

EDITORIAL AND BUSINESS ADDRESS:

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CHEMICAL ENGINEERING EDUCATION (ISSN 0009-2479) is published quarterly by the Chemical Engineering Division, American Society for Engineering Education, and is edited at the University of Florida. Correspondence regarding editorial matter, circulation, and changes of address should be sent to CEE, Chemical Engineering Department, University of Florida, Gainesville, FL 32611-6005. Copyright © 2006 by the Chemical Engineering Division, American Society for Engineering Education. The statements and opinions expressed in this periodical are those of the writers and not necessarily those of the ChE Division, ASEE, which body assumes no responsibility for them. Defective copies replaced if notified within 120 days of publication. Write for information on subscription costs and for back copy costs and availability. POSTMASTER: Send address changes to Chemical Engineering Education, Chemical Engineering Department, University of Florida, Gainesville, FL 32611-6005. Periodicals Postage Paid at Gainesville, Florida, and additional post offices.

Mississippi State's

Kirk Schulz

JULIE M. LEMONS

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Balance. It's one thing that all of us strive for daily, but it seems to come quite naturally for Kirk Schulz, dean of the James Worth Bagley College of Engineering at Mississippi State University. If you know him or have ever worked with him, then you know what I'm talking about. He seems to get more accomplished in one day than most of us do in a week. And although his dedication to his work is obvious, his commitment to his family is even more evident.

Kirk has been called approachable, accessible, and a great listener, and he has also been characterized as quick-witted, decisive, and driven—quite a combination for a 42-year-old dean. One MSU engineering alumnus and advisory board member recently spoke of Kirk saying, “He is open to new ideas and new ways of doing things, but more than that he follows through and implements those ideas.” Kirk is not one to sit around and wait for things to happen; he is a man of action and integrity with a strong desire to move his engineering program into the Top 50.

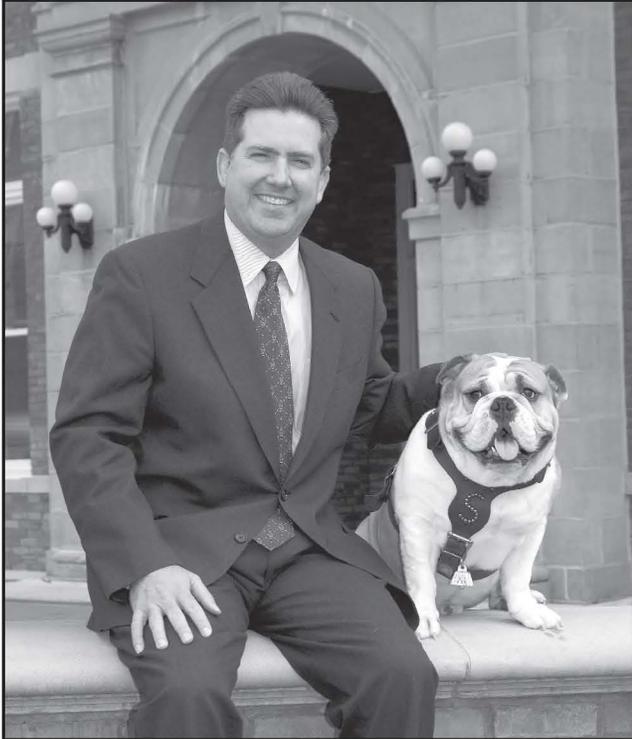
Faculty excellence is at the top of every dean's list of priorities. Deans want to see their professors excel as mentors and leaders, knowing that their efforts are molding the young minds of our world's future leaders. Kirk knows that faculty excellence is the foundation of a top-tier institution and such excellence is crucial to the success of all its programs. Recognizing faculty for their accomplishments and successes in teaching, research, and service is important to him and to the continued excellence of the engineering program at Mississippi State. Simply put, Kirk is an administrator who enables faculty to do what they do best—teach others to become contributing leaders in their fields.

MSU Provost Dr. Peter Rabideau remarks, “Kirk is one of the most enthusiastic and energetic administrators with whom I have been associated. He supports quality as the number one issue, and he wants to work with faculty, staff, and students to develop a vision that will move MSU engineering to the next level of excellence.”

As the new dean of the Bagley College of Engineering, Kirk has established the Academy of Faculty Fellows to recognize those who have risen



Kirk updates alumni and friends of the Bagley College during Engineering Day on campus this past fall.



to the rank of Fellow in their respective engineering professional societies. This past year, 15 faculty members were inducted into the academy. Another way that the college is recruiting new faculty and celebrating current faculty members' excellence is by honoring them through endowed positions. Currently, the Bagley College has 23 endowed positions, and in Kirk's inaugural year as dean he has made it a priority to fill these important faculty positions in the college. He has already filled nine endowed chairs or professorships as well as several other key leadership positions around the college including two associate dean positions, two department head positions, and a center director. With a stellar leadership team now in place, Kirk hopes to help Mississippi State's Bagley College of Engineering gain the recognition it deserves as one of the top research universities in the country.

HIS BACKGROUND

Born into a family of educators in Portsmouth, Va., during the summer of 1963, Kirk was destined to become a teacher. He was raised in Norfolk, Va., by parents who were both university employees—his father a mathematics professor at Old Dominion University, his mother an associate registrar and director of compliance.

In speaking of his parents, Kirk characterizes his father as an "outstanding teacher who does a great job engaging his students," and his mother as "very active as a researcher, doing very creative and innovative research in historical geography."

"Kirk is one of the most enthusiastic and energetic administrators with whom I have been associated. He supports quality as the number one issue, and he wants to work with faculty, staff, and students to develop a vision that will move MSU engineering to the next level of excellence."

—MSU Provost Dr. Peter Rabideau

As a student at Norfolk Christian High School, Kirk first realized that he had a natural bent toward mathematics and chemistry. He excelled as a leader throughout his high school years, and as a graduating senior he was awarded both the leadership and science awards. It was during his high school years that Kirk first gained hands-on engineering experience while participating in the Soapbox Derby. He learned how to machine different steels, use a lathe, and paint. Building a car and steering it down a long track seemed to suit him. He won the local Tidewater Virginia race, going on to represent his home state in the World Championships in Akron, Ohio, in 1977.

After graduating from Norfolk Christian in 1981 with 44 of his peers, Kirk actually wanted to study medicine and was advised to work as a volunteer in the emergency room to see if he would really like being a doctor. He recounts, "After about one year of volunteering at Norfolk General Hospital, I decided that I really wanted to go into engineering and not medicine." Kirk's father had always spoken highly of the engineering profession, which initially planted the thought in his head. After a family friend took it upon himself to give Kirk a tour of the chemical plant where he worked, the decision to pursue engineering was solidified. In 1984, with three years of undergraduate work under his belt, Kirk decided to transfer from Old Dominion to Virginia Tech to pursue his chemical engineering degree, receiving his bachelor's in 1986. At Virginia Tech, Kirk was actively involved in the Baptist Student Union, serving as president and statewide vice president. Kirk realized as an undergraduate that he wanted to continue his education at the graduate level and become an educator himself. While in graduate school, Kirk remained active in various organizations, even helping start a Scout troop at his church in Blacksburg, Va. The troop is still active today.

Kirk was the first Ph.D. student that Dr. David F. Cox ever advised at Virginia Tech, so needless to say they both learned much during their time together. Kirk was conducting research in metal oxide surface chemistry. Dr. Cox recounts his time with Kirk: "He helped set up my laboratory, did all the interfacing of computers and experimental apparatus, and wrote all the code for data collection and analysis. When he wasn't



Kirk as a Ph.D. student under Dr. David F. Cox at Virginia Tech.

working in the lab, he was founding a new graduate student association in our department, working on committees with the dean's office, and generally helping out with any departmental, college, or university task with which he was approached. It drove me crazy.

"I was a young assistant professor, and I kept thinking he would be able to accomplish so much more if only he would focus more of his effort on his research. In the end, we published 12 papers from his graduate research. Fifteen years and many students later, I feel extremely lucky when I have a graduate student that manages to produce one-third of what Kirk did. With each passing year my appreciation increases for Kirk's skill, dedication, and technical abilities. Unfortunately for him, I did not realize how good I had it when he was working in my lab."

Dr. Cox explains, "When Kirk was still a Ph.D. student, I asked him about his career goals in the hope that I could offer him some sound career advice. He told me even then (I kid you not) that he wanted to become a dean. I suggested to him that such a career path would be a waste of a good scientific career. Thank goodness he ignored my advice.

"Throughout his academic career he has continued to turn out excellent scientific work even as he became more and more involved in administration. Kirk is the most well-rounded academician I know. I continue to be amazed by his ability to perform so well in so many different arenas. These days, I go to Kirk for career advice rather than the other way around. Whenever I am asked, I take credit for all of Kirk's success, but the bottom line is I have learned more from him than he ever learned from me."

Kirk feels blessed to have had a large number of people play an integral part in the success of his career. "My father and my research adviser, Dr. David Cox, both stressed the need to work hard and to finish the things I started. Tom



With wife Noel at the Tower of London, above.



Left, Kirk presents Dr. Rand German with a medallion in honor of his new position as director of the Center of Advanced Vehicular Systems and holder of the CAVS endowed chair.

Owens, my first department chair at the University of North Dakota, really stressed the need to communicate with people clearly and to set high standards. Ed Fisher, my department head at Michigan Tech, and Wayne Bennett, former dean at MSU, both stressed the need to aggressively seek external support and private gifts for big, visionary ideas."

After receiving his Ph.D. from Virginia Tech in 1991, Kirk accepted a position as an assistant professor of chemical engineering at the University of North Dakota in Grand Forks, N.D.

His wife, Noel, an associate professor in electrical engineering and TVA Professor at MSU, recalls, "For two years during my Ph.D. work, I lived 325 miles away from our son Timothy and him. He was a single parent during the week so I could get my Ph.D. It was a challenging time, but we made it through because of Kirk's commitment to my advancement."

The two met during Noel's freshman year at Virginia Tech and connected during a mission trip to Kentucky that Kirk led.

"She has been my number one fan and has been willing to pick up her research program and move it when an opportunity came up for me," says Kirk of his wife of 18 years.

She echoes the sentiment saying, "Kirk has always been an extremely supportive spouse. Since he is several years ahead of me in his professional career, he has been a mentor all along—sometimes making the mistakes, then warning me about them."



Above, as director of the Swalm School of Chemical Engineering, Kirk taught the unit ops labs. Here, he is assisting students as they review their results.

Right, all active in Scouting, Kirk and sons Tim (now 15) and Andrew (now 11) have long enjoyed spending time together outdoors.



Kirk spent four years at the University of North Dakota before moving to Michigan Tech University as assistant professor in 1995. His leadership abilities were quickly recognized, and he was promoted to associate professor in 1998. That same year, he assumed the chairmanship of the Department of Chemical Engineering.

After several years heading chemical engineering at Michigan Tech, Kirk accepted a position at Mississippi State University in 2001 as director of the Dave C. Swalm School of Chemical Engineering and holder of the Earnest W. Deavenport, Jr., Chair.

Dr. Wayne Bennett, dean emeritus of the Bagley College of Engineering, recalls, "I recognized his leadership skills when he interviewed for the director's position of the Swalm School of Chemical Engineering. Under his leadership, the school progressed on every front. The undergraduate programs flourished, graduate enrollments increased, and the research set new records."

Success doesn't come without ample opportunities. This idea is something that Kirk recognizes, and he acknowledges that there have been several people throughout his career who have given him an opportunity when conventional wisdom would have said otherwise. One such individual was Bob Warrington, dean of engineering at Michigan Tech, who was willing to give a 35-year-old associate professor a chance to be a department chair very early in his career. Another administrator willing to take a chance was MSU Provost Dr. Peter Rabideau, who agreed to let a 41-year-old lead the university's flagship college. "Both of these individuals gave me an opportunity in my career that many people never get," comments Kirk.

HIS MOTIVATION

His motivation is simple: to make a difference in the lives of others, especially the students. Working with students and faculty is what Kirk enjoys the most about his job.

"Teaching at the university level in my mind is the real chance to make a difference in someone's life. If you ask an engineer who they had for chemical engineering reactor design, most can give you a name—even 20 years later. When you talk with alumni, you realize just how big an influence we have on a person during their formative years," says Kirk.

Kirk receives great joy and satisfaction from seeing his former doctoral students become successful in their careers. Dr. Alan Nelson, one of Kirk's first doctoral students, is now an associate professor and associate chair in the University of Alberta's Department of Chemical and Materials Engineering. Regarding Kirk's abilities as a professor, Dr. Nelson says, "I have a great deal of respect for Kirk, not only because he is a scholar and educator, but because he has been and continues to be a benevolent mentor to so many individuals. I would certainly not be where I am today without the research supervision and professional guidance Kirk has provided to me over the years."

Dr. Nelson goes on to say, "Kirk's ability to maintain personal and professional balance should be a model for all new chemical engineering faculty. He is a case study of how to be an effective and efficient educator, while not sacrificing his personal goals or time with his family."

Professors work hard to impart some vast wisdom or knowledge to the students they teach. The students will, of course, remember some of a teacher's meager efforts in the lab and

classroom and how he or she graded them, but in the end it is one's character that students take note of the most. It is how they are treated as students and how faculty respond to life and all its clichés that demonstrate what true "balance" in life is all about.

HIS FAMILY

Family is the most important part of Kirk's life. One favorite family activity at the Schulz house is Scouting, which probably has a little to do with having an Eagle Scout for a dad. Currently, Kirk is the assistant Scoutmaster of Troop 14 in Starkville. Son Timothy (15) is a Life Scout, while Andrew (11) is in Webelos. The Schulz family also enjoys spending time outdoors as well as traveling to a wide variety of destinations, such as Disney World, London, and San Diego—not to mention following the MSU Bulldogs to the SEC Basketball Tournament in Atlanta.

Kirk shares a good relationship with Noel's parents, and they have always been supportive of his professional career. While at Virginia Tech, Kirk was a student worker for Dr. Charles Nunnally, the assistant dean of engineering at Virginia Tech—and Noel's father.

Being a dean and having a wife who is an associate professor oftentimes means that the weeknights are booked with college or university events. It is not unusual for Timothy and Andrew to be present at some of these functions, and they are often a crowd favorite at such events.

Kirk made it a point when he first became dean of the Bagley College to let his staff and faculty know that the dean's office was a family-friendly environment. "We all have families and from time to time there are family situations that come before work. I want my staff and faculty to know that I support them personally and am here if they ever need anything," said Kirk.

Throughout the academic year Mississippi State will often host MathCount competitions and Science Fairs, and you will see the Schulz boys in and out of the dean's office visiting Dad. One of the most enjoyable visits to campus for his sons was during Engineering Week at MSU this past year. It was toward the end of the week and just so happened to be the same day as Timothy's MathCount competition. All week, engineering students had purchased tickets to "pie" a faculty member or fellow student as part of a fund-raiser. The activity on the Drill Field drew a crowd of curious onlookers, as Kirk and two other department heads sat bravely in anticipation of the firing squad of students and faculty that stood before them. It is not often that students, or faculty for that matter, get to throw a pie at their dean. Needless

to say, Kirk took it in stride and Timothy and Andrew were *greatly* amused.

HIS CAREER

Throughout his career Kirk's talent for administration and leadership have been recognized and have afforded him some wonderful opportunities. Of course, no one begins their career as a dean of a college; there are dues to pay and work to be done along the way. Kirk has traveled that path, working his way from a summer school chemical engineering instructor at Virginia Tech all the way to dean of a major state university.

Each engineering program that Kirk has been involved in has benefited from his leadership. As an administrator, much of his time and energy have been devoted to improving alumni relations, growing graduate programs, increasing the diversity of faculty and students, recruiting new faculty, and increasing external funding. With a strong desire to see faculty collaborating across the college at Michigan Tech, he assisted in the initiation of the Carbon Technology Center. This is a multidisciplinary research center involving faculty from chemical engineering, mechanical engineering, civil engineering, and chemical engineering technology in research focused on polymer composites. At Mississippi State, Kirk saw a need to make pursuing a Ph.D. in chemical engineering more enticing. So as director of the Swalm School of Chemical Engineering, he led the efforts to establish the first direct-admit doctoral program, increasing the number of Ph.D. students from three to 15 in three years.

"Whenever I am asked, I take credit for all of Kirk's success, but the bottom line is I have learned more from him than he ever learned from me."

**—Dr. David Cox,
Kirk's Ph.D. advisor
at Virginia Tech**

Kirk has shared his knowledge and research findings through 42 journal articles that he has authored or co-written; he has presented numerous conference papers and given 100 presentations. He has had over \$1.8 million in funded research projects and has provided guidance to six doctoral students and 14 master's students.

