,  $l$ , allows the calculation of the time step from the above equation:

$$t_{\text{step}} = \sqrt{l^2/3S^2} \quad (6)$$

At each time step, each cell moves to one of the adjacent empty lattice sites. The choice of site is determined by comparing the probability of migration to each neighboring site to a random number drawn from the uniform distribution between 0 and 1. The probability of migration to a particular site is dependent on the number of cell-cell and cell-wall interactions that the cell will experience in that site and the relative importance of these interactions. This probability is normalized by the sum of migration probabilities to all the sites neighboring the starting site at that time step:

$$P_{i,j} = A_j / \sum_{nn} A_k \quad (7)$$

$$A_k = nc * cp + nw$$

where  $P_{i,j}$  is the probability of moving from site  $i$  to site  $j$ ,  $nc$  is the number of neighboring sites occupied by cells,  $nw$  is the number of neighboring sites occupied by polymer wall,  $cp$  is the ratio of cell-cell cohesivity to cell-polymer adhesivity, and  $\sum_{nn} A_k$  is the sum of  $A_k$  over all sites that are nearest neighbors to site  $i$ .

In addition to migrating, the cells can proliferate. Each cell is initially set to proliferate at a time randomly drawn from a normal distribution. At each time step, a counter indicating the cell's time to proliferation is decreased until it becomes negative, indicating that the cell should now divide. If space is available in one of the adjacent lattice sites, the cell will divide and the resulting new cell will occupy that site. The counters for both cells are again set randomly from the normal distribution of proliferation times.

The cells infiltrating the scaffold must maintain some physical connection to solid support, so no cluster of cells can be completely disconnected from the wall. Moves that isolate a cluster of cells from the walls must be disallowed. Therefore, before a move is accepted, one must check that every cell neighboring the one about to be moved has some connection to the walls and that the cell in its new location will have some connection to the walls. This is done by a depth-first search (DFS) algorithm<sup>[13]</sup> adapted from that of Kevin Murphy, found at <<http://www.cs.ubc.ca/~murphyk/Software/>>. The DFS is the most computationally expensive part of the program.

It is instructive to compare the lattice model formulation of

this “diffusion and reaction” problem with an attempt to cast it as a system of differential equations. The physical condition that no cell or cluster of cells can float unconnected to the solid support of the walls is particularly difficult to describe in the language of differential equations.

Since such a project involves a fair amount of coding effort, we provided the MATLAB code to the students. We asked them to run it for various values of macropore spacing, micropore fraction, and  $cp$  and to examine how these factors affect the time taken for cells to reach the top of the lattice and how the concentration profile of cells in the pore space varies. At low  $cp$ , the cells tend to penetrate into the lattice by crawling up the walls and leaving the centers of the macropores relatively empty. At higher values of  $cp$ , however, the increased preference for other cells over polymer walls results in a fairly uniform front of cells penetrating through the lattice. In this latter case, the cell proliferation rate determines the progress of the front, rather than the rate of migration along the walls. All of this is only possible if the micropore fraction is high enough to permit percolation from one end of the lattice to the other. Above this critical value, the micropore fraction has minimal impact on the rate of cellular invasion.

For a reasonably large system of a few hundred lattice sites in each direction, the naive neighbor-searching algorithm we implemented (in which all cells are examined as possible neighbors) runs into recursion limits during the depth-first search. We wanted the students to run simulations for several different sets of parameters in a relatively short time, so we initially disabled the depth-first search, decreasing the run times to a minute or less even for large systems. Of course, this also meant that groups of cells could detach from the walls, unlike the work of Shea and Pasquini. Since we wanted the students to examine how the code actually worked, we refrained from explaining the physical meaning of  $cp$ , instead requiring the students to infer its meaning from the way in which it is used in the code. We also had the students modify the code to make the function call to the depth-first search routine and run simulations within a single small macropore, which took a few minutes per simulation. Students were additionally questioned about ways in which to make the full simulation more efficient by using a better neighbor-searching algorithm. Given sufficient time, the implementation of a grid-cell based neighbor-searching algorithm could be a useful programming exercise.

Thus, although the students were saved much of the grunt work involved in writing the code, they had to become fairly familiar with its workings to receive full credit. The code is fairly well commented except for the deliberate omissions regarding  $cp$  and the routine in which the depth-first search is called. Most students were able to do this assignment without much assistance after being provided with the above details on the physical system and the overview of the code contained in the README file.