Kirk is currently co-chairing the Chemical Engineering Division of ASEE's 2007 Summer School for Chemical Engineering Faculty, which will be hosted on the campus of Washington State University. His service to engineering professional organizations does not end here. He is very involved with ABET and has served as a program evaluator, a member of the AIChE Education and Accreditation Committee, and now a member of the Engineering Accreditation Commission (EAC).

He has served as the division chair and program vice chair for ASEE's New Engineering Educators; he has held offices such as secretary/treasurer, program chair, and director for the Chemical Engineering Division; and he is a senior member of AIChE. Since 2003, he has been a member of the Advisory Board for the University of Tennessee's Department of Chemical Engineering.

Kirk, center, along with Drs. Tony Vizzini (head of aerospace engineering) and Glenn Steele (head of mechanical engineering), getting pie-faced to the delight of students, faculty, and especially Kirk's sons Timothy and Andrew during last year's E-week activities.



Along the way, Kirk has been recognized in numerous capacities for his work. Early in his career, he was named Outstanding Professor of the Year at the University of North Dakota. In 1997, while at Michigan Tech, Kirk was recognized by the Chemical Engineering Division of ASEE with the Raymond W. Fahien Award for his outstanding accomplishments and commitment to his profession. He has also received an NSF CAREER Development Award (1995-1999), the Dow-ASEE Outstanding Young Faculty Award (1995-1996), and ASEE's Outstanding Teaching Award for the North Midwest Section (1999). His alma mater, Virginia Tech, named him as the Outstanding Young Alumnus in 2001. The next year, Kirk was recognized by Mississippi State University as Outstanding Professor in Chemical Engineering.

HIS VISION

Over the past 20 years, Kirk has observed a dramatic change taking place in the field of engineering education, noting the increased importance now placed on the quality of undergraduate teaching and faculty development at research universities. He has also seen the communication skills of engineering graduates improve dramatically from what they were 20 years ago.

In the Bagley College of Engineering a strong emphasis is placed on both of these areas. Through the newly established Center for Engineering Student Excellence, programs such as the Shackouls Technical Communication Program, Six Sigma, Study Abroad, congressional internships, and the Entrepreneurship Program emphasize the need to take technical degrees a step further. Students are encouraged to complement their technical degrees with programs such as these, providing them with better global awareness as well as im-

proved communication and business skills.

Kirk's vision for the Bagley College is to see it recognized as one of the top research institutions in the United States. He knows that this must be done by investing resources in carefully selected areas where MSU can be internationally renowned. He strongly believes that MSU will be one of the leading institutions in providing a diverse engineering workforce, and he is committed to the education of African-American engineering students at all degree levels. The Bagley College of Engineering, in fact, already ranks among the top 15 schools in graduating African-American engineers, and Kirk wants his college's ranking to go even higher.

Ultimately, Kirk wants to see the MSU Bagley College of Engineering thrive and become one of the Top 50 engineering colleges in the country. The core of his strategic plan focuses on providing first-rate education while continuing to recognize faculty for their research endeavors and teaching excellence. He believes that MSU has an obligation to the state of Mississippi and the nation, and to support growth and economic development with the expertise and knowledge found in the faculty of the Bagley College of Engineering.

HIS MOTTO

The advice he extends to each of the engineering students at Mississippi State is the same adage he chooses to live by: "Seek out challenging opportunities during your career—look for something that people say can't be done—and then go out and do it."

Now 42 and almost a year into his deanship, is there anything that Kirk would have done differently along the way?

Not a chance. □

Chemical Engineering at Columbia University

CARL C. GRYTE,
with contributions from
LENORA BABB AND
EDWARD F. LEONARD
*Columbia University
New York, NY 13699-5705*

Columbia Chemical Engineering is quintessentially New York, a central part of a university whose legal name is Columbia University in the City of New York. It is a university united to its city perhaps more than any other urban university in the United States. In 2005 Columbia Chemical Engineering celebrated its 100th anniversary, but it is rooted even farther back into the chemical, financial, and public works history of its home city; the special characteristics of contemporary chemical engineering at Columbia trace far into the department's, the city's, and the country's past.

A STORIED HISTORY

Columbia's engineering school was founded in 1864, initially named the School of Mines. It originated out of science departments that had participated in the 19th-century struggle in much of the Western World to reconcile philosophical and practical views of science.

In 1896, separate schools of engineering, chemistry, and architecture were set off from the School of Mines, resulting, finally, in Columbia's first curriculum in chemical engineering being offered by the School of Chemistry in the fall of 1905 (having been approved the preceding February).

A towering figure at Columbia and in New York at the time was **Charles Frederick Chandler**, a Bostonian whose pivotal education in chemistry was, notwithstanding his origins, in Germany. There he met some of Europe's leading



== CELEBRATING 100 YEARS ==

scientists, including Wöhler, Liebig, von Humboldt, and Pasteur—all of whom had progressed from a purely philosophical to a decidedly practical bent. On his return with a doctorate from Göttingen, Chandler joined Columbia, where he taught for 46 years.

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Chemical Engineering Education

Professor Chandler actually campaigned for 14 years before 1905 for a program that would produce what we could now only call chemical engineers. He was strongly resisted by professors who saw chemistry as pure science, beautiful in its own right and with deep philosophical meaning. Such battles raged in many universities and account for the earliest realization of chemical engineering as a distinct discipline being born in technological institutions such as MIT.

INFLUENCES FAR AND NEAR

New York in 1905 was one of the high-thinking, intellectual centers of the young United States. It was an international business center where agents of European—especially German—chemical firms issued and oversaw limited licenses to operate processes developed in Europe. In reaction, strong incentives existed for establishing an American capacity to develop and improve chemical processes, even before this became a desperate priority when the first World War broke out.

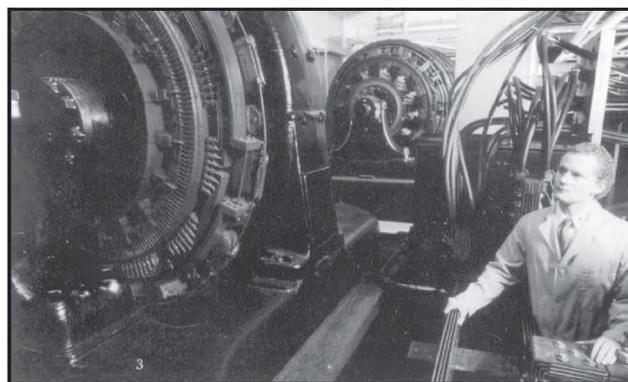
Professor Chandler was close friends with **Nicholas Murray Butler**—Columbia's president from 1902 until 1949. Both men consulted and were on good terms with the New York business community centered on Wall Street. Columbia's role in international business and politics was then, and remains today, preeminent, affecting every department of the university. These connections, and Professor Chandler's popularity as a teacher deeply involved in his subject, impelled the Columbia program to flourish.

In 2005 Columbia Chemical Engineering celebrated its 100th anniversary, but it is rooted even farther back into the chemical, financial, and public works history of its home city.

New York City after the Civil War was also a dirty, overcrowded, unhealthy, and unsafe place. In addition to his extensive involvement with the chemical industry, Professor Chandler played a central role in the public health of New Yorkers, dealing officially for the city with "the adulteration of milk, kerosene accidents, gas-factory nuisances, and general sanitation," as well as an issue that persists today—lead in drinking water. Professor Chandler was also very concerned with the chemical education of physicians and pharmacists and presented lectures to those professions regularly. We at Columbia like to think of him as our first biomedically oriented chemical engineer.

BUILDING THE PROGRAM

Records show the first chemical engineering curriculum at Columbia laid out four solid years of unremitting "chemis-



An early view of the large electrical generators at Columbia ChE's now-closed Heat Transfer Research Facility. For more than 50 years the laboratory tested electrically heated models of nuclear fuel-rod assemblies. Practically every configuration used in the Western World's boiling-water nuclear reactors was tested at this facility. Tests were run late at night to reduce dimming of lights in Manhattan.

try, engineering, metallurgy, mathematics, mechanics, physics, and mineralogy," having presumed prior preparation in "algebra, geometry, plane trigonometry, chemistry, physics, freehand drawing, English literature, composition and grammar, American and English history, French, and German."

Professor A.W. Hixson, who joined the faculty in 1922 and later became the preeminent department historian of Columbia, put forth the claim that despite the preexistence of other programs entitled chemical engineering, Columbia's was "the first well-balanced and completely integrated curriculum in chemical engineering to be established in America." In what is arguably a less disputable first, only five years after its 1905 founding Columbia admitted students to study for the degree "doctor of philosophy in chemical engineering."

Professor Chandler's handpicked colleague and later successor, **Milton C. Whitaker**, also became a leading figure in chemical engineering education. He was recognized with two honorary degrees and was an early president of AIChE.

Engendered by these early innovators, Columbia Chemical Engineering's current specializations all have origins and histories that reach back to the department's founding.

Polymer Surfaces

In the earliest years, polymers were mostly natural and the coursework was concerned with materials such as cellulose, gutta percha, and rubber. The esters of cellulose were already in wide use, however, and as the department was being founded **Leo Baekeland** was inventing the phenol-formaldehyde resin that was to bear his name. Indeed, Baekeland was an honorary professor in the department, an advisor to Columbia's President Butler, and an overseer of the chemical engineering program nearly until his death in 1944.



Left, Columbia's Unit Ops Lab, circa 1929, with students dressed "properly" for lab work in those days. Columbia's department was one of the earliest proponents of the unit operations concept and such laboratories evolved continuously along these lines through the first half of the 20th century. Above,

Professor Elmer Gaden and family. Gaden was named "Father of Biochemical Engineering" by Chemical Engineering News in 1971; this photo appeared on the magazine's cover.

With the nation's drive for independence from European technology, major emphasis was placed on process and plant design. A steady stream of doctoral theses based on process and plant design flowed out of the department from 1915 through the beginning of the second World War. While these dissertations covered a wide range of processes, many were concerned with raw materials for synthetic substances.

In 1939, **James M. Church** arrived at Columbia and for more than 20 years ran an undergraduate unit processes laboratory in which students conducted carefully scaled-down versions of industrial, mostly organic, processes. The real resurgence of interest in polymers began in the mid-'60s, however, with the hiring of **George Odian** in 1966 and **Harry Gregor** in 1967. They were joined by **Carl Gryte** in 1972 and **Christopher Durning** in 1983. The trend continued when **Ben O'Shaughnessy**, a condensed-matter physicist, joined the faculty in 1988, followed by **Rasti Levicky** in 1998, and **Jeffrey Koberstein** in 2000. The lasting theme of this resurgence has been an interest in polymer surfaces in an exceptionally wide range of applications.

Electrochemical Engineering

Electrochemistry and electrochemical engineering have had a similarly long run through the department's history. For a long time the ability to generate electricity from the potential energy of water far outweighed the ability to transmit electricity over long distances. In that era, a major center of electrochemical manufacturing evolved at Niagara Falls, N.Y.

The first professor of electrochemical engineering, **Samuel A. Tucker**, was appointed in 1910 and rapidly built up what historian Hixson has called the most com-

plete electrochemical laboratory in the country. The strength of a great university was brought to bear on this enterprise through the influence of Columbia's Department of Physics, with its interests in electricity.

In 1922, **Colin G. Fink** joined the department to begin a long and distinguished career in electrochemical engineering. Professor Fink was a 1903 Columbia graduate who subsequently received his Ph.D. in chemistry (from the University of Leipzig) in 1907. Fink's personal research accomplishments were extraordinary, including—during earlier employment with General Electric—the process for drawing tungsten wire that was essential to light-bulb manufacture, as well as the development of chromium plating. He became the executive secretary of the Electrochemical Society, revitalized it, and negotiated a home for it on the Columbia campus.

Fink (who retired in 1950) was joined by **Henry B. Linford** in 1942. Linford, too, served as executive secretary of the Electrochemical Society, retiring in 1976. Joining late in Linford's tenure was **Huk Y. Cheh** (who retired in 2001 to become director of research for the Duracell Company). Cheh was honored in 1982 with the Ruben-Viele chair named in honor of Samuel Ruben—a protégé of physics professor Michael Pupin—who made important contributions to the electrochemistry of metals. Cheh was joined in 1991 by **Alan West**, a specialist in electroplating. West was joined in 2000 by **Scott Calabrese Barton**, specializing in fuel cells.

Bioengineering

Bioprocessing, biochemical engineering, and biomedical engineering have also long figured in the department's history. Professor Chandler's influential involvement with the healthcare community and public health has already been mentioned. Following in his footsteps was **D.D. Jackson**, who led the department for 23 years, from 1917. Jackson was trained in chemistry, engineering, and biology, and had a major interest in biochemical processes (second only to his interest in processes for the production of heavy chemicals). Professor Jackson was succeeded by the aforementioned Professor Hixson—who had a major interest in yeast chemistry. Such chemistry was fundamental to much early bioprocessing.

The real prominence of Columbia in the area of bioprocessing, however, came with the rise of **Elmer L. Gaden** in the years immediately following World War II. The discovery of penicillin and its manufacture by fermentation, combined with the extensive demand for it during the war, had enormously accelerated interest in bioprocessing. Professor Gaden, an eminently practical man but also an ideologue, quickly grasped the significance of oxygen delivery in fermentations and developed, over many years, methods for measuring and increasing it.

His students were soon continuing his efforts, both in other schools and in industry. **Juan Asenjo** and **Alex Seressiotis** followed Gaden, who left Columbia in 1974 to ultimately become a professor of chemical engineering at the University of Virginia.

Such was the influence of his work that, on the cover of its May 31, 1971, issue, *Chemical and Engineering News* declared Professor Gaden, "the father of biochemical engineering." But beyond Gaden's contribution to biochemical engineering was his early recognition of the development of biomedical engineering. Largely through his efforts, by 1965 Columbia had graduate and undergraduate programs in "bioengineering" with a decidedly medical orientation. The graduate program was run by an interdisciplinary commit-

tee, but the undergraduate program remained within chemical engineering until 1997, when a separate department of biomedical engineering was established.

Many faculty members contributed to the bioengineering program, which was seen as a broad effort to focus the tools and methods of chemical engineering on biological and medical problems. These influential individuals included **Jordan**

Spencer, Harry Gregor, Frank Castellana, Mary Anne Farrell-Epstein, Huk Cheh, and Rakesh Jain. No faculty member was more involved in this effort than **Edward Leonard**, however, who has worked on problems related to artificial organs since 1956—two years before he joined the Columbia faculty.

In more recent times, the department has initiated a program in *genomic engineering*, the first of its kind in the country. **Professor Jingyue Ju** is the director of sequencing in the Columbia Genome Center, while Professors Ju, Levicky, **Banta**, and Leonard are all involved in research that relates to the modeling and manipulation of gene expression.



Professor Carl Gryte (on staircase) with Isao Noda (top left) and other doctoral students installing the Cobalt-60 radiation source used in polymer research (about 1971).

SHAPED BY WORLD EVENTS

Thus, the three areas of current concentration in the department have extensive histories. The full story, however, is necessarily a bit more complicated. Two great wars stamped the department indelibly.

World War I matured chemical engineering throughout the country. Europe, most notably Germany, no longer served as the fountainhead of chemical engineering—professors were no longer "finished" in European universities—and the American chemical industry moved rapidly toward reliance on chemical engineers wholly formed in the United States. This shift led inexorably to the dominance that American chemical engineering now possesses.

World War II had more specific effects. Columbia was the home of the Manhattan Project. While the project later moved to other universities and to the national laboratories, its beginnings were at Columbia, and no other university was as

much affected. Chemical engineers participated, especially in the early conceptualization of the gaseous diffusion process for the separation of uranium isotopes. While the detailed story remains to be told, **Professor Thomas Drew** was pivotal in these efforts. He remained at Columbia until 1965.

Another legacy of the Manhattan Project was Columbia's Heat Transfer Research Laboratory. This laboratory, founded in 1951, served as the major research and testing facility for thermal-hydraulic design of nuclear reactors until its closure in 2003. In major tests it could consume 13 mW of electrical energy, which had to be accessed out of peak usage times yet could *still* dim lights on the west side of Manhattan during tests! The first director was **Professor Charles F. Bonilla**. Later directors included a number of chemical engineering professors, notably Huk Y. Cheh in the laboratory's later years.

THE BIG PICTURE

Throughout the history of chemical engineering at Columbia there has been a steady concern with the "core" of chemical engineering. Notwithstanding the historical specialties emphasized above, Columbia Chemical Engineering has always been a broad endeavor, not a boutique dedicated to select applications. The more than 50 individuals who have held profes-



The current faculty. Seated: Scott Banta, Rasti Levicky, Nina Shapley, Jingyue Ju, Jeff Koberstein. Standing: Edward Leonard, Alan West (chair), Ben O'Shaughnessy, Scott Calabrese Barton. Not pictured: Carl Gryte.

sor positions—too many to mention here—have represented almost every area of research: process design and development; energy conversion; particular unit operations such as distillation, heat transfer, fluid mechanics, solids separations, extraction, and most of the rest, as well as kinetics and reactor design; process control and optimization; and oil and gas recovery.

Columbia Chemical Engineering today has 10 faculty, currently chaired by Alan West. Table 1 lists their interests. □

Electrochemical Engineering									
1911	1922	1942	1970	1984	1991	2000			
Samuel Tucker	Colin Fink	Henry B. Linford	Huk Yuk Cheh	Ulrich Stimming	Alan West	Scott Calabrese Barton			
Biomedical Engineering									
1866	1946	1958	1977	1983	1988	2000	2001	2004	
Charles Chandler	Elmer Gaden, "Father of Biochemical Engineering"	Edward Leonard	Rakesh Jain	Juan Asenjo	Alex Seressiotis	Jingyue Ju	Nina Shapley	Scott Banta	
Polymer Engineering									
1914	1917	1939	1966	1967	1972	1983	1988	1998	2000
Leo Baekeland, inventor of Bakelite, the first important thermosetting resin	D.D. Jackson	James Church	George Odian	Harry P. Gregor	Carl Gryte	Chris Durning	Ben O'Shaughnessy	Rasti Levicky	Jeff Koberstein

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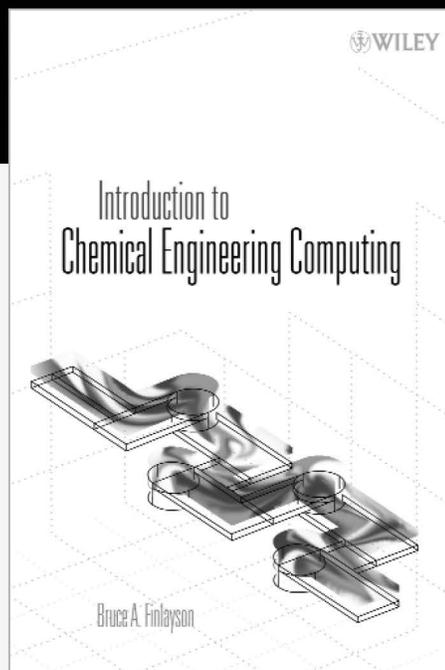
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NUMERICAL PROBLEM SOLVING USING MATHCAD

in Undergraduate Reaction Engineering

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With the development and availability of fast, efficient computers, the role of computing in analysis and solution of engineering problems and graphical communication of results has increased dramatically—leading to greater need for computer-application skills in the curricula and practice of various engineering disciplines.^[1] Efficient solution of problems is essential for enhanced understanding of chemical engineering principles at all course levels.^[1] Commercially available computational packages, such as Maple, Mathcad, Mathematica, and Matlab, have considerably reduced the time and effort required for engineering calculations. Such programs allow engineers with limited or no formal training in programming to solve relatively complex problems.^[2-4]

One of these packages, Mathcad, combines some of the best features of spreadsheets and symbolic math programs, allows efficient manipulation of large data arrays, and provides a good graphical user interface.^[2,4,5] Ability to perform calculations with units is an important feature of Mathcad for engineering students.^[2] While students need to understand the problem they are trying to solve, they may know little or nothing about numerical analysis; Mathcad allows them to work on problems even if they know very little of the program's syntax.^[4] Some of the advanced and special capabilities of Mathcad, such as solution of stiff differential equations, statistical methods for nonlinear parameter estimation, and programming, have been used in undergraduate courses.^[3,5-8]

Experience in using Mathcad in the undergraduate chemical reaction engineering course at the Illinois Institute of Technology (IIT) is discussed here. Pertinent illustrations are provided to demonstrate the ease with which problems with varying complexity can be solved using Mathcad. Example problems considered for illustration deal with simultaneous solution of: linear algebraic equations (*i.e.*, kinetic parameter estimation); nonlinear algebraic equations (*i.e.*, equilibrium calculations for multiple reactions and steady-state behavior of isothermal/nonisothermal CSTR with single/multiple reactions); integral equations (*i.e.*, design of steady-state plug flow reactor, or PFR); integral-algebraic equations; and nonlinear ordinary differential equations (*i.e.*, solution of conservation equations for steady-state PFR and unsteady state CSTR). Based on these illustrations, the benefits of this user-friendly software in accelerating learning and strengthening the fundamental knowledge base should be evident. With hand calculations being replaced by computation, it is more impor-

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tant than ever to consistently validate and verify the results.^[9] This is done, where appropriate, in the illustrations that follow. The Mathcad worksheet for each illustration is provided in a table and contains problem input, solution algorithm, and presentation of results in appropriate (numerical and/or graphical) format.

NUMERICAL ILLUSTRATIONS

Illustration 1

This illustration pertains to estimation of kinetic parameters using linear regression, which requires solution of several simultaneous equations that are linear in unknown parameters.

Consider the following relation among variables y and x_j ($j = 1, 2, \dots, m$) that is linear in terms of the unknown parameters θ_j ($j = 1, 2, \dots, m$).

$$y = y_p + e, \quad y_p = x_1\theta_1 + x_2\theta_2 + \dots + x_m\theta_m \quad (1)$$

Information on y and x_j ($j = 1, 2, \dots, m$) is available in the form of n samples ($n > m$). The parameter estimation

problem then involves finding the parameter set

$$\hat{\Theta} (\theta_j = \hat{\theta}_j, j = 1, 2, \dots, m)$$

for which $\sum_{i=1}^n e_i^2$ is minimized. After some algebra, the necessary and sufficient condition for this can be deduced to be

$$A\hat{\Theta} = b, \quad A = X^T X, \quad b = X^T Y \Rightarrow \hat{\Theta} = (X^T X)^{-1} X^T Y \quad (2)$$

with

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad X = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1m} \\ x_{21} & x_{22} & \dots & x_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nm} \end{bmatrix}, \quad \Theta = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_m \end{bmatrix} \quad (3)$$

Each column in array X represents the collection of values of a particular variable x_j ($j = 1, 2, \dots, m$) for different samples. The goodness of fit of the least squares can be examined by calculating the relative error for each data point or sample (ϵ_i) defined as $\epsilon_i = (y_i - y_{ip})/y_i$, $i = 1, 2, \dots, n$.

The specific example considered here pertains to Problem 5-13 of Fogler^[10] and involves a three-dimensional linear fit ($m = 3$). The dependence of the rate r of a solid-catalyzed association reaction between A and B on partial pressures of A and B, p_A and p_B , respectively, is expressed as $r = k p_A^\alpha p_B^\beta$ with k , α , and β being the kinetic parameters to be estimated. The units for k , p_A , p_B , and r are $\text{mmol}/\{\text{g cat.h} \cdot (\text{atm})^{(\alpha + \beta)}\}$, atm , atm , and $\text{mmol}/\{\text{g cat.h}\}$, respectively. Upon linear transformation of the expression, a relation linear in terms of three unknown parameters can be obtained as in Eq. (1), with $x_1 = 1$, $x_2 = \ln(p_A)$, $x_3 = \ln(p_B)$, $y = \ln(r)$, $\theta_1 = \ln(k)$, $\theta_2 = \alpha$, and $\theta_3 = \beta$. The data for p_A , p_B , and r are listed in Table 1, where the Mathcad worksheet for this problem is also shown.

Mathcad allows input only of column vectors. Two-dimensional arrays can be constructed from column vectors already introduced using the "stack" feature. The predicted reaction rates, r_p , are compared with the reaction rates available from measurements, r , and provide a very close fit (Table 1). The reason for presenting the relevant equations in this and other illustrations, where necessary, is to enable the reader to see how the equations to be solved and the Mathcad syntax are almost identical.^[4] In the illustrations that follow, the subscript 0 denotes variable values at the start of a batch reactor or in the feed for a flow reactor.

Illustration 2

This illustration pertains to an autocatalytic reaction and involves comparison of space times (τ) required for steady-state isothermal operations of a CSTR and a PFR. The reaction $A + B \rightarrow 2B$ occurs as per the kinetics $r = k C_A C_B$.

TABLE 1
Worksheet for Illustration 1

$r := \begin{pmatrix} 0.42 \\ 0.96 \\ 0.18 \\ 0.78 \\ 1.2 \\ 0.28 \\ 2.88 \end{pmatrix}$	$p_A := \begin{pmatrix} 0.1 \\ 0.2 \\ 0.05 \\ 0.3 \\ 0.4 \\ 0.05 \\ 0.5 \end{pmatrix}$	$p_B := \begin{pmatrix} 0.1 \\ 0.2 \\ 0.05 \\ 0.01 \\ 0.02 \\ 0.4 \\ 0.5 \end{pmatrix}$	$X_1 := \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$
$X_2 := \ln(p_A)$	$X_3 := \ln(p_B)$	$Y := \ln(r)$	$Q := \text{stack}(X_1^T, X_2^T, X_3^T)$
$X := Q^T$	$\theta := (X^T \cdot X)^{-1} \cdot X^T \cdot Y$		
$k := \exp(\theta_1)$	$\alpha := \theta_2$	$\beta := \theta_3$	$r_p := \exp(\theta_1 \cdot X_1 + \theta_2 \cdot X_2 + \theta_3 \cdot X_3)$
$k = 6.652$	$\alpha = 0.997$	$\beta = 0.205$	
$\frac{(r - r_p)}{r} = \begin{pmatrix} 4.871 \times 10^{-3} \\ -1.481 \times 10^{-3} \\ -9.417 \times 10^{-3} \\ 1.073 \times 10^{-3} \\ 2.959 \times 10^{-3} \\ 6.006 \times 10^{-3} \\ -4.098 \times 10^{-3} \end{pmatrix}$			

The feed contains A and B in the ratio 100:1. For the feed composition under consideration, the reaction rate is expressed as

$$r = kC_{A0}^2 f(X), \quad f(X) = (1-X)(0.01+X) \quad (4)$$

A comparison of the required space times for a CSTR and a PFR is equivalent to the comparison of the corresponding Damkohler numbers, $Da (= kC_{A0} \tau)$ which can be obtained explicitly in terms of the exit conversion X_e . The Mathcad worksheet for this problem is shown in Table 2. Rather than calculating Da for one value of X_e at a time, the Da 's for CSTR and PFR are expressed as a function of X_e , a floating variable (Table 2). The Da 's for a particular X_e are then readily obtained by plugging the value of X_e into the symbolic solutions. Keeping X_e floating also enables the student to represent the results graphically over a specified range of X_e ($0 < X_e < 1$ in Table 2). This beneficial feature in Mathcad is also used in Illustrations 7 and 8. For minimizing the required space time, a CSTR is the reactor of choice up to a critical conversion, X_c , and a PFR beyond this conversion (Table 2). Identifying X_c requires solution of an integral-algebraic equation in X_e —the numerical solution of which is certainly challenging for an undergraduate student. Using Mathcad, the solution is obtained rather easily and its accuracy is demonstrated in Table 2.

Illustration 3

The gas phase reaction, $SO_2 (A) + \frac{1}{2}O_2 (B) \rightarrow SO_3 (C)$, occurs as per the kinetics $r = kC_A C_B$. For the feed composition under consideration, the reaction rate is expressed as^[10]

$$r = kC_{A0}^2 f(X), \quad f(X) = \frac{(1-X)(0.54-0.5X)}{(1-0.14X)^2} \quad (5)$$

with k being the kinetic coefficient, C_{A0} the feed concentration of A, and X the fractional conversion of A. The reaction is carried out in three CSTRs of equal volume in series with the exit conversion being specified. Computation of the intermediate fractional conversions and the required total space time, or of the corresponding $Da (= kC_{A0} \tau)$, requires simultaneous solution of design equations for the three reactors, viz.,

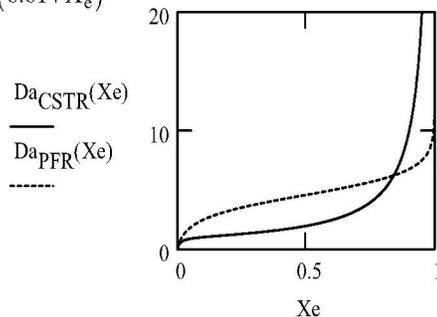
$$X_i - X_{(i-1)} - \frac{Da}{3} f(X_i) = 0, \quad i=1, 2, 3 \quad (6)$$

In the above, X_i refers to fractional conversion of A in reactor i ($X_0 = 0$) and Da corresponds to the total space time for the three-reactor battery. The Mathcad worksheet for this problem is shown in Table 3. The solution proceeds by providing initial guesses for Da , X_1 , and X_2 . The validity of the solution is verified by substituting Da , X_1 , and X_2 generated by the solution into Eq. (6).

TABLE 2
Worksheet for Illustration 2

$$Da_{PFR}(X_e) := \int_0^{X_e} \frac{1}{(1-X) \cdot (0.01+X)} dX$$

$$Da_{CSTR}(X_e) := \frac{X_e}{(1-X_e) \cdot (0.01+X_e)}$$



When is $Da_{CSTR} = Da_{PFR}$?

$$X_e := 0.7$$

Given

$$\int_0^{X_e} \frac{1}{(1-X) \cdot (0.01+X)} dX - \frac{X_e}{(1-X_e) \cdot (0.01+X_e)} = 0$$

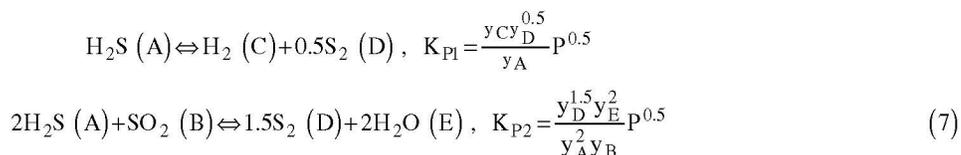
$$X_c := \text{Find}(X_e) \quad X_c = 0.841 \quad Da_{CSTR}(X_c) = 6.222$$

Verify

$$\int_0^{X_c} \frac{1}{(1-X) \cdot (0.01+X)} dX - \frac{X_c}{(1-X_c) \cdot (0.01+X_c)} = -4.187 \times 10^{-8}$$

Illustration 4

This illustration pertains to estimation of the equilibrium composition of a reaction mixture and is adopted from Problem 4.14 of Cutlip and Shacham.^[11] The reactions



occur in a gas phase batch reactor. In the above, K_{P1} and K_{P2} denote the equilibrium coefficients, P the total pressure, and y_j the mole fraction of species J . The initial pressure P_0 is 1.2 atm and the initial composition is (I = inerts): $y_{A0} = 0.45$, $y_{B0} = 0.25$, and $y_{I0} = 0.3$. For $K_{P1} = 0.45 \text{ atm}^{0.5}$ and $K_{P2} = 28.5 \text{ atm}^{0.5}$, obtain the composition of the reaction mixture at equilibrium in constant volume and constant pressure operations of the reactor. Let n_{j0} denote the initial number of moles of species J , while ξ_1 and ξ_2 equal the extents of reactions 1 and 2, respectively, and n_j equals the number of moles of J after certain extents of the two reactions. The expressions for y_j 's in terms of ξ_1 and ξ_2 then, are: $y_j = n_j/n$, $n_i = \sum_J n_j$, $n_0 = \sum_J n_{j0}$, and $J = A, B, C, D, E, I$, with $n_A = (n_{A0} - \xi_1 - 2\xi_2)$, $n_B = (n_{B0} - \xi_2)$, $n_C = (n_{C0} + \xi_1)$, $n_D = (n_{D0} + 0.5\xi_1 + 1.5\xi_2)$, $n_E = (n_{E0} + 2\xi_2)$, $n_I = n_{I0}$, and $n = (n_0 + 0.5\xi_1 + 0.5\xi_2)$. The mole fractions in the equilibrium relations in Eq. (7) and the reactor pressure for constant volume operation are then expressed as

$$\begin{aligned} y_A &= \frac{(y_{A0} - \rho_1 - 2\rho_2)}{\Psi}, \quad y_B = \frac{(y_{B0} - \rho_2)}{\Psi}, \quad y_C = \frac{\rho_1}{\Psi}, \quad y_D = \frac{(0.5\rho_1 + 1.5\rho_2)}{\Psi}, \\ y_E &= \frac{2\rho_2}{\Psi}, \quad \Psi = (1 + 0.5\rho_1 + 0.5\rho_2), \quad \rho_1 = \frac{\xi_1}{n_{I0}}, \quad \rho_2 = \frac{\xi_2}{n_{I0}}, \\ P &= P_0 \Psi \text{ (constant volume)}, \quad P = P_0 \text{ (constant pressure)} \end{aligned} \quad (8)$$

TABLE 3
Worksheet for Illustration 3

	$X_3 := 0.9$	$Da := 2$	$X_1 := 0.3$	$X_2 := 0.6$
Given				
	$\left[X_1 - \frac{Da}{3} \cdot \frac{(1-X_1) \cdot (0.54 - 0.5X_1)}{(1-0.14 \cdot X_1)^2} \right] = 0$	$\left[X_2 - X_1 - \frac{Da}{3} \cdot \frac{(1-X_2) \cdot (0.54 - 0.5X_2)}{(1-0.14 \cdot X_2)^2} \right] = 0$		
	$\left[X_3 - X_2 - \frac{Da}{3} \cdot \frac{(1-X_3) \cdot (0.54 - 0.5X_3)}{(1-0.14 \cdot X_3)^2} \right] = 0$	$\begin{pmatrix} Da \\ X_1 \\ X_2 \end{pmatrix} := \text{Find}(Da, X_1, X_2)$		
	$Da = 19.502$	$X_1 = 0.635$	$X_2 = 0.823$	
Verify	$\left[X_1 - \frac{Da}{3} \cdot \frac{(1-X_1) \cdot (0.54 - 0.5X_1)}{(1-0.14 \cdot X_1)^2} \right] = -9.212 \times 10^{-9}$			
	$\left[X_2 - X_1 - \frac{Da}{3} \cdot \frac{(1-X_2) \cdot (0.54 - 0.5X_2)}{(1-0.14 \cdot X_2)^2} \right] = -3.984 \times 10^{-9}$			
	$\left[X_3 - X_2 - \frac{Da}{3} \cdot \frac{(1-X_3) \cdot (0.54 - 0.5X_3)}{(1-0.14 \cdot X_3)^2} \right] = 0$			

The Mathcad worksheet for constant volume operation is shown in Table 4. The equilibrium relations are nonlinear coupled equations in the dimensionless extents, ρ_1 and ρ_2 , initial guesses for which need to be supplied (Table 4). The extents calculated are substituted into equilibrium relations to verify that these indeed are satisfied. Computations for constant pressure operation, not shown here, proceed in a similar fashion. Illustration 4 reveals to the students the uniqueness of the physically realizable equilibrium composition for a given initial composition.