## STUDENT RESPONSE

Despite the grumbling that ensues when students are prodded out of their comfort zones, most of them were able to complete these assignments without a great deal of difficulty. In general, we noticed that the qualitative and open-ended questions proved more taxing than actually solving the differential equations or running the agent-based simulations. Most of the students were interested in biological applications but had not encountered many at this stage of their education. This, coupled with the novelty of agent-based modeling, added to interest in the tissue engineering example. Though the students would have learned more through coding the entire lattice model themselves, we feel reasonably satisfied that they have been exposed to using and modifying a relatively large piece of code, an accomplishment in itself, in the short span of a couple of weeks. If one wished to use this example in a course with more programming, the project could be extended by having students implement a more efficient neighbor-searching algorithm or modify the code further to reproduce some of Shea and Pasquini's other results,<sup>[11]</sup> such as those for multiple cell types invading the scaffold or for cells initially being seeded throughout the scaffold.

## ACKNOWLEDGMENT

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# USING A READILY AVAILABLE COMMERCIAL SPREADSHEET

## To Teach a Graduate Course on Chemical Process Simulation

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For chemical engineering graduates, being able to use a chemical process simulator is considered as a *sine qua non* of the discipline, yet relatively few students have a direct appreciation of what is involved in constructing a chemical process simulator. The complex chemical process simulators, such as ASPEN and HYSYS, that are almost universally known to chemical engineers, have significantly streamlined the task of chemical process design. Efficient these simulators are, however, they also mask myriad complex calculations. Thus one of the end results is that users of these software packages may not have a full appreciation of how elegantly and succinctly process simulators intertwine almost all aspects of chemical engineering from thermodynamics to equipment design to cost estimation.

An ancient Chinese proverb says, “Tell me and I’ll forget; show me and I may remember; involve me and I’ll understand,” and it was with this mind-set that Professor P.R. Bishnoi (one of the founders of Hyprotech) developed, in the mid-1980s, a post-graduate course in process simulation in which students would enhance their understanding of process simulation by constructing all, or part, of a chemical process simulator. In the initial years of its existence, individual students constructed relatively simple simulators, using FORTRAN 77, to solve a specific problem rather than to serve as a general process simulator. In the 1990s, there was a shift from FORTRAN 77, a procedure-oriented language, to C and then finally to C++, which is an object-oriented language. The use of an object-oriented language allowed for the creation

of re-usable blocks of code that could be connected in a near infinite number of configurations, thereby greatly extending the generality of the students’ simulator. As the scope of the term project became more complex over the years, it necessitated a migration from individual term projects to a format in which all of the class member would contribute to a single final project. To the best of the author’s knowledge, this course is unique and is not offered, in this format, at any other institution.

Following Professor Bishnoi’s retirement, this course took an extended hiatus from the list of courses available to graduate students in Chemical and Petroleum Engineering at

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the University of Calgary. At the time of its resurrection, in 2007, much had changed in the world of chemical engineering education and computing, particularly with respect to students' familiarity with structured programming languages. Thus, the decision was made to do the project with a more familiar platform: that of MS Excel with VBA. While it is not possible to construct a stand-alone simulator using Microsoft Excel, it was an attractive choice because it provides a convenient platform for entering and displaying data and because it is almost universally known to post-graduate students in chemical engineering. The use of spreadsheets for various chemical engineering calculations is not new and has been documented in many sources.<sup>[1-5]</sup> What makes this course unique is that Excel is being used to create an "all-purpose" simulator, with a built-in graphical user interface (GUI), for solving simultaneous heat and energy balances.

Additionally, unlike traditional graduate courses in chemical engineering, this course is distinctive in that it is a group effort, rather than a solo pursuit. Because of the sheer size of the project, it is not feasible to expect each student to construct his or her own simulator in a one-semester course. Thus, each student is given a task and, toward the end of the semester, the pieces are fit together to produce a working simulator.

Because of the unique nature of this course, this paper is being written to evaluate the delivery format of the course and the effectiveness of teaching chemical process simulation in a "hands-on" format.

## COURSE DESCRIPTION AND DELIVERY FORMAT

The idea of learning by doing is not a new one; the great Italian renaissance polymath Leonardo Da Vinci once said "Knowing is not enough; we must apply. Being willing is not enough. We must do." The objective of this course is to give to the students hands-on experience at developing a general-purpose, steady-state, chemical process simulator and to understand the various types of computations involved in such a simulator. In this respect, it's as much a course in software design as it is a course in chemical engineering.

In the university's calendar, the course was allocated three hours per week for lectures, of which half was used for lecturing and presenting new material and the other half was used for a weekly seminar in which students would individually discuss their previous week's progress and their goals for the following week. This seminar was particularly important since two of the students were employed full time. The material covered in the lectures was, for the most part, not entirely new to the students and consisted of a review of basic heat and energy balances and unit operations, selected topics from numerical methods and computational thermodynamics, and sequencing. Sequencing, which will be discussed in more detail later, was the only section that was completely new to the students. At several points throughout the semester, an invited speaker who worked in the chemical process simulation field

gave lectures on object-oriented programming fundamentals and on how to put all of the components together to form the final product.

Because the course was primarily a group effort, evaluation of the students' progress was not a trivial task. As alluded to earlier, each student was given a specific task to work on and then at the end of the semester, the pieces were assembled into their final magnum opus. Thus, for roughly the first two-thirds of the semester, each student worked independent of the others and it was felt that the appropriate method for midterm evaluation was a combination of a written report and an oral exam for each student. These components were each worth 15% of the final grade. In the latter portion of the semester, the students were collaborating much more closely than in the early part of the semester and thus the term-end evaluation consisted of a final oral presentation and exam for each student, worth 25% of their grade, plus a single final report submitted by all group members, worth 45% of the final grade.

## WHAT THE STUDENTS THOUGHT THEY WERE TAKING

The aforementioned course was first offered to graduate students more than 20 years ago. Due to the original instructor's retirement, however, the course had not been offered in almost five years. Thus, students were not able to learn about the course by word of mouth and the only information available to the students regarding the course came from the university's catalog description, which, at the time read

*"Chemical Process Simulation: Synthesis. Analysis and screening of process alternatives. Steady state simulation. Material and energy balances for systems of process units. Modular approach. Heat exchanger network and separation processes."*

When this course description was first conceived, two decades ago, it quite adequately conveyed what the course was about. Most of the 12 students that arrived to class on the first day of the semester were expecting something completely different, however. When I asked the students what they were hoping to achieve in taking this course, responses ranged from "HYSYS training" to "I need an easy course for my professional registration." When I handed out the course outline to the students, a great silence fell across the room and faces paled at the revelation that this was not a software training course, that this would not be an easy course, and that they would have to do the programming themselves. The end result was that the class size dropped from 12 to four by the second lecture. (It should be noted that, because of the necessary division of labor, four students is the minimum number necessary to run the course.)

After re-examining the calendar description quoted above, I felt it could be written to better elucidate the course content. For the upcoming year, the calendar entry has been changed to make it explicitly clear that it is an

object-oriented programming course. It now reads:

*“Chemical Process Simulation: Object-oriented programming applied to the design of a steady state chemical process simulator via the sequential modular approach and by the equation-based approach. Material and energy balances for systems of process units.”*

It was felt the above wording would not only inform students that it is not a software training course, but it would also inform other students that it is a programming course.

## WHAT SKILLS THE STUDENTS HAD TO LEARN

The students enrolled in the course had a diverse academic background and each brought certain strengths to the project. As previously mentioned the lecture content included topics from basic chemical engineering, numerical methods, thermodynamics, and sequencing. Thankfully, all students were well versed in the basics of chemical engineering and numerical methods and thus it was not necessary to devote significant lecture time to these topics.

Computational thermodynamics, on the other hand, was a subject with which the students had little direct experience. Thus, this section included a review of vapor/liquid equilibrium, equations of state, activity coefficient models, bubble point and dew point calculations for nonideal systems, isothermal/isobaric flash calculations, isenthalpic/isobaric flash calculations, isentropic/isobaric flash calculations, and Gibbs free energy minimisation for reacting systems.

Sequencing, as mentioned previously, was the lone topic that was completely new to the students and the lectures were devoted to presenting various algorithms for determining in which order the unit operations should be solved.

The biggest deficiency in the students' knowledge base, however, was not in any of the chemical engineering topics; it was in object-oriented programming. Maixner<sup>[6]</sup> observed that after taking basic engineering computing, students “usually allow their programming skills to stagnate.” While some of the students were out of practice with respect to programming, it was found that for 100% of the students, their knowledge was limited to procedure-oriented programming. The advantage of an object-oriented approach is the ability to solve and test individual modules together and the ease with which modules can be combined, solved, analyzed, and swapped.<sup>[7]</sup>

After the semester, the three remaining students were asked, among other things, what skills they had to learn and their responses are listed below:

- “Thermodynamics, unit operations, programming, logical thinking, teamwork.”
- “During the course, we learned some concepts of OOP, thermodynamics, simulation solver other than extensive use of computer programming.”
- “Teamwork.”

## ORGANIZATION OF THE SIMULATOR

The construction of a steady state, sequential, modular simulator is a daunting task when first approached by students and it's not feasible for individual students to construct their own simulator in a one-semester course. Thus, the project was done as a group project in which each student was assigned a part of the object-oriented simulator to construct. Initially, one student was assigned to create a GUI and component database, one student was assigned to create the thermodynamic routines, one person was responsible for the unit operations, and the remaining member was responsible for sequencing. Midway through the semester, the student in charge of the thermodynamics routines withdrew from the class and these duties were subsequently divided among the remaining group members. Fortunately, one of the remaining students had previous exposure to computational thermodynamics.