Illustration 5

Illustration 5 pertains to multiplicity of steady states in an isothermal CSTR. The reaction under consideration, catalytic hydrogenation of olefins, obeys the kinetics $r = C_A/(1+C_A)^2$, with r being expressed per unit reactor volume. The operating conditions for the reactor are: $C_{A0}=13 \text{ mol/L}$, $V=10 \text{ L}$, $v_0=0.2$

L/s.^[12] The Mathcad worksheet for this illustration is shown in Table 5. The symbolic solution of the steady-state mass balance for A, viz., $(C_{A0}-C_A)/\tau = r(C_A)$, reveals that the reactor can operate at three steady states. The students observe that the steady-state mass balance is a cubic equation in the unknown, C_A , and therefore has three solutions, not all of which may be real. The verification of solutions of the steady-state mass balance, generated as a vector, follows as usual and is done at once for all three solutions. The start-up conditions are important in determining which steady state is eventually reached. This requires solution of the mass balance for the transient operation, viz.,

$$\frac{dC_A}{dt} = \frac{(C_{A0}-C_A)}{\tau} - r(C_A), \quad C_A(0) = C_{Ai} \quad (9)$$

The results of computations pertaining to two C_{Ai} are shown

TABLE 4			
Worksheet for Illustration 4			
$P_0 := 1.2$	$K_{P1} := 0.45$	$K_{P2} := 28.5$	$y_{A0} := 0.45$
$y_{B0} := 0.25$	$y_{I0} := 1 - y_{A0} - y_{B0}$		$y_{I0} = 0.3$
	$\rho_1 := 0.085$	$\rho_2 := 0.132$	
Given			
$\frac{\rho_1 \cdot (0.5 \cdot \rho_1 + 1.5 \cdot \rho_2)^{0.5} \cdot P_0^{0.5}}{(y_{A0} - \rho_1 - 2 \cdot \rho_2)} - 0.45 = 0$			
$\frac{(0.5 \cdot \rho_1 + 1.5 \cdot \rho_2)^{1.5} \cdot (2 \cdot \rho_2)^2 \cdot P_0^{0.5}}{(y_{A0} - \rho_1 - 2 \cdot \rho_2)^2 \cdot (y_{B0} - \rho_2)} - 28.5 = 0$			
$\begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} := \text{Find}(\rho_1, \rho_2) \quad \rho_1 = 0.06 \quad \rho_2 = 0.157$			
Verify			
$\frac{\rho_1 \cdot (0.5 \cdot \rho_1 + 1.5 \cdot \rho_2)^{0.5} \cdot P_0^{0.5}}{(y_{A0} - \rho_1 - 2 \cdot \rho_2)} - 0.45 = 1.805 \times 10^{-10}$			
$\frac{(0.5 \cdot \rho_1 + 1.5 \cdot \rho_2)^{1.5} \cdot (2 \cdot \rho_2)^2 \cdot P_0^{0.5}}{(y_{A0} - \rho_1 - 2 \cdot \rho_2)^2 \cdot (y_{B0} - \rho_2)} - 28.5 = -4.707 \times 10^{-7}$			
Equilibrium Composition	$y_A := \frac{(y_{A0} - \rho_1 - 2 \cdot \rho_2)}{(1 + 0.5 \cdot \rho_1 + 0.5 \cdot \rho_2)}$	$y_B := \frac{(y_{B0} - \rho_2)}{(1 + 0.5 \cdot \rho_1 + 0.5 \cdot \rho_2)}$	$y_C := \frac{\rho_1}{(1 + 0.5 \cdot \rho_1 + 0.5 \cdot \rho_2)}$
	$y_D := \frac{(0.5 \cdot \rho_1 + 1.5 \cdot \rho_2)}{(1 + 0.5 \cdot \rho_1 + 0.5 \cdot \rho_2)}$	$y_E := \frac{2 \cdot \rho_2}{(1 + 0.5 \cdot \rho_1 + 0.5 \cdot \rho_2)}$	$y_I := \frac{y_{I0}}{(1 + 0.5 \cdot \rho_1 + 0.5 \cdot \rho_2)}$
	$y_A = 0.068$	$y_B = 0.083$	$y_C = 0.054$
		$y_D = 0.24$	$y_E = 0.284$
			$y_I = 0.271$
	$y_A + y_B + y_C + y_D + y_E + y_I = 1$		$\psi := 1 + 0.5 \cdot \rho_1 + 0.5 \cdot \rho_2$
			$\psi = 1.109$

in Table 5. In this illustration and Illustration 6, integration of appropriate differential equations has been accomplished using the Runge-Kutta method with adaptive step size (Rkadapt). Let the steady state concentrations of A be denoted as C_{As1} , C_{As2} , and C_{As3} , with $C_{As1} < C_{As2} < C_{As3}$. The reactor operation started from C_{Ai1} (very close to but less than C_{As2}) leads to the lowest concentration steady state ($C_{Af1} \rightarrow C_{As1}$, Table 5), while that started from C_{Ai2} (very close to but greater than C_{As2}) leads to the highest concentration steady state ($C_{Af2} \rightarrow C_{As3}$, Table 5). The steady state corresponding to C_{As2} is therefore unstable. Working with other values of C_{Ai} , the students deduce that for $0 < C_{Ai} < C_{As2}$, C_A converges to C_{As1} at large times and for $C_{Ai} > C_{As2}$, C_A converges to C_{As3} at large times (additional computations not shown).

Illustration 6

This illustration pertains to a membrane reactor employed to obtain higher conversions for reversible reactions, and is adapted from Example 4-10 of Fogler.^[10] A gas phase dissociation reaction $A \rightleftharpoons B + C$ is carried out in a steady-state plug flow reactor, the wall of which consists of a membrane which allows transport exclusively of B. The feed to the membrane reactor contains only A, with $F_{A0} = 10$ mol/min. The reactor

and the feed are kept at 8.2 atm and 500 K. Since A and C remain in the reaction phase throughout the reactor, it follows from the reaction stoichiometry that $F_C = F_{A0} - F_A$. As there are two independent unit operations (reaction and membrane separation), the two independent mass balances are those for A and B, *viz.*,

$$\frac{dF_A}{dV} = -r, \quad \frac{dF_B}{dV} = r - r_B \quad (10)$$

The expressions for the volume-specific rates of reaction, r , and removal of B, r_B , are^[10]

$$r = k \left(C_A - \frac{C_B C_C}{K_C} \right) = k_1 \left[\frac{F_A}{F_T} - C_1 \frac{(F_{A0} - F_A) F_B}{F_T^2} \right],$$

$$r_B = k_B C_B = k_{B1} \frac{F_B}{F_T}, \quad F_T = (F_{A0} + F_B),$$

$$k_1 = k C_{T0}, \quad C_1 = \frac{C_{T0}}{K_C}, \quad k_{B1} = k_B C_{T0}, \quad C_{T0} = \frac{P}{RT} \quad (11)$$

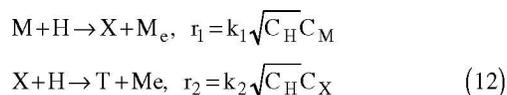
with $k = 0.7 \text{ min}^{-1}$, $K_C = 0.05 \text{ mol/L}$, and $k_B = 1 \text{ min}^{-1}$. It is desired to obtain profiles of F_A and F_B in a 300 L reactor via numerical integration of Eq. (10). The Mathcad worksheet

TABLE 5			
Worksheet for Illustration 5			
$v_0 := 0.2$	$C_{A0} := 13$	$V := 10$	$\tau := \frac{V}{v_0}$
$r(C_A) := \frac{C_A}{(1+C_A)^2}$		$f(C_A) := \frac{(C_{A0} - C_A)}{\tau} - r(C_A)$	
$C_{As} := f(C_A) \text{ solve, } C_A \rightarrow$		$\xrightarrow{f(C_{As})} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$	
Unsteady state CSTR—Which steady state do we reach? — $C_1 = C_A$			
$t_i := 0.0$	$t_f := 10000.0$	$N_{pts} := 200$	$C_{Ai1} := 2.1305$
$D(t, C) := \frac{(C_{A0} - C_1)}{\tau} - \frac{C_1}{(1+C_1)^2}$		$Sol := \text{Rkadapt}(C_{Ai1}, t_i, t_f, N_{pts}, D)$	
$C_{Af1} := \text{Sol}_{N_{pts}, 2}$		$C_{Af1} = 0.752$	$C_{Ai2} := 2.1315$
$Sol := \text{Rkadapt}(C_{Ai2}, t_i, t_f, N_{pts}, D)$		$C_{Af2} := \text{Sol}_{N_{pts}, 2}$	$C_{Af2} = 8.118$

for this illustration is shown in Table 6. The students observe that the profile of F_B exhibits a maximum (Table 6), since B is not supplied in the feed and is subject to two serial processes, namely generation by reaction and removal by membrane. If B is not removed by membrane separation (reaction-only operation, $F_B = F_C = F_{A0} - F_A$ per reaction stoichiometry), working with the driving force for the reaction, the lowest F_A ($= F_{Ae}$, corresponding to reaction equilibrium) is calculated via symbolic manipulations to be 5.528 mol/L (Table 6), which corresponds to 45% conversion of A. From the profile of F_A in Table 6, the students observe that for the effluent from the membrane-wall reactor, F_A is much lower than F_{Ae} and therefore the conversion of A is much higher. The last two illustrations deal with multiple reactions.

Illustration 7

This illustration, adopted from Example 6-7 of Fogler,^[10] pertains to the series-parallel reactions



with M, H, X, Me, and T being abbreviations for mesitylene, hydrogen, m-xylene, methane, and toluene, respectively. The reactions are carried out in a CSTR. The feed contains only M and H. In view of the stoichiometry of these mole-conserving reactions, it can be deduced that the concentrations of species influencing the kinetics are related to one

TABLE 6
Worksheet for Illustration 6

$$P:=8.2 \quad R:=0.082 \quad T:=500 \quad C_{T0}:=\frac{P}{R \cdot T} \quad C_{T0}=0.2$$

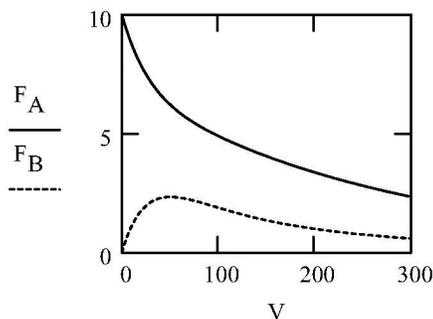
$$k:=0.7 \quad K_C:=0.05 \quad k_B:=1.0 \quad F_{A0}:=10 \quad F_{B0}:=0$$

$$k_1:=k \cdot C_{T0} \quad k_{B1}:=k_B \cdot C_{T0} \quad C_1:=\frac{C_{T0}}{K_C} \quad IC:=\begin{pmatrix} F_{A0} \\ F_{B0} \end{pmatrix}$$

$$Npts:=100 \quad V_i:=0.0 \quad V_f:=300.0 \quad F_1=F_A \quad \& \quad F_2=F_B$$

$$D(V,F):=\begin{bmatrix} -k_1 \cdot \left[\frac{F_1}{F_{A0}+F_2} - C_1 \cdot F_2 \cdot \frac{(F_{A0}-F_1)}{(F_{A0}+F_2)^2} \right] \\ k_1 \cdot \left[\frac{F_1}{F_{A0}+F_2} - C_1 \cdot F_2 \cdot \frac{(F_{A0}-F_1)}{(F_{A0}+F_2)^2} \right] - k_{B1} \cdot \frac{F_2}{(F_{A0}+F_2)} \end{bmatrix}$$

$$Sol:=Rkadapt(IC,V_i,V_f,Npts,D) \quad V:=Sol^{(1)} \quad F_A:=Sol^{(2)} \quad F_B:=Sol^{(3)}$$



Equilibrium for reaction-only operation

$$G(F_1):=\left[\frac{F_1}{F_{A0}+F_2} - C_1 \cdot F_2 \cdot \frac{(F_{A0}-F_1)}{(F_{A0}+F_2)^2} \right]$$

$$G(F_1) \text{ substitute } F_2 = F_{A0} - F_1 \rightarrow \frac{F_1}{(20-F_1)} - 4.00000000000000000000 \cdot \frac{(10-F_1)^2}{(20-F_1)^2}$$

$$\left[\frac{F_1}{(20-F_1)} - 4 \cdot \frac{(10-F_1)^2}{(20-F_1)^2} \right] \text{ solve } F_1 \rightarrow \begin{pmatrix} 10+2\sqrt{5} \\ 10-2\sqrt{5} \end{pmatrix} \quad F_{Ae}:=10-2\sqrt{5} \quad F_{Ae}=5.528$$

another as

$$C_M = \frac{1}{2}(a + C_H - C_X), \quad a = 2C_{M0} + C_{X0} - C_{H0} \quad (13)$$

Since there are two independent reactions, one needs to solve only two mass balances, *e.g.*, those for hydrogen and m-xylene, in conjunction with the stoichiometric relation in Eq. (13). The Mathcad worksheet for solution of the design equations is shown in Table 7. The kinetic and operating parameter values are^[10]: $k_1 = 55.2$ (ft³/lb mol)^{0.5}/h, $k_2 = 30.2$ (ft³/lb mol)^{0.5}/h, $C_{H0} = 0.021$ lb mol/ft³, and $C_{M0} = 0.0105$ lb mol/ft³. The profiles of C_H and C_X are shown in Table 7, with the space time for CSTR— τ_c —being in hours. The profiles reveal that the concentration of m-xylene, an intermediate, exhibits a maxi-

um as expected, since it is not supplied in the feed.

For each τ_c , one has to provide initial guesses for C_H and C_X , and solve the mass balances iteratively. The same initial guesses may work for certain range of τ_c . This happens to be the case in this illustration. The solutions of mass balances are therefore obtained using τ_c as a floating variable (Table 7). To verify the solution, the normalized residues associated with the mass balances for H and X— reH and reX , respectively—are calculated by substituting C_H and C_X generated by the solution into the mass balances. From the definitions of reH and reX and magnitudes of these displayed in the profiles in Table 7, it is evident that the profiles of C_H and C_X in Table 7 are indeed solutions of the mass balances.

TABLE 7
Worksheet for Illustration 7

$$k_1 := 55.2 \quad k_2 := 30.2 \quad C_{H0} := 0.021 \quad C_{M0} := 0.0105 \quad C_{X0} := 0.0$$

$$a := 2 \cdot C_{M0} + C_{X0} - C_{H0} \quad a = 0$$

$$C_H := 0.0089 \quad C_X := 0.00312$$

Given

$$\frac{(C_H - C_{H0})}{\tau_c} = -k_1 \cdot (C_H)^{0.5} \cdot (a + C_H - C_X) \cdot 0.5 - k_2 \cdot (C_H)^{0.5} \cdot C_X$$

$$\frac{C_X}{\tau_c} = k_1 \cdot (C_H)^{0.5} \cdot (a + C_H - C_X) \cdot 0.5 - k_2 \cdot (C_H)^{0.5} \cdot C_X$$

$$\text{Soll}(\tau_c) := \text{Find}(C_H, C_X) \quad C_H(\tau_c) := \text{Soll}(\tau_c)_1 \quad C_X(\tau_c) := \text{Soll}(\tau_c)_2$$

$$reH(\tau) := \frac{\tau \cdot [-k_1 \cdot (C_H(\tau))^{0.5} \cdot (a + C_H(\tau) - C_X(\tau)) \cdot 0.5 - k_2 \cdot (C_H(\tau))^{0.5} \cdot C_X(\tau)]}{C_H(\tau) - C_{H0}} - 1$$

$$reX(\tau) := \frac{\tau \cdot [k_1 \cdot (C_H(\tau))^{0.5} \cdot (a + C_H(\tau) - C_X(\tau)) \cdot 0.5 - k_2 \cdot (C_H(\tau))^{0.5} \cdot C_X(\tau)]}{C_X(\tau)} - 1$$

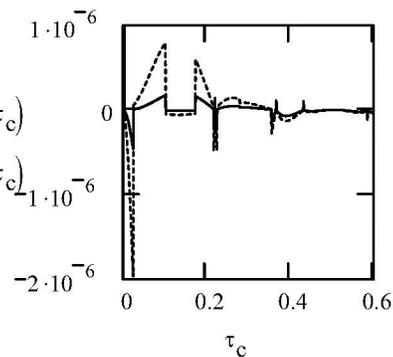
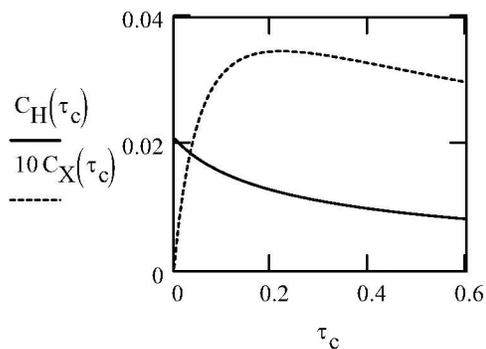


Illustration 8

This illustration, adopted from Example 8-12 of Fogler,^[10] pertains to elementary liquid phase reactions $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ taking place in an adiabatic steady state CSTR. The expressions for C_A and C_B obtained from solution of mass balances for A and B are

$$C_A = \frac{C_{A0}}{(1 + \tau k_1)}, \quad C_B = \frac{\tau k_1 C_A}{(1 + \tau k_2)} \quad (14)$$

The energy balance has the form (specific heats of all species being considered equal, $C_{pA} = C_{pB} = C_{pC} = C_p$)

$$C_{A0} C_p (T - T_0) + (k_1 C_A \Delta H_1 + k_2 C_B \Delta H_2) \tau = 0, \\ k_i = k_{i0} \exp\left(-\frac{E_i}{RT}\right), \quad i=1, 2 \quad (15)$$

Upon substituting Eq. (14) into the above, the master equation for the adiabatic reactor is obtained as

$$G(T) = R_m(T), \quad R_m(T) = C_p (T - T_0), \\ G(T) = -\frac{\tau k_1(T)}{[1 + \tau k_1(T)]} \left[\Delta H_1 + \Delta H_2 \frac{\tau k_2(T)}{(1 + \tau k_2(T))} \right] \quad (16)$$

with the reactor temperature T being the only unknown. The values of various parameters are: $C_p = 300 \text{ J}/\{\text{mol.K}\}$, $\Delta H_1 = -55,000 \text{ J/mol}$, $\Delta H_2 = -71,500 \text{ J/mol}$, $C_{A0} = 0.3 \text{ mol/L}$, $T_0 = 300 \text{ K}$, $\tau = 0.01 \text{ min}$, $E_1 = 9,900 \text{ cal/mol}$, $E_2 = 27,000 \text{ cal/mol}$, $k_1 = 3.03 \text{ min}^{-1}$ at 300 K , $k_2 = 4.58 \text{ min}^{-1}$ at 500 K . With the exception of C_p , all other parameter values have been taken from Fogler,^[10] where C_p has been considered to be $200 \text{ J}/\{\text{mol.K}\}$ and the reactor operation has been considered to be nonadiabatic. The Mathcad worksheet for this illustration is shown in Table 8. By plotting $G(T)$ and $R(T)$ versus T , the students observe that the two profiles intersect at five T 's for $T > T_0$, implying existence of five steady states. The temperature at each steady state can be calculated via iterative solution of Eq. (16). Alternately, the relative error associated with Eq. (16), denoted as $\text{dif}(T)$ in Table 8, can be calculated at various temperatures to directly zoom in on the steady state temperature. For the parameters under consideration, the steady state T values are 309.59, 354.33, 473.85, 540.29, and 719.58 K.

TABLE 8
Worksheet for Illustration 8

$$C_p := 300 \quad \Delta H_1 := -55000 \quad \Delta H_2 := -71500 \quad C_{A0} := 0.3 \quad T_0 := 300 \quad \tau := 0.01$$

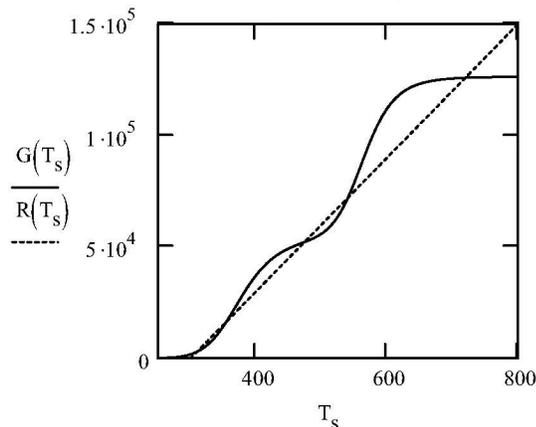
$$E_1 := 9900 \quad E_2 := 27000$$

$$k_{10} := 3.3 \cdot \exp\left(\frac{E_1}{1.987} \cdot \frac{1}{300}\right) \quad k_{20} := 4.58 \cdot \exp\left(\frac{E_2}{1.987} \cdot \frac{1}{500}\right)$$

$$k_1(T) := k_{10} \cdot \exp\left(\frac{-E_1}{1.987 \cdot T}\right) \quad k_2(T) := k_{20} \cdot \exp\left(\frac{-E_2}{1.987 \cdot T}\right)$$

$$G(T) := \frac{-\tau \cdot k_1(T)}{(1 + \tau \cdot k_1(T))} \cdot \left[\Delta H_1 + \Delta H_2 \cdot \frac{\tau \cdot k_2(T)}{(1 + \tau \cdot k_2(T))} \right]$$

$$R(T) := C_p \cdot (T - T_0) \quad \text{dif}(T) := \frac{G(T)}{R(T)} - 1.0$$



$$\text{dif}(309.59) = 6.249 \times 10^{-5}$$

$$\text{dif}(354.33) = 2.788 \times 10^{-5}$$

$$\text{dif}(473.85) = -4.697 \times 10^{-6}$$

$$\text{dif}(540.29) = -5.812 \times 10^{-6}$$

$$\text{dif}(719.58) = -1.027 \times 10^{-6}$$

DISCUSSION

The students also use Matlab in parallel to Mathcad. Both packages are available on computers across the IIT campus and in the chemical engineering computer laboratory. The purpose of exposing students to different packages is to provide them with a broad spectrum of skills needed for solving engineering problems and to demonstrate the differences in the packages' capabilities for solving different engineering problems.^[1] The students recognize that some of the problems can be formulated, but not solved, by hand. They can quickly develop worksheets for these problems and solve them, the emphasis thus being on understanding the fundamentals of the problems.

Care must be taken to ensure that use of computational software enhances students' understanding and enriches their logic and problem-solving skills, rather than simply allowing them to solve problems with only a superficial understanding of the problems.^[13] With this in mind, the undergraduate chemical reaction engineering course using this software at IIT includes handouts and tutorials providing an introduction to the software and to different numerical methods. Further, the author has integrated computational software throughout the course, with the use of software always following solution of related simpler problems by hand.^[13]

CONCLUSION

The use of computational packages enhances teaching and learning, allowing the teacher to cover more material.^[2, 14] In the process, the students learn more and faster and appreciate the course even more, while developing the skills and flexibility necessary for ready adoption of different software packages for professional activities in industry.^[1, 4, 10, 14] The graphics capabilities of Mathcad help in quick visualization of results as well as in reinforcing expected results and under-

standing not-so-expected results. The capabilities of Mathcad in symbolic manipulations are of considerable use in developing analytical skills of students in solving complex problems. The time spent outside the courses on gaining further familiarity with different computational software and their applications will allow students to reap the benefits of these programs.^[14]

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EXPERIMENTAL AIR-PRESSURE TANK SYSTEMS

for Process Control Education

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Process control education is a significant aspect of the chemical engineering curriculum, as it provides a fundamental basis for modern chemical process operation. The subject is highly applied yet rooted deeply in theory. Bridging the gap between the theory and application is often a difficult task, particularly in the classroom setting. Experimental laboratories have been shown to be useful in motivating students and reinforcing the information taught in the classroom,^[1-4] often with the additional benefit of small-group learning.^[5,6] The use of hands-on experimental laboratories that are closely tied to the traditional process control lecture course allows students to actually link the theoretical content of the courses to its use on real-world systems. For this reason, process control experiments have been developed across the country.^[7-9]

The development of useful, dynamic, process control experiments requires a number of considerations. Safety is the primary consideration because an environmentally friendly system that can be operated with minimal risk to both the equipment and the user is necessary. The ideal system would also be a cost-effective means to demonstrate the pertinent material with some industrial relevance. It should be of moderate complexity, as simple systems may be too trivial to motivate students while a full-scale industrial process may be too overwhelming. Giving it flexible configuration options will allow for its use in a variety of contexts. Reasonable process time constants are also essential so that the sys-

tem dynamics are slow enough to demonstrate that process changes are not instantaneous, while also reacting quickly enough to limit student boredom when examining dynamic process transitions.

Undergraduate students typically have very limited experience with dynamic systems since many undergraduate courses work under assumptions of steady-state operation. The use of the dynamic experiment(s) provides this experience and demonstrates all aspects of the textbook theory.^[10-17]

There are a number of well-designed, low-cost experiments available commercially, from vendors such as Lego, for use

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in process control education.^[18] These systems, however, fail to offer the flexibility to be utilized in many different contexts. Furthermore, they often fail to provide any semblance of being industrially relevant.

At the University of South Carolina, both a simple, dynamic, nonlinear, two-tank, air-pressure system and a more complex, multivariable, four-tank, air-pressure system have been developed. These pressure-tank systems prove quite useful in process control education, as they address the objectives for an ideal process control experiment. Inspired by experimental liquid-level systems,^[19-23] these experiments are exceptional instructional tools for chemical engineers. As opposed to liquid-level systems, in these systems pressure differences drive the flow. This variation removes the limitations in system flexibility typically associated with gravity-driven liquid systems. The two-tank system is quite portable, thus lending itself well to classroom and outreach demonstrations. A variety of undergraduate topics including open-loop modeling and traditional single-input, single-output (SISO) closed-loop control strategies can be readily demonstrated on the two-tank system. The more complex, multivariable, four-tank system can be used in a small group setting to illustrate more advanced topics such as multi-input, multi-output (MIMO) modeling, interacting systems, and multivariable decoupling, to name a few. This paper presents a detailed description of both systems and summarizes their current and future uses for both educational and research purposes.

THE TWO-TANK SYSTEM

A compact, experimental, air-pressure tank system involving a pair of tanks in series has been developed (<http://www.che.sc.edu/faculty/gatzke/software.htm>). A schematic and photograph of the system are provided in Figures 1 and 2. This section describes the system itself as well as presenting its uses in the context of undergraduate process control education.

System Description

The two-tank pressure system is comprised of two constant-volume aluminum tanks assembled in series supported by aluminum framework (22 inches long \times 24 inches high \times 17 inches wide). The two cylindrical tanks are each a foot in length. Their diameters are two inches and one inch, respectively. Supply air enters the system through a single one-half-inch, air-actuated, BadgerMeter control valve.^[24] The air flows through quarter-inch tubing into the two tanks in series and exits to the atmosphere. A small muffler is utilized at the exit to reduce system noise. The tanks are separated by Swagelok^[25] metering valves with repeatable vernier handles. This provides a means to accurately transform the system between various system configurations. Note that completely opening a valve between the two tanks effectively “joins” the tanks, resulting in one large tank of uniform pressure, as

opposed to two tanks in series. Pressure measurements are available from each of the two pressure tanks. Gauges are installed on each tank to provide visual indications of the pressures while pressure transducers are used to more accurately measure and transmit pressure readings to a computer. The larger tank is also fitted with a small release valve that vents to the atmosphere. This valve can be used to create a disturbance on the system that might simulate a leak in the given tank, providing the opportunity to examine disturbance rejection as a possible control objective in addition to refer-

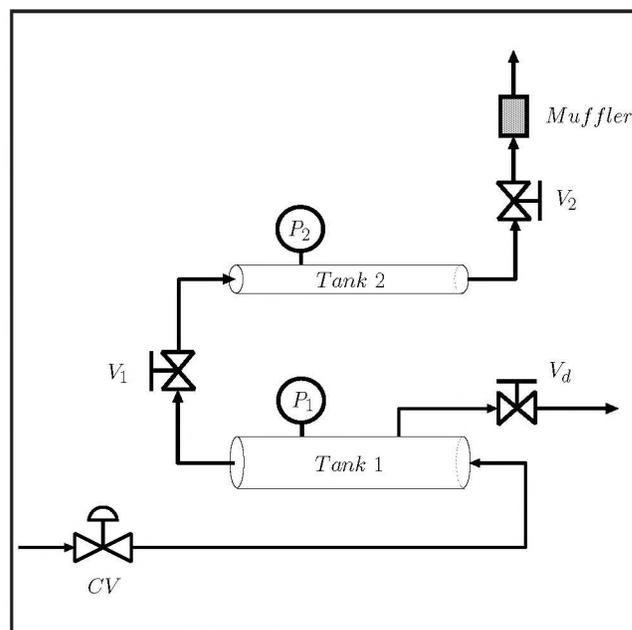


Figure 1. Two-tank schematic.

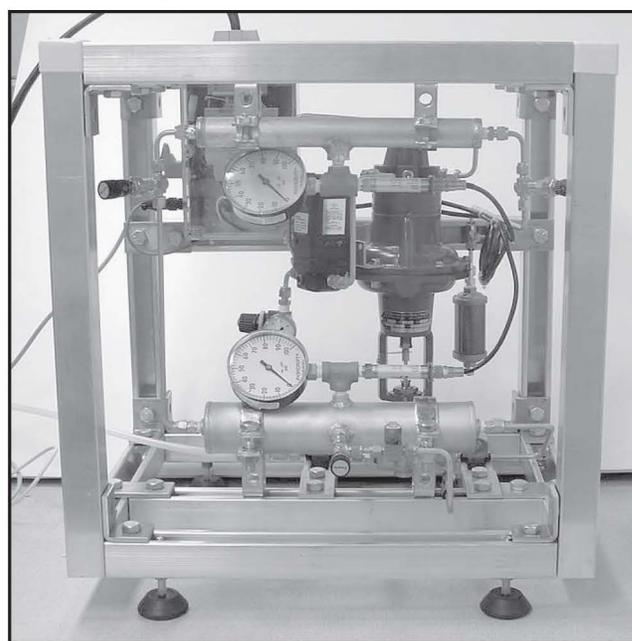


Figure 2. Photograph of the two-tank system.