The program is composed of a GUI, information sheets, thermodynamic routines, unit operations routines, and the sorting/tearing algorithm—all of which interact with each other, as shown in Figure 1. In the ensuing subsections, a brief description of each section of the program is provided.

### Information Sheets

The information sheets, which are merely Excel worksheets, provide a platform for entering and displaying data and for storing thermodynamic component data. Data is read from and written to the appropriate worksheet using the built-in *cells()* function.

### GUI and Component Database

The graphical user interface was constructed in Excel using the built-in VBA editor. Once the equation of state and the components for the new project have been selected, the program closes all dialogs and takes the user to the main interface window, where the Process Flow Diagram is built.

On this page, the program shows the core of the graphical user interface: the “Unit Operations” tool bar. This tool bar is divided in five main sections: adding new unit operations,

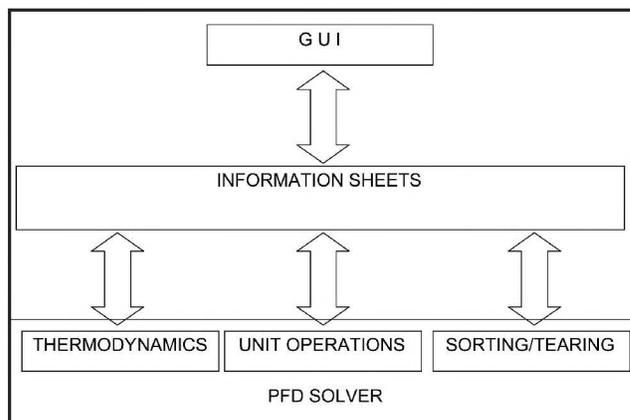
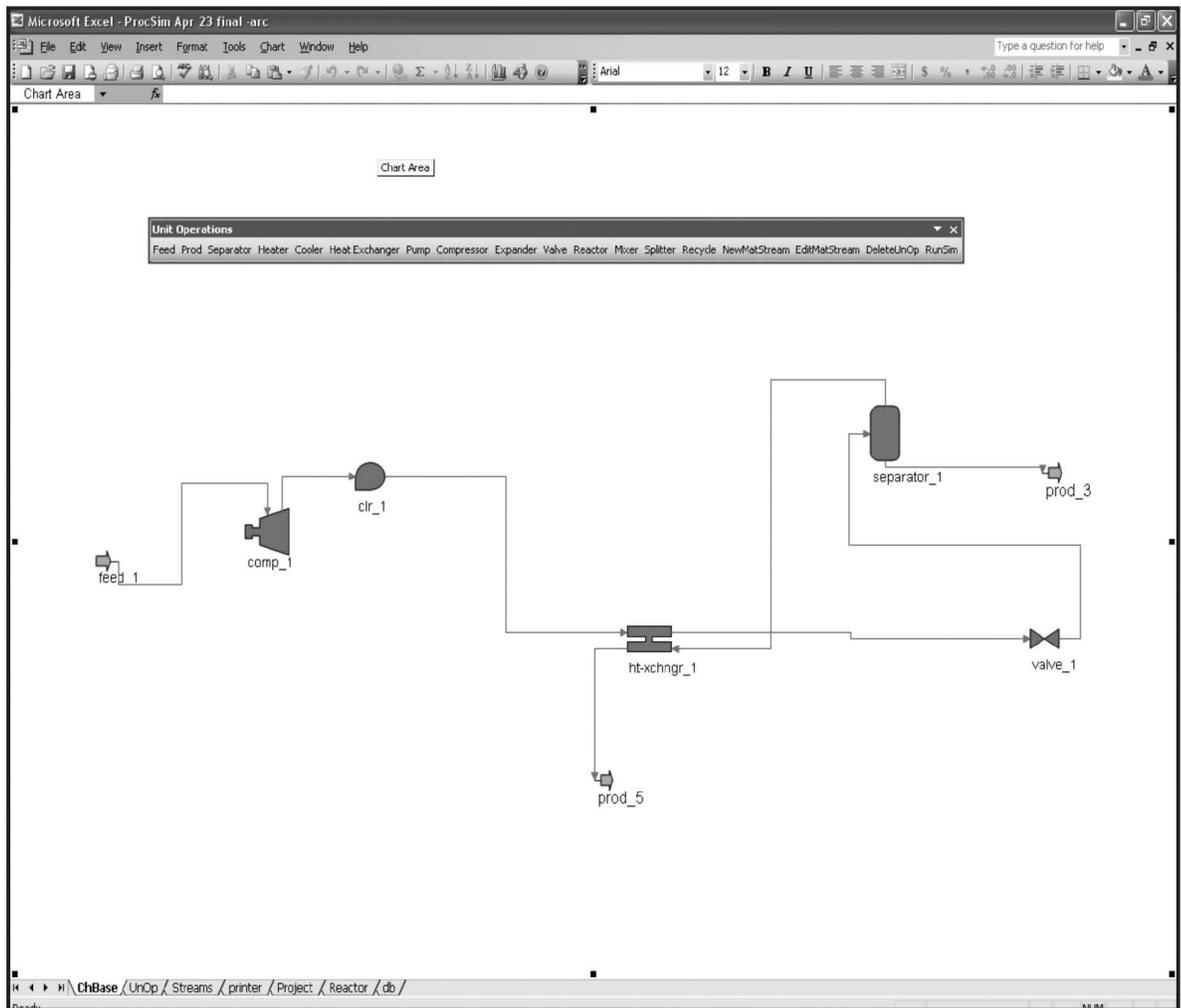