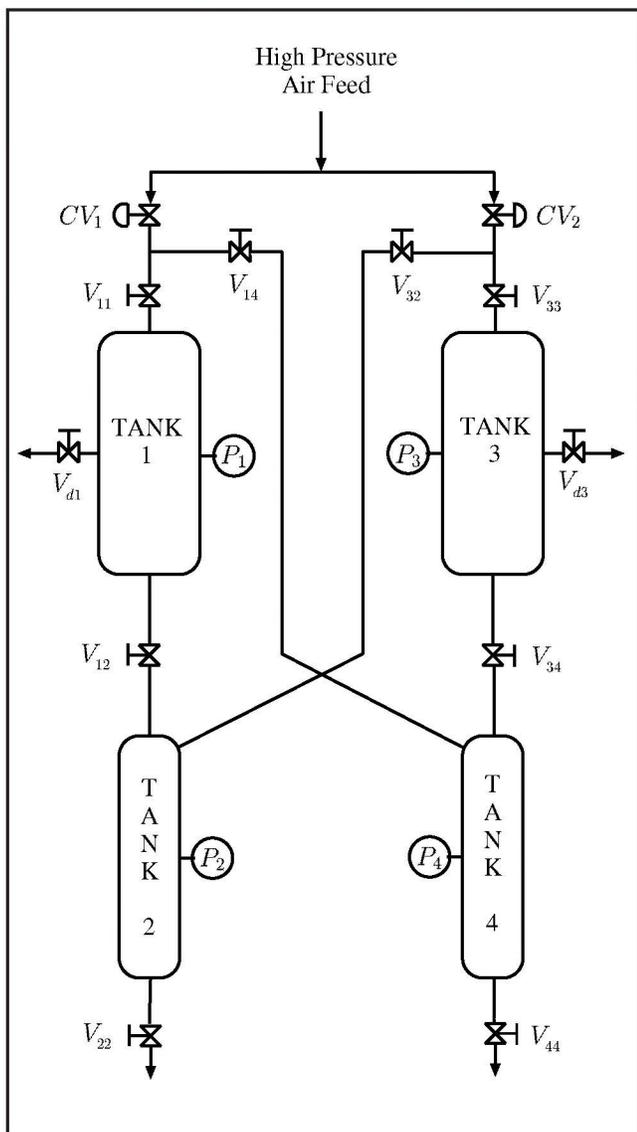


Figure 3. Schematic of the four-tank pressure system.

ence tracking. The apparatus is equipped with a National Instruments Data Acquisition system which can be interfaced to both Matlab/Simulink^[26] and LabVIEW.^[27] A complete materials listing can be obtained by contacting the authors.

It should be noted that initially the control valve exhibited substantial hysteresis, making accurate modeling impossible. A valve positioner was required in order to generate reproducible open-loops results on the system. This also helps introduce students to cascade control and the complexity of real industrial systems.

In the lab environment, the feed air pressure can be supplied in a more permanent manner from a compressor. On the other hand, small compressed-gas cylinders or lecture bottles can be used so that the system can be taken into the classroom for demonstrations. Similarly, a dedicated desktop computer can be used in the labs, while a laptop can be conveniently carried to the classroom.

Educational Uses

This new experimental system is quite valuable for educational purposes. In the classroom setting, it lends itself well for demonstration to larger audiences. Alternatively, smaller groups can experiment with the system in a laboratory setting and reap the benefits of learning in a hands-on environment. The typical undergraduate class can be broken into small groups that can be rotated between the actual pressure-tank system and nearby computer labs. In the computer labs, students can use a high-fidelity model of the system to carry out simulation work that closely parallels what is to be done experimentally. This way, those entering the computer labs first can prepare for the actual experiment, while those that see the actual system first can later reaffirm what has been done experimentally. These advantages are supported by the rapid dynamics of the system. Note that the open-loop time constant is on the order of 30 seconds. In an extended class period, it is possible that numerous groups could get a substantial amount of time working with the apparatus.

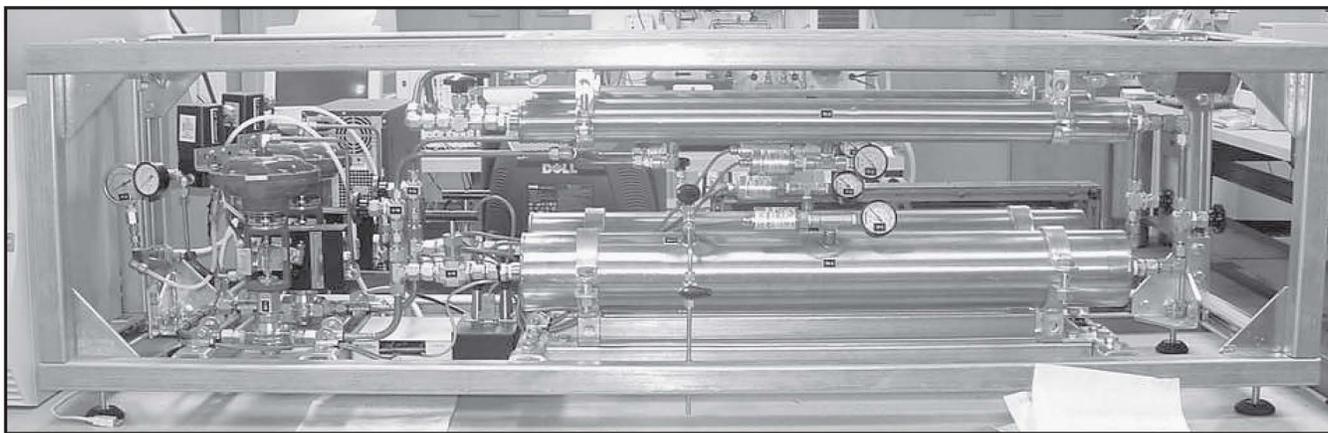


Figure 4. Photograph of the four-tank pressure system.

Using this system, many topics from the undergraduate process control curriculum can be illustrated. Open-loop modeling can be performed to identify both first- and second-order SISO models of the two tanks, depending on the configuration. Both frequency- and time-domain models can be considered, including input/output descriptions such as Autoregressive Moving Average (ARMA) models. Linearization of an available nonlinear first-principles model can also be carried out. Traditional closed-loop control methodologies such as Proportional-Integral-Derivative (PID) and Internal Model Control (IMC) can be implemented. Additionally, related topics such as closed-loop stability can be demonstrated.

THE FOUR-TANK SYSTEM

This section describes the four-tank system in comparison to the two-tank apparatus. A schematic and photograph of the system are provided in Figures 3 and 4. This system's uses for undergraduate, intermediate, and advanced process control education are presented along with its utility in process systems engineering research.

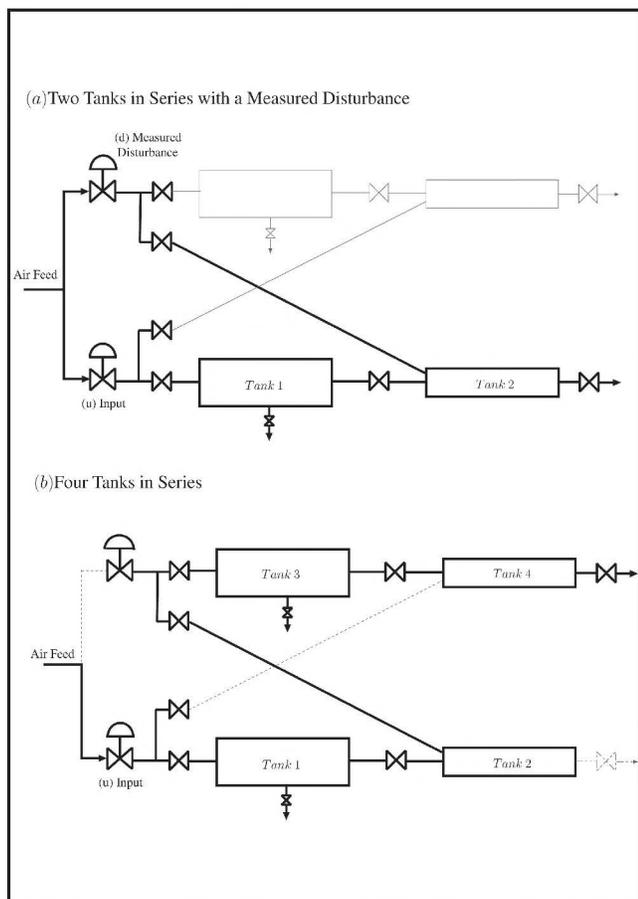


Figure 5. Flow diagram for alternative configurations of the four-tank system.

System Description

The MIMO experimental system consists of four interconnected air tanks arranged in two parallel trains of two tanks, in series, built upon a steel framework. Each tank is 35 inches in length with diameters of 4 inches and 2.5 inches for the upstream and downstream tanks, respectively. Supply air flows into the system through two air-actuated BadgerMeter control valves which serve as the manipulated variables for the system. The air flows through copper tubing and the tanks before exiting to the atmosphere. Again, mufflers have been installed at the system exit to reduce the noise level. Specifically, the air flowing through control valve 1 (CV_1) proceeds into tank 1 and subsequently into tank 2 downstream before exiting the system. Additionally, a portion of the flow from the control valve can be routed into the downstream tank of the adjacent train (tank 4). In a similar manner, control valve 2 (CV_2) affects the pressure in tanks 3 and 4, with cross-flow effects on tank 2. Valves V_{14} and V_{32} are directly responsible for the cross-train flow. In some cases, the interacting nature of the system as a result of the cross-train flow leads to the presence of an adjustable, multivariable, right-half plane zero and inverse response. Physically, this is a result of the fast and direct response of the downstream tank pressures to cross-train flow, in contrast to the slow indirect effects of the flow from the large upstream tanks into the smaller downstream tanks.

The flow of air through the system is driven by pressure gradients. Check valves are not used, therefore air could flow back upstream provided that the pressure gradient is in the appropriate direction. (Similar liquid levels have limitations in these regards as the flow path is dictated by gravity.) The result is a more flexible, dynamic experiment. As with the two-tank system, the various tanks are separated by a number of Swagelok metering valves; their placement allows the system to be configured in a variety of ways. By opening or closing select valves between the tanks, the system can be quickly transformed from one configuration to another. The possible configurations include: a single tank of numerous possible sizes (depending on the number of tanks utilized), two to four tanks in series, a pair of tanks in parallel, and other setups that would have tanks in both series and parallel. For example, V_{14} , V_{22} , and CV_2 can be completely closed, resulting in an SISO fourth-order system with air flowing through all tanks in series (see Figure 5b). Note that in the interest of saving laboratory space, the system is "folded" so that the smaller tanks are placed above the larger ones, leaving a system with total dimensions of 72 inches long, 22 inches high, and 22 inches wide.

Educational Uses

Although not portable enough to be taken to the classroom, this system is well suited for use in the laboratory environment. This apparatus can again be used for large group demonstrations or in a more personal setting for individual-to-

subspace identification methods in Matlab to develop a linear state-space representation of the system. Using this model, implement a traditional Model Predictive Controller on the system and test the closed-loop performance of the system by introducing both setpoint changes and disturbances. Test the impact of the various tuning parameters on the stability and performance of the controller.

These assignments exemplify those used in the different control courses. They provide students with the opportunity to explore the modeling and control the experimental pressure-tank system. Again, note that in the interest of time, some students can develop their control methodology using a high-fidelity process model as the system to be controlled before implementing their work on the actual system.

Related Research

In addition to its utility in the instruction of process control theory, this four-tank system has potential for use in research in the field of systems engineering. To date, this particular system has been the focus of a number of research endeavors.

For instance, system modeling is an important precursor to many advanced model-based control schemes. In limited regions of operation a simple linear model could suffice. Process nonlinearities, however, often require more complex model forms. The nature of this system is such that the process can exhibit hybrid dynamic behavior as the flow of air through the valves of the system can discretely switch between distinct, multiple, continuous regimes of operation. Under low pressure-drop conditions, the air flowrate across a given valve is dependent on both the up- and downstream pressures. In high pressure-drop conditions, however, a sonic, or choke, flow regime is encountered in which the flowrate across a valve becomes solely dependent on the upstream pressure. The respective valve manufacturers, Swagelok^[25] and BadgerMeter,^[24] provide “hybrid” flow expressions based on first principles to capture these dynamics. For the BadgerMeter control valves the flow can be described by:

$$q = NC_v P_a \sqrt{\frac{P_a \Delta P}{G_g T_a}} \quad \text{if } P_b > 0.5P_a$$

or

$$q = NC_v \sqrt{\frac{(3/2)P_s^2}{G_g T_a}} \quad \text{if } P_b \leq 0.5P_a$$

while for the Swagelok needle valve the flows can be de-

scribed by:

$$q = NC_v P_a \left(1 - \frac{2\Delta P}{3P_a}\right) \sqrt{\frac{\Delta P}{P_a G_g T_a}} \quad \text{if } P_b > 0.5P_a \quad (1)$$

or

$$q = 0.471 NC_v P_a \sqrt{\frac{1}{G_g T_a}} \quad \text{if } P_b \leq 0.5P_a \quad (2)$$

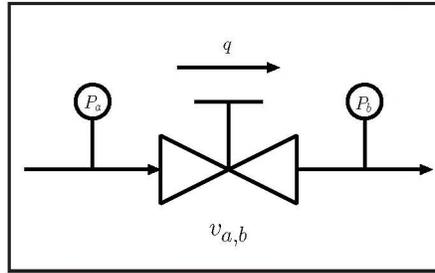


Figure 8. Schematic showing the relationship of the pressures involved in calculating the gas flowrate across a valve. Adapted from Reference 25.

where q is a volumetric air flowrate across the valve at standard conditions, N is a numerical constant for units, C_v is the valve coefficient, P_a is the upstream pressure, G_g is the specific gravity of the fluid, and T_a is the temperature of the system. Temperature measurements are not available at the various points in the system. For convenience it is assumed that the temperature of the air in the system is approximately constant throughout. The first flow expression defines the low pressure drop regime where the flow across the valve is a function of both the upstream and downstream pressures. The second flow expression defines the

choked flow regime where the downstream pressure has no influence on the flowrate. Under ideal conditions, these flow expressions can be used in conjunction with the ideal gas law to develop discrete-time models of the pressure in each tank.

To model the rate of change of pressure in a given tank (\dot{P}_i), the ideal gas law is assumed as the system is operated at both a reasonable temperature and pressure.

$$\dot{P}_i = \frac{\dot{n}_i RT}{V_i} \quad (3)$$

where V_i is the volume of the tank, \dot{n}_i is the molar rate of change of air in the tank, R is the gas constant, and T is the temperature inside the tank.

Provided that flow expressions define a volumetric flow across a valve at standard conditions, the ideal gas law can be utilized a second time to convert to a molar flow across a valve.

$$\dot{n} = \left(\frac{P_{atm}}{RT_{std}}\right) q \quad (4)$$

where P_{atm} is the standard (atmospheric) pressure, T_{std} is the standard temperature, and again q is a volumetric flowrate. Thus

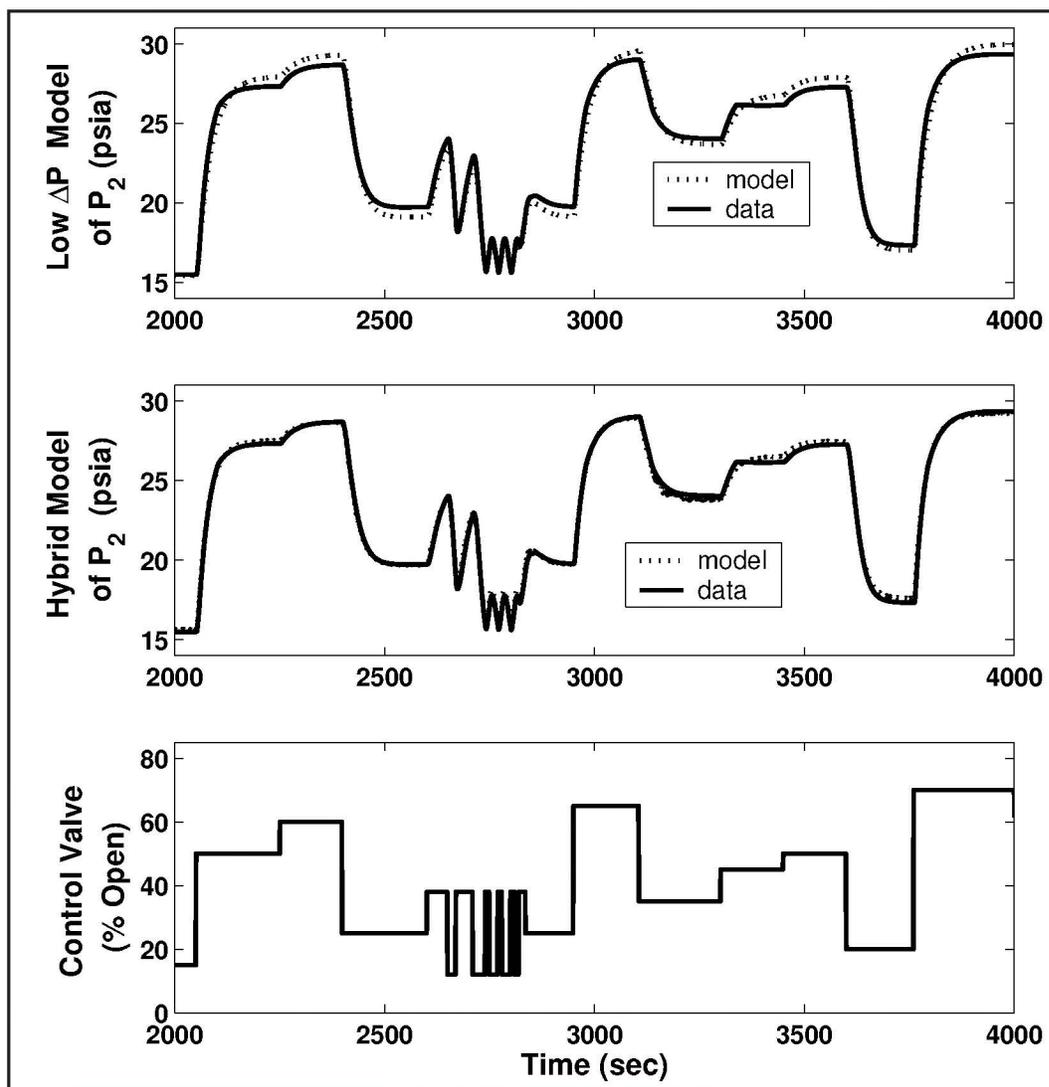
$$\dot{P}_i = \left(\frac{P_{atm}}{V_i}\right) \left(\frac{T}{T_{std}}\right) (\sum q_{in} - \sum q_{out}) \quad (5)$$

Based on this general expression, a discrete-time model of the system can be developed. Using the switching conditions prescribed by the valve manufacturers, a least squares regression can be performed to identify model coefficients that represent parameters such as the valve coefficients, temperature influences, etc. For the simple case of modeling the pressure within a single tank, the results are presented in Figure 9. It can be seen that the hybrid model that considers both low-pressure drop and choke flow regimes is better able to capture the system dynamics than a model based solely on low-pressure drop flow.