Figure 1. Block diagram for the simulator.



**Figure 2.** Screen capture of a typical flow diagram.

1	Type	STREAM S1	STREAM S2	STREAM S3	STREAM S5	STREAM S6	STREAM S7	STREAM S4
2	Name	S1	S2	S3	S5	S6	S7	S4
3	Inlet1							
4	Inlet2							
5	Inlet3							
6	Inlet4							
7	Outlet1							
8	Outlet2							
9	Outlet3							
10	Outlet4							
11	Pressure	2100000	2100000	2100000	2099000	2100000	2102000	2100000
12	Temperature	273	273	273				273
13	flowrate(mol/s)	1000	773.8285	226.1715	1000	1000	773.8285	1000
14	Vapour fraction	0.767096	1	0				1
15	Enthalpy(J/mol)				1000	1000		1000
16	Entropy(J/mol K)							
17	Molecular weight(g/mol)	28.04	24.3801	40.56207	28.04	28.04	24.3801	28.04
18	Molar Composition							
19	CH4	0.55	0.68049	0.103538	0.55	0.55	0.68049	0.55
20	C2H6	0.04	0.040441	0.03849	0.04	0.04	0.040441	0.04
21	C3H8	0.4	0.267451	0.853506	0.4	0.4	0.267451	0.4
22	CO2	0.01	0.011618	0.004466	0.01	0.01	0.011618	0.01
23	vapour phase							
24		0.685985	0.68049	0	0	0	0.68049	
25		0.040491	0.040441	0	0	0	0.040441	
26		0.261881	0.267451	0	0	0	0.267451	
27		0.011643	0.011618	0	0	0	0.011618	
28	liquid phase							
29		0.102117	0	0.103538	1	1	0	
30		0.038384	0	0.03849	1	1	0	
31		0.854911	0	0.853506	1	1	0	
32		0.004588	0	0.004466	1	1	0	

**Figure 3.** Screen capture of the "Streams" worksheet.

adding a material stream, editing a material stream, deleting a unit operation, and running the simulation.

### Thermodynamics

Thermodynamic calculations represent the basis of the simulator, since all the unit operations are assumed to reach the equilibrium. To develop the current simulator, two equations of state have been selected: the Soave-Redlich-Kwong (SRK) equation of state<sup>[8]</sup> and the Peng Robinson (PR) equation of state.<sup>[9]</sup> As part of the process simulator, we are generating the value of thermodynamic properties (enthalpy and entropy), thus, the designation of a reference state becomes essential. For this simulator, the reference state that was chosen was an ideal gas at 273.15 K and 1 Pa.

The thermodynamic routines provide a necessary support for the unit operations in that they calculate necessary outlet conditions such as temperature, pressure, and/or composition. Depending upon the specific unit operation, these values are calculated with the aid of a constant-temperature/constant-pressure flash routine, a constant-enthalpy/constant-pressure flash or a constant-entropy/constant-pressure flash. The values of the thermodynamics quantities, such as entropy and enthalpy, are calculated by using the appropriate departure function<sup>[10]</sup> in conjunction with an equation of state. In addition, a Gibbs free energy minimisation routine was implemented to support the reactor unit operation. The algorithms for each of these routines are available in the open literature.<sup>[10-12]</sup>

### Unit Operations

To code the unit operations, an object-oriented programming philosophy was adopted. For this section it is important to introduce some related terminology, mainly the object, class, properties, and method. An object is defined as a programmable entity with specific characteristics and features,<sup>[13]</sup> a class is what defines the object and serves as the template or blueprint for all the objects created from that class; any of the object's particular features, including properties, methods, and events, are handled by the class module.<sup>[13]</sup> Properties are all the characteristics and features of the object without executing any action, and method is an entity that provides the actions supported by the objects created from the class.<sup>[13]</sup> Methods are defined as the abilities, or actions, that the object can carry out.<sup>[13]</sup>

Basically, a module class was created for every single unit operation; this class contains the most important properties and methods. In addition, modules were included to collect the inputs from the interface, which become the properties of the class and present the results again on the interface. Unit operations that were included in the project were separators, valves, pumps, compressors, expanders, heaters, coolers, heat exchangers, mixers, splitters, recycle loops, and a Gibbs free energy minimization reactor. The details of the individual unit operations are available in any standard chemical engineering textbook.<sup>[14]</sup>

### Sequencing

Sequencing is a term that essentially refers to the process of figuring out the order in which each of the unit operations should be solved. The sequential modular approach is the most popular approach and there are a number of commercial simulators that use this solution methodology. "Sequential modular" simply means that calculations start with known feeds, and continue on a unit-by-unit basis until all unit operations in the flowsheet are calculated.<sup>[15]</sup>

In sequential modular approach, the material balances for an entire process are solved one module (process block) at a time. For sequential modular material balance calculations, the output streams can be calculated if the input streams and the module parameters are known.

### VALIDATION OF THE NEW SIMULATOR

A case study was initiated to study how the new Process Simulator compares with the popular commercial simulator, Aspen HYSYS. The simple case illustrated the capability of the new Process Simulator for performing reliable chemical process calculations for the Linde Process. Methane is usually liquefied in a Linde process. Initially, the vapor is compressed to 6MPa and cooled at 300K. Subsequently the vapor passes through a heat exchanger before reducing its pressure (to 0.1MPa) through a valve. The unliquefied fraction leaves the separator at the saturation point and passes through the heat exchanger exiting at the end at 295K. A screen capture of the flow diagram and the constructed worksheet for the process used in the case study is presented in Figures 2 and 3 (previous page).

The components that were present in the case study were methane, ethane, propane, n-butane, and carbon dioxide. The fluid properties were calculated with the PR equation of state. It was found that all of the stream compositions, temperatures, and pressures as calculated by the new simulator were within 1.5% of the values calculated by the commercial simulator.

### EVALUATION OF THE COURSE FROM A STUDENT'S POINT OF VIEW

As previously mentioned, at the conclusion of the course, the students were asked for their feedback. In addition, one student (who is the second author on this paper) provided a detailed evaluation of the course. The following paragraphs are his evaluation of the course:

*"The construction of a steady state, sequential modular simulator represented an immense challenge for all the members of the group since none of us had done anything similar in previous courses. The experience acquired until that moment with programming languages was limited to very "simple" algorithms dedicated for particular cases. Thus, when the distribution of the work was assigned by the professor, a sensation of confusion came up in the group because nobody was really sure about how to tackle the*

problem. Since the beginning of the semester, this course was different from the ones a regular graduate student usually takes, where the professors impart lots of information in the lectures. In this case, the classes were divided in two sessions per week; one of them was a lecture reviewing the basic tools that we required to complete this course successfully and the second one was a group meeting to show everyone's progress, difficulties, and critical points, etc.

During the first few weeks, the work was done independently; each of the members of the group wrote his or her own code without considering anybody else's problems or difficulties. Integration of the code was not the main concern in that particular moment. But, fortunately, the professor invited as guest lecturer a former student who had taken the course a few years ago; he basically commented about his experience in creating a process simulator. His main contributions to us were definitely the concept of working as a group and the fact that it is necessary to completely define the structure of the simulator on a piece of paper before any coding is done; in addition, he highlighted that the final product should be written with the mind-set that it is going to be used by an external user. From that moment on, teamwork began and it was established how the simulator was going to work and what kind of special characteristics should be included. For instance, definition of the variables that would be supplied by the user, the variables that would be public (available for all the program) or private and the possible inconsistencies due to errors when wrong data were supplied by the users, final outputs, etc.

Once the designing stage was finally done, all of the members of the group had to recode a big part of our programs to make them suitable for the final integration. After having succeeded on this, the skeleton of the whole simulator was ready. The following phase was to complete the rest of the thermodynamic algorithms and unit operations, which was a lot easier due to main parts being already done. The first simulator was really big and it was really difficult to handle, thus, some parts of the program were recoded once again to make them better. In this part of the work a very helpful support was provided from one student at U of C whose knowledge in Visual Basic for Applications was far beyond any of the other members of the group. His main contributions were the implementation of useful techniques and hints to reduce the number of lines in the program and increase the speed of processing. One of the most challenging parts was the debugging of the code; from our point of view the best way to debug any long program is by ensuring that every piece of code is working properly rather than to verify the whole program. It is also important to keep in mind that a minimum knowledge is required of programming, creation of algorithms, numerical methods focused on the solution of single and simultaneous systems of non-linear algebraic equations, sorting, matrixes, etc. But the most important thing is to always be motivated and be open to learning new concepts. At the end of the term, the group was really satisfied with the final product; since we were able to reproduce the results of commercial simulators by using simple programs."

Additional comments by the other students are given below:

Which parts were the most challenging?