Alternatively, mixed integer methods^[28-30] can be used to develop strictly empirical hybrid descriptions of the process. Propositional logic can be used to formulate Mixed Integer Linear Programs (MILP) whose solution yields optimal coefficients and switching conditions for a variety of model forms including hybrid Volterra, autoregressive moving average (ARMA), and more general nonlinear state-space representations.

On a similar note, six process states can be considered in the modeling of the dynamics of the system. The pressures in each of the four tanks can act as states in the model, as well as two states that are not so obvious. The placement of the two supplemental valves leading into the two larger tanks causes some resistance to air flow, regardless of their position. This, in effect, makes the small sections of entrance tubing between the control valves and the supplemental valves act as two additional but very small tanks. The pressure in these two regions will act as the remaining process states. No pressure measurements are available in the areas, yet the size of these “tanks” and the nature of the system imply that the associated dynamics are extremely fast. A set of ordinary differential equations (ODEs) can be developed for the tank system to describe each respective state. Under the assumptions that these two extra tanks exhibit fast dynamics in comparison to the rest of the system, however, an approximation can be made that reduces the respective ODEs to algebraic relationships as the derivative term can be approximated as

Figure 9.
Comparison of a fundamental low-pressure-drop flow model and a hybrid dynamic model in their ability to describe the pressure in a downstream tank.



zero. This leads to the use of a system of differential algebraic equations (DAE) to describe the system, as well as motivating studies in the area.

Additionally, the system has been utilized as a testbed for the development of advanced control strategies. In one case, the prioritized objective inferential control of unmeasured process states is considered. The system is operated in a 2-by-2 fashion with measurements of the downstream tank pressures available. The two upstream tank pressures are considered as the unmeasured process states to be controlled. Traditional MPC methods are often limited to the control of measured outputs and typically rely on a heuristic tuning to address the trade-off between satisfying different control objectives. A state-space modeling approach can be utilized to explicitly describe unmeasured process states. Using information from this state-explicit model and using propositional logic, a mixed-integer MPC algorithm^[31] can be developed that relies on the online solution of an MILP or MIQP for the optimal control move. Such a formulation can allow for a more intuitive tuning in which control objectives, possibly involving unmeasured states, are met in order of their assigned priority.

CONCLUSIONS

Chemical process control education is often limited by the availability of practical hands-on educational tools. Few industrially relevant systems are available that offer both reasonable size and cost while providing interesting dynamics with the flexibility to be used in numerous contexts. This paper describes two such systems that provide students with the opportunity to actually apply and demonstrate experimentally many of the theoretical concepts that are fundamental to the subject. A small, experimental, two-tank system has been developed for use as a tool in process control education. The size and simplicity of the system lend themselves well to particular use in the undergraduate classroom. A similar yet more complex multivariable four-tank has also been developed. Its flexibility enables its use in a variety of applications. Many aspects of both the undergraduate and graduate-level process control curriculum can be presented. Additionally, the system is the focus of a variety of interesting research problems. Among these are studies on the hybrid dynamic nature of the flow through the system, and the systems' use as a testbed for advanced control schemes such as prioritized objective MPC.

ACKNOWLEDGMENT

The authors would like to acknowledge financial support from the National Science Foundation Early Career Development grant CTS-0238663.

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This column provides examples of cases in which students have gained knowledge, insight, and experience in the practice of chemical engineering while in an industrial setting. Summer internships and co-op assignments typify such experiences; however, reports of more unusual cases are also welcome. Description of the analytical tools used and the skills developed during the project should be emphasized. These examples should stimulate innovative approaches to bring real-world tools and experiences back to campus for integration into the curriculum. Please submit manuscripts to Professor W.J. Koros, Chemical Engineering Department, University of Texas, Austin, TX 78712.

PARTNERING WITH INDUSTRY *for a Meaningful Course Project*

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Engineering students can gain valuable benefits from an industry-sponsored project. Not only do students gain exposure to a full-scale chemical process, they also work closely with process engineers to collect and evaluate data. Students may even be allowed to collect data themselves by running product-testing equipment on-site. Once the data are analyzed, students can present their findings in a formal environment in front of industry personnel.

Many chemical engineering programs provide opportunities for students to tour regional industries, thus exposing them to the complexities of a full-scale chemical process. Rarely, however, are students given the chance to do coursework on a real problem with an actual state-of-the-art industry process. Yet such experience is especially valuable to students who do not receive a co-op or internship opportunity.

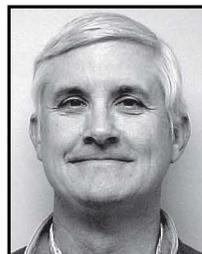
The University of Kentucky at Paducah has an advantageous location in close proximity to many industries. Calvert City, 17 miles east of Paducah, is home to 16 multinational industrial plants including Arkema Chemicals (formerly Atofina Chemicals), ISP Chemicals, Degussa Corporation, Celanese Chemicals, Westlake Vinyl Corporation, Wacker Polymer Systems, and Air Products and Chemicals. Many of these industries were involved in establishing the UK-Paducah engineering program, and now participate on an Industrial Advisory Board (IAB) that provides input into course content.

Through the IAB, contact was made with one member interested in collaborating on a course project. Wacker Polymer Systems, whose manufacturing site is on the Air Products plant site, provided the opportunity for an industry project applicable to Introduction to Particle Technology, a course offered biannually to upper-level undergraduates. Air Products is a minority partner in a joint venture with Wacker Polymer Systems on the operation of a spray-dryer system. The system manufactures a powder used in dry-mix mortars and other construction-related products.



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Mary Beth Hudson is the site manager of Wacker Polymer Systems in Calvert City, Ky. She received a B.S. in chemical engineering from the University of Kentucky in 1989. She began her career as a process engineer for Air Products and Chemicals in 1989 and joined Wacker Polymer Systems in her present role in 1998.



Ralph Young is the environmental manager at the Air Products and Chemicals plant in Calvert City, Ky. He received a B.S. in chemical engineering from Cornell University in 1971 and an M.B.A. from State University of New York (SUNY) at Buffalo in 1981. In 1991 he received a master's in environmental technology from Murray State University in Murray, Ky.

Three projects were identified that: were of interest to Wacker; involved the spray-dryer system; and applied to the course content. One important project-selection criterion was that students would have the opportunity to perform particle-sizing analyses using the company's Beckman Coulter Counter laser diffraction analyzer. Therefore, each student would be involved in data collection on a real project, and would gain experience running a particle-sizing instrument.

This industry project, taking the place of the usual term paper assignment, counted as 20% of the final grade. The requirements of the industry project were: to tour the process site; obtain all available data from sponsors; collect additional data; compile and analyze the data; formulate conclusions and recommendations; write the report; and present to sponsors. One of the first steps was separating the 10 students enrolled in the course—all undergraduate seniors—into one of the three projects.

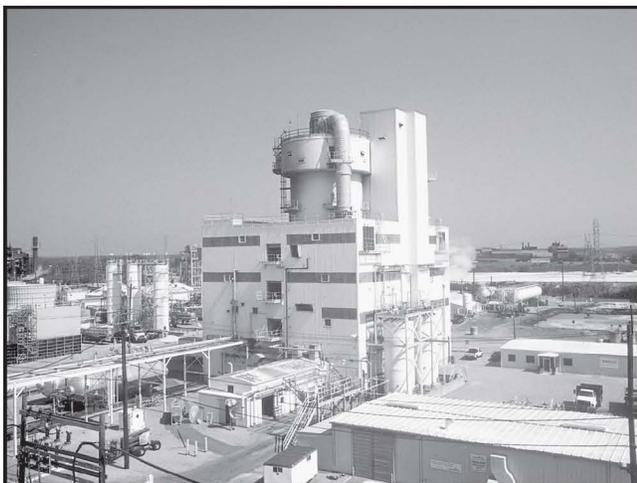


Figure 1. The Wacker spray-dryer system in Calvert City, Ky.

The industry projects were introduced during the fourth week of class, after students had been exposed to particle-size analysis, mixing and segregation of particles, and separation of particles from a gas—subjects related to the three chosen projects. Given a form containing a short description of the projects, the students were asked to rank their interest in each. All students were then assigned to their first or second project choice. One project group had four students and the other two groups each had three.

The industry tour of the spray-dryer process site (See Figure 1) took place during the fifth week of the course. The regular class meeting time was at 2 p.m. on Tuesdays/Thursdays for 75 minutes each. Arrangements were made to carpool on a Thursday to the Air Products plant site, leaving at the beginning of regular class time, and returning before 5 p.m. (one student had a 5 p.m. class). This three-hour time span allowed for 20 minutes travel to plant site, 30 minutes for introductions and a safety/orientation video, a one-hour plant tour, a 30-minute break-out session with engineers to discuss specific projects, and 20 minutes return travel. On the day of the tour, students were instructed to wear long pants, no open-toe shoes, and no sleeveless shirts. Our industry contacts provided flame-retardant smocks, hard hats, and safety glasses for the students at the plant site. After the tour, groups were responsible for making arrangements with a Wacker engineer for any experiments or analyses required by the projects.

THE INDUSTRY PROJECTS

Figure 2 shows a schematic of the Wacker spray-dryer process indicating the locations of the three projects.^[1] In this process, the facility produces vinyl acetate-ethylene copolymer redispersible powders.^[2] The conglomerated polymer powder that forms during the process is redispersed when contacted with water. These powders are used to improve

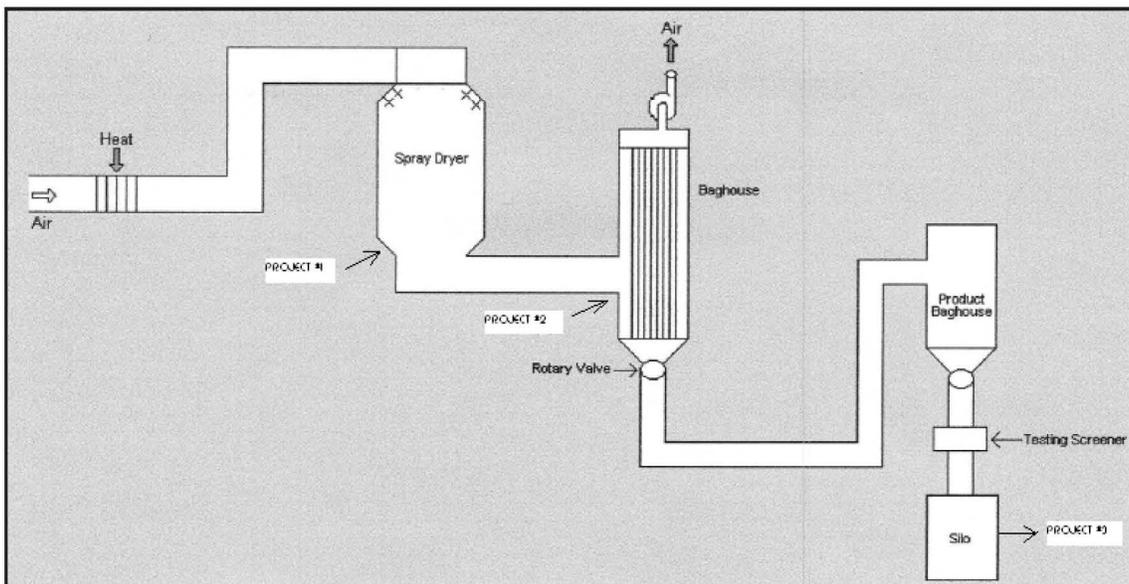


Figure 2. Spray-dryer process flow diagram.

adhesion, impact resistance, flexible strength, water and freeze-thaw resistance, and abrasion resistance properties of Portland cement and other architectural coatings. In the process, polyvinyl alcohol (PVOH) is mixed with emulsions and fed to the spray dryer.

High-pressure air and the solution are supplied to the top of the tower through spray nozzles. In the tower, water is driven from the mix leaving a dry powder at the bottom of the tower. The dried powder is pneumatically transported from the spray dryer to the main baghouse, where particles are separated from the gas before being transported to the product baghouse; there particles are screened and then stored in a silo. From the silo, the product powder is packaged and warehoused until delivery to the end user.

Project 1. Nozzle Configuration versus Particle-Size Distribution (PSD) of Spray Dryer Product

In the spray-dryer tower, polymer is supplied to the top of the tower through a high-pressure ring of spray nozzles. The high pressure forces the liquid droplets through a small orifice, causing them to atomize into a fine spray. The first project investigates the effect of the nozzle configuration—that is, the sequence of nozzles that are operational—to the final PSD of the product. Students measured the PSDs based on three different



Figure 3. Student Melissa Barrett and Professor Lee-Desautels use the Beckman Coulter Counter at the plant.

ent spray-nozzle configurations using the Beckman Coulter Counter (See Figure 3). Students compared the PSDs and analyzed the results based upon differences in trajectories between the various configurations.

The students

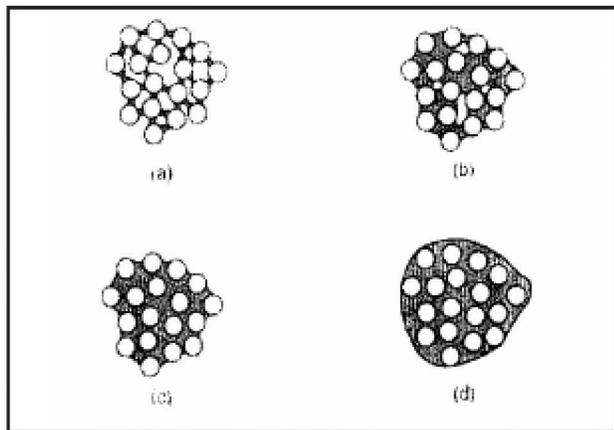


Figure 4. Types of agglomeration occurring throughout the spray dryer.

found little variation between sample distributions for the three nozzle configurations. Wacker provided an airflow model of the spray dryer to aid the students in their analysis.^[3] The airflow model showed a vortex forming in the tower, causing much turbulence. The students attributed the small variation in PSDs to the presence of this highly turbulent vortex region, which formed in the tower independently of nozzle configuration. The students connected the project to their coursework by proposing the various forms of agglomeration that can occur throughout the tower (See Figure 4) with capillary (c) and droplet (d) occurring at the top of the tower, nearer to the atomized liquid spray, and pendular (a) and funicular (b) agglomeration dominating toward the bottom of the column, where much of the liquid has evaporated.^[4] This student group recommended a study to maximize polymer feed to the tower without causing excessive agglomeration by controlling nozzle configuration, nozzle pressure, and airflow.

Project 2. Baghouse Segregation Analysis

Once the polymer powder has exited the spray tower, it has an average diameter of about 100 microns. It is mixed with clay particles (average size 60 microns) and pneumatically transported down flexible ductwork to the main baghouse. The main baghouse serves to separate the transport gas from the powder while controlling particulate emissions. The pneumatic ductwork splits into six separate ducts (labeled A, B, C, D, E, and F as shown in Figure 5) before entering the main baghouse.