- "Finding the best way to represent the unit operations and connect the graphical part to the database in Excel."
- "The most challenging part was debugging. The algorithm initially written was not the best one. The program went very big and was just too big to handle."

Problems to comment on for future students?

- "Teamwork is a key component in this course."

Which skills you got to the end of the course?

- "Computer programming skills, basic structure of simulator, simulation solver knowledge. Above all we learned how to put together a simulator."

## EVALUATION AND RECOMMENDATIONS FROM THE INSTRUCTOR'S POINT OF VIEW

The structure and content of the course make it unique among graduate courses in chemical engineering at the University of Calgary and thus it presented many challenges to the instructor. As previously mentioned, this was the first time in almost five years that the course had been offered, and in spite of that fact, the overall sentiment of the instructor was that the course achieved its desired outcomes.

Over the course of the semester, there were only two negative events to dampen evaluation of the course. The first was that, as previously stated, a large number of students enrolled believing the course would be a software-training course. It is also hypothesized that some students—who may have been keen programmers—avoided the class for the same reason. Secondly, the number of students was below the optimal number for the course. When one of the students withdrew from the course, a tremendous burden was placed upon the remaining students.

Conversely, many aspects of the course were extremely positive. The total project was divided into manageable parts and, at the end of the semester, each student was able to say that they had not only learned how to program a part of the simulator, but they also benefitted from having to work in a team environment. The regular weekly debriefings not only allowed the students to receive weekly feedback from the instructor, but they also served to educate each group member as to what challenges the other members were facing with their programming. Additionally, the use of Excel as the programming platform was advantageous. While Excel may not have all of the capabilities of high-level programming language, such as the ability to create a stand-alone executable file, the fact that students had previous exposure to it and the fact that student access to Excel is practically universal made it the best choice for the course.

For any instructor that is contemplating offering a graduate course in simulation, I would make the following recommendations:

1. Ensure that the calendar description clearly conveys that it is a course in software design and not merely a software-training course.
2. Advertise a detailed synopsis of the course well in advance of the beginning of the term.
3. Stipulate a minimum of six students. This ensures that if one or two students withdraw partway through the term, the remaining students are not overly burdened.
4. To attract and retain a larger number of students, include minimal hands-on work with a commercial simulator, perhaps as a means of illustrating lecture topics.
5. Spend the majority of lecture time covering object-oriented programming fundamentals, computational thermodynamics, and sequencing.

## CONCLUSION

A post-graduate course on chemical process simulation was offered in the Department of Chemical and Petroleum Engineering at the University of Calgary in which students were given the opportunity to construct a chemical process simulator as a group project. Microsoft Excel, along with its built-in Visual Basic for Applications (VBA) programming environment, was used to create a fully functioning modular chemical process simulator. An object-oriented approach was used to create and combine the necessary sections of the simulator; mainly the graphical user interface and component database, the thermodynamic routines, the unit operations, and the sequencing algorithms. The result is a fully functioning, steady state, chemical process simulator that is capable of matching the results of the far more expensive commercial simulator, as was seen with the validation study. Student feedback on the course indicated that the students learned a great deal with respect to both software design and to working in a team environment. From the instructor's point of view, the

course was successful in achieving its goals and recommendations for future offerings of the course were made.

## ACKNOWLEDGMENTS

The authors would like to acknowledge Dr. Ryan Krenz from the Virtual Materials Group in Calgary, Alberta, for sharing his experiences in creating object oriented process simulation tools.

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## ARE THE STEAM TABLES DEAD?

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Are the steam tables dead? I have recently had two strong hints that appeared to indicate that what we know as the “steam tables” (tabulations of volumetric and energetic properties of saturated and superheated water) have slowly but surely died. In the first place I managed to buy, through a used book dealer, a very nice copy of the Keenan steam tables. This is a 1930 edition that included in an inside flap a beautiful Mollier diagram as large as my own desk. The book is in pristine condition, properly printed and beautifully hardbound, and all—for the staggering price of 50 cents. This is not only a collector’s item, but also a very useful tool still. Extensive tables with a very fine grid of temperatures and pressures allow precise calculation of the thermodynamic properties of water. Looking up, for example, at 520 °F and 39 psi, this table reports a specific volume of 14.838 ft<sup>3</sup>/lb. Considering that the density of water has not changed with time, the result is still of acceptable accuracy for most purposes (a reliable<sup>[1]</sup> value today would be 14.845 ft<sup>3</sup>/lb—a difference of less than 0.05%). The other parallel event that sparked my imagination was that I managed to download to my PDA a steam table program<sup>[2]</sup> (which also gave me the expected 14.84424 ft<sup>3</sup>/lb answer for the state point in question). So, why have my steam tables not gone the same way as logarithm tables, which disappeared sometime after I left high school?<sup>[3]</sup> For some reason thermodynamic tables have endured the passage of time, and most major modern thermodynamic textbooks have abridged versions as appendices. You can buy many versions of these “smaller” classroom tables<sup>[4]</sup> (so they must be used extensively by someone). Furthermore, you can buy a “new” edition<sup>[5]</sup> of my recently acquired Keenan tables. In fact, they are obviously not things of the past, if one notices that this year a new version of the International Steam Tables was published.<sup>[6]</sup>