The second project involved analyzing the uniformity of particle loading on the main baghouse after the splitting of the ductwork. Samples were collected by industry personnel at each of the six separate ducts leading into the baghouse. The students analyzed the samples with the Beckman Coulter Counter and compared distributions. The students found that the mean particle size differed widely among the ducts. Duct A contained the largest particles at a median size of 159 microns; Duct B particles had a median size of 76 microns; Ducts E and F averaged 60 microns; and Ducts C and D averaged

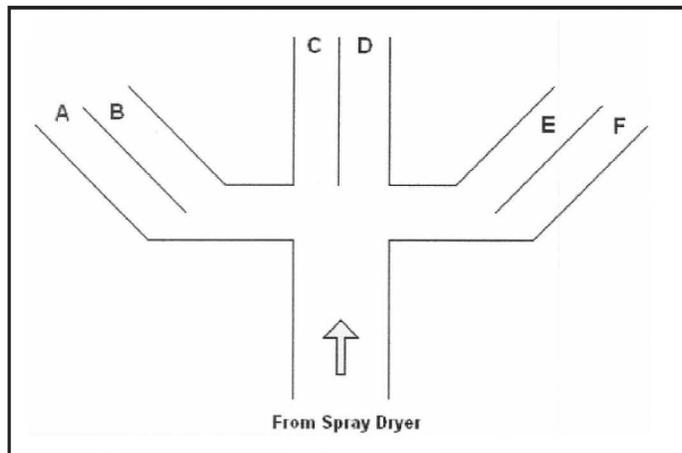


Figure 5. Pneumatic ductwork to main baghouse.

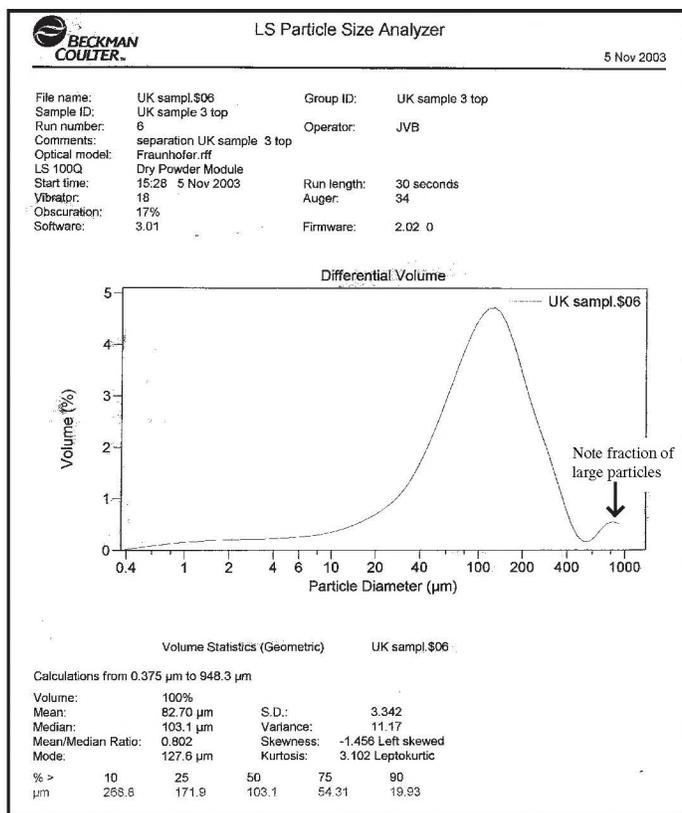


Figure 6. PSD of particles sampled from top of container.

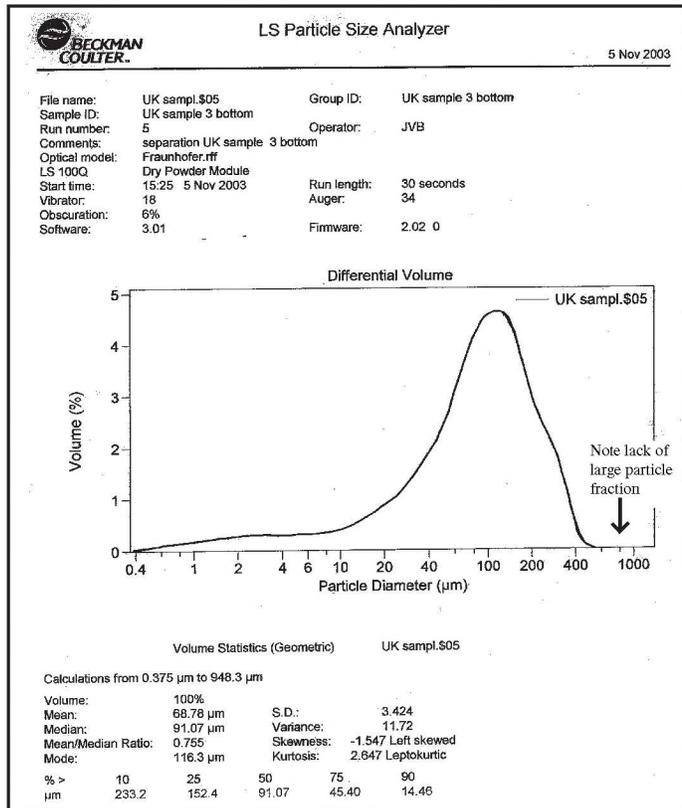


Figure 7. PSD of particles sampled from bottom of container.

45 microns. The students realized they couldn't explain these results in terms of inertial considerations alone, as the larger particles would be more likely to settle out when making the turn to Ducts A, B, E, and F—an effect that would lead to smaller particles in those ducts. The students decided they needed to gather more information about the ducting. On speaking with plant personnel, they were made aware that the lines had never been cleaned. The students also learned that directional plates had been installed in the transport lines to direct powder flow, but were nonfunctional due to buildup of wet product—essentially “gluing” them in place. Students proposed in their analysis that blockage due to material buildup was occurring in the pneumatic lines, and proposed it was concentrated around Ducts C and D, creating a region of restricted flow and high pressure drop. This restriction to flow in turn resulted in the smaller average particle sizes in these ducts, they theorized.

In addition to regular sampling of the transport lines to monitor particle distributions, the students recommended the directional plates in the ductwork be made operational to control powder fed to each duct. To prevent recurring problems, students proposed that since the majority of this buildup occurred during start-up of the process, developing stricter process start-up guidelines was recommended.

Project 3. Product Segregation During Transport

Once the powder has been sent through both sets of baghouses, it is transported to a silo where it is bagged and transported to consumers by truck. The third project investigated the segregation of powder product during the transport process. Some additional PVOH powder is added to the spray dryer product before reaching the product baghouse, and the company suspected some segregation might be occurring with handling and transport due to the PVOH having a smaller average particle size than the product. Having learned about the mechanisms of particle segregation,^[4] students decided the mechanism of percolation was responsible due to the rise of coarse particles with agitation.

To test if segregation could occur, the students used a Ro-Tap device to agitate a sample container for a given amount of time to simulate the transport process. The students then took samples from the top and bottom of the shaken sample container and measured PSDs in the Beckman Coulter. The students also had an unshaken control sample that was measured. They found that the control had little difference in particle-size distributions between the top and bottom samples, with mean sizes of 95 and 96 microns, respectively. The shaken samples showed a greater percentage of large particles in the top samples than in the bottom samples, indicating the percolation and coarse particle-rise phenomena. In one shaken sample, after shaking for 30 seconds particles removed from the top of the container had a mean size of 83 microns, while particles from the bottom had a mean size of 69 microns (See Figures 6 and 7).

“One of the most valuable aspects of this assignment from an industry perspective was the ‘Presentation to Plant Technical Professionals.’ Many entry-level engineers do not have the communication skills to clearly share their ideas with technical management. In many cases, engineering supervisors spend significant amounts of time working with entry-level engineers on their presentation and communication skills.”

—Industry feedback

The students concluded that particle segregation is a negative effect for a product intended to meet certain requirements and specifications for its end use. Because this product had received no complaints, however, the students recommended no changes to the transportation of these powders. In spite of this concession, they further recommended making customers aware that this phenomenon occurs as a courtesy in case end users might want to homogenize the powder post-transport.

PROJECT PRESENTATIONS

At the end of the semester, each team presented its project findings to industry personnel at a seminar held in the Air Products Engineering Building conference room. Attending the proceedings were the three industry participants plus an additional invited engineer.

All students were required to participate in the presentation, and were given an outline on the required presentation format:

- ▲ *Background (Define the System and the Problem)*
- ▲ *Experimental (What You Did to Collect Data)*
- ▲ *Results/Analysis (Present the Data and Analysis)*
- ▲ *Discussion (Your Interpretation of the Results)*
- ▲ *Conclusions*
- ▲ *Recommendations*

The students in each group took turns presenting portions of the findings and were graded on the quality of the visual aides and delivery. The conference room was equipped with state-of-the-art audiovisual equipment including a projector and screen. The students were told to bring their presentations on a CD, with additional copies to hand out to industry attendees. Most students had never presented in this kind of corporate environment.

INDUSTRY PERSPECTIVE

In an effort to capture the industry viewpoint on the project experience, industry participants were asked to submit comments on the project. Their comments are summarized below. The comments are valuable, not only for students, but also for faculty to gain insight into what qualities industry values from their engineering employees. From the responses, it is obvious that the industry participants looked at the project more as a way to prepare students for the workforce, offering words of advice and critique, than a means of obtaining free labor. The industry participants had a genuine desire to provide a distinctive learning experience for our engineering students.

THE COMMENTS

Concerning the Performance of the Students

- ▲ *“From an industry perspective, I found the students enthusiastic and ready to do a ‘hands-on’ project. I’m not sure if everyone was trying to build their resume, but each student approached the project with an open mind and was prepared to learn something new. They quickly learned how to operate the test equipment and collect useful data.”*
- ▲ *“In most cases, once the ‘newness’ of running the Coulter Counter and other test equipment wore off, the tedium of repetitive testing and analysis was apparent. In this respect each student was exposed to real industrial experience: 10-25% new and exciting opportunities versus 75-90% less exciting work. Every student has their own threshold of tedious, repetitive work. These types of assignments provide the opportunity to help students decide career paths such as process engineering in a plant environment or research assignments in lab environments.”*
- ▲ *“In this project, it was obvious each student had some prior presentation*

training and experience. Many engineering curricula include this training in their degree requirements. Project leaders divided the presentation so that it flowed logically and used graphics to help the audience understand the project and results.”

- ▲ “The only element that was lacking in these presentations was the business case that would make or break a decision to allocate more resources. Since this aspect was not expected from the students, the technical staff was able to question the students and guide their thinking during the presentations. When the business case was made for a project—such as to increase plant production yields or benefit customers—many light bulbs seemed to go on in students’ minds about the importance of the work. The interaction between students and industrial professionals was invaluable and one of the most important aspects of these projects.”

Concerning What is Valued in an Employee

- ▲ “One of the most valuable aspects of this assignment from an industry perspective was the ‘Presentation to Plant Technical Professionals.’ Many entry-level engineers do not have the communication skills to clearly share their ideas with technical management. In many cases, engineering supervisors spend significant amounts of time working with entry-level engineers on their presentation and communication skills.”
- ▲ “Most new engineers get bogged down in project details and sophisticated analysis, and cannot summarize pros and cons to drive a management decision.”
- ▲ “Key qualities I value in employees are: problem solving ability, creativity, communication, teamwork, ability to accomplish goals with minimal direction, initiative, dependability, time-management skills, and the ability to successfully manage multiple constraints. The students’ analytical ability is proven by their successful completion of the engineering curriculum. This project allowed them to demonstrate the other key qualities above as well.”
- ▲ “Among the biggest constraints in industry are time and personnel. We are expected to accomplish more with less. Therefore, we need goal-oriented employees who can drive projects to completion. I have seen many engineers spend too much time evaluating options in trying to find the ‘best’ solution, only to create more problems by not achieving anything. I was told as a young engineer that you will be seen as more successful if you attempt to solve a problem five times over a year and only succeed on the fifth try than if you spend the whole year developing the perfect solution for the first try.”
- ▲ “We do not have clearly defined problems with one correct answer in our work environment. Often, data to analyze the problem are missing or incomplete.

Resources such as money, personnel, and time are limited. Engineers are challenged to determine the best solution to the problem based on the information and resources at hand. There is always an economic impact that has to be evaluated.”

Concerning the Benefit to Industry

- ▲ “The results from the three projects reinforced our knowledge and confidence in what was happening.”
- ▲ “The data will be useful to support the allocation of resources to cleaning the ducting to the main baghouse, alleviate any concerns with nozzle configuration influencing final product quality, and increase awareness of product segregation with transport.”
- ▲ “The particle-size data collected in these projects have been used to address customer issues associated with particle size. Examples are a recent modification to a powder grade to decrease particle size/increase bulk density in response to a bulk handling issue with one of our largest customers, and a recommendation of powder grades to address an application which will require a coarser particle size.”
- ▲ “One of the main benefits to industry in participating in these programs is that we get a better introduction to the students who will be entering the job market.”

STUDENT EVALUATIONS

The students were asked to evaluate the industry project in the optional-items section of the evaluation form. Four queries were made on the project. Students were also asked to provide personal comments specifically about the industry project. Eight of the 10 students taking the course were present for the evaluation.

- ▲ **Query 1. Rate your overall perception of the industry project.**
Response: One rated it outstanding, four rated it good, two rated it average, and one rated it poor.
- ▲ **Query 2. The industry project has allowed me to learn more about a specific area of particle technology.**
Response: One rated it outstanding, four rated it good, two rated it average, and one rated it poor.
- ▲ **Query 3. The industry project has helped me feel better prepared to seek employment with a company that manufactures/uses particles.**
Response: Two rated it outstanding, three rated it good, two rated it average, one rated it poor.
- ▲ **Query 4. The industry project was a valuable component of the course.**
Response: One rated it outstanding, four rated it good, and three rated it as poor.

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Random Thoughts . . .

THE WAY TO BET

The race is not always to the swift, nor the battle to the strong, but that's the way to bet.

—Damon Runyon

RICHARD M. FELDER

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There is no such thing as certainty in science—everything we believe ultimately rests on unprovable assumptions and imprecise observations. Our current theory may seem to work beautifully, but if we really understand science we know that new data can overthrow it at any time. Nevertheless, if there's enough evidence to back it up, we can base predictions on it and sleep peacefully without worrying that we might be wrong. If I pick up a heavy object and drop it, I feel comfortable predicting that it will fall down. I can't prove Newton's theory of gravitational attraction and I'm clueless about *why* gravity works the way it does (as was Newton), but I'm confident that down is the way to bet.

As much uncertainty as there may be in science (and by extension, engineering), there is far more in education. Students are infinitely more complex and unpredictable than cantilever beams and airborne projectiles and fruit flies. Even in education, however, there are some propositions that give you a great chance of coming out ahead if you bet on them often enough. I've got a few like that to offer you.

STUDENTS

- ▶ *If a student who fails a test claims afterwards that he/she really understood the material, then either he/she really **didn't** understand it or the test was unfair (too long, too tricky, . . .). The first one happens far more often than most students believe and the second far more than most professors believe.*
- ▶ *Students who argue vehemently for additional points on every test will have difficult lives as both students and professionals. I also worry about their marriages.*
- ▶ *Students who routinely come up with bizarre but valid ways of approaching problems may struggle in school but will do very well as researchers and engineers (if they survive school).*

- ▶ *Students who drop out of engineering are on average no worse academically than students who stay in. We like to believe that our absurdly high dropout rates in engineering mean we are eliminating weak students and retaining good ones, but that's not how it goes. Lots of students who leave have fine academic records but just don't like what they see in our classes. (Don't bet against this one—I've got the data to back it up.)*

GOOD AND BAD TEACHERS

*An engineering faculty member is a **good** teacher (i.e., a teacher who motivates his/her students to learn and facilitates their learning) or a **bad** teacher (i.e., a teacher who does not motivate or facilitate learning and may even interfere with it) if he or she:*

- ▶ *(good) gets all of his/her students actively involved in class and knows all of their names (or at least most of them in large classes).*
- ▶ *(bad) makes classes PowerPoint shows, or spends most of every period deriving equations, or puts high-level problems on exams that are qualitatively different from anything students have seen in class or on homework "to see if they can think for themselves."*



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- ▶ **(good)** *always has students waiting in the hall during office hours and coming with questions before and after class.*
- ▶ **(bad)** *uses words like “spoonfeeding” and “coddling” when talking about student-centered teaching methods (e.g., problem-based learning) and colleagues who use those methods, and dismisses all educational research as nonrigorous. I’m also betting that individuals who do this have never read an educational research study and could not name a journal that publishes them.*
- ▶ **(good)** *gets consistently excellent student ratings. It’s possible that the ratings are high because of easy grading or whatever other spin colleagues with lousy ratings put on it, but I’m betting (again with a lot of research backup) that a highly rated engineering instructor would also show up as a good teacher in peer ratings and assessments of learning outcomes.*
- ▶ **(bad)** *gets consistently poor student ratings. Someone who is regularly shredded by most students may claim it is because he is “rigorous” or “unwilling to lower standards,” or because she “refuses to be an entertainer,” and “the students don’t appreciate me now, but after they graduate they’ll see how good I was.” Maybe, but if I always bet that those instructors are simply poor teachers I say I’ll come out way ahead in the long run.*
- ▶ **(good)** *has students coming back years later saying what an outstanding teacher he or she was. I’d bet my life savings on this one—and I’d do so even if that individual has never gotten a grant