A rapid (non-exhaustive) search<sup>[7]</sup> showed me that steam tables are also available as spreadsheet plug-ins,<sup>[8]</sup> as commercial<sup>[9]</sup> and academic<sup>[10]</sup> stand-alone programs for PCs, and as phone<sup>[11]</sup> applications, just to mention a few. Special mention has to be made to the NIST Webbook.<sup>[1]</sup> This is an outstanding resource that allows the precise and efficient determination of

thermophysical properties of a rather significant amount of fluids with all the usual features one would typically require: choice of units, choice of conditions, display of an array of volumetric, energetic, and derivative properties, generation of tables and graphs that can be “cut and pasted” to other places, etc. Three things make it stand out among all other options, however

- It is accessible through the Internet via a Web page, so it is not device-specific. All calculations are done on the remote machine, so it is also fast.*
- It is free, with no needless registration procedure or cost to the user. A very generous and highly appreciated gesture.*
- It is state-of-the art and in constant update in terms of the equations of state used to generate the data. All this means that any computer connected to the Web can automatically be converted into a “steam e-table,” therefore the utility of the site cannot be underestimated.*

So, is there any point in continuing the discussion? A common argument in favor of insisting on the use of “paper” tables is that learning to use them will teach students about the different regions of the phase diagram (since the boundaries where the tables end usually coincide with the boundaries of the change of behavior: saturation, ideal gas, etc.). It is hard to think that this is not a biased opinion, for the programs have limits also. I started to look at other data points using my palm-held program, for example raising the pressure at the given temperature. For 2500 psi (@520 °F) it refused to give me an answer. Granted, the table did not have an answer either. It would take some basic knowledge on thermophysical properties to recognize that by increasing the pressure above the saturation line the system would be in the liquid state, and

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if no other information were available, the low compressibility of the liquid phase would allow one to use the specific volume at saturation (0.37693 ft<sup>3</sup>/lb) as a likely estimate.<sup>[12]</sup> Another repeated argument is that given a computational tool—be it a process simulator or simply a spreadsheet add-in—a lecturer can focus on more elaborate problems which may involve, for example, taking the thermodynamics into its context for typical engineering applications.

Does this then back the hypothesis that we should shelve our tables forever? Please think again. A problem with using computer programs (or Web pages, or phones), apart from the fact that they are useless when no electricity is present, is that one can easily fall prey of the “black box syndrome,” a condition in which the brain ceases to perform its usual analytical functions while the user simply inputs numbers and accepts the response from his or her electronic instrument without questioning. Prausnitz<sup>[13]</sup> warned us of this many years ago when he stated, in the onset of the computer age, “Never be impressed by calculated results merely because they come out of a computer. The virtue of a computer is speed, not intelligence.” I think, however, that the student who recently reported reading from a table the density of liquid water at STP to be “roughly 1, umm, kg/m<sup>3</sup>” wasn’t actually thinking much anyway.

Although it is not the subject matter of these lines, computers offer (at least in theory) the ability to visualize 3-D thermodynamic surfaces (for example the P-v-T surface) interactively. This is particularly useful when studying phase equilibria of mixtures, where the usual graphs are slices of a more elaborate and complex surface. Prof. K. Jolls (Iowa State) has made a lifetime effort of providing thermodynamics students with such interactive and pictorial representations.<sup>[14]</sup> In spite of the fact that there is no doubt about the enormous pedagogical value of these and similar representations, it is clear that they are still emerging technologies, and e-tables still dominate the field.

An important argument is that while for water the thermophysical properties are well known and documented, they are not so for many other simple fluids, let alone the more complex or exotic ones. Therefore, even today, the chemical engineer will have to deal with sometimes just a few sparse data or an odd table, from which he or she must interpolate,

correlate, and sometimes even estimate data. This is a daily task for any practicing engineer, and it is up to the thermodynamics lecturer to train students for this awful reality. Perhaps the best course of action is to do both: teach the use of the programs and resources while simultaneously showing students the “facts of engineering life”—one of them being that you will never have as much information as one would desire for a given system. Probably we still have to teach them some “old school” methods. So with this in mind, I sent my dutiful students out to buy their abridged steam tables sold in the bookstore, wondering if next year the answer to the question will be different.

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<http://cee.che.ufl.edu/index.html>

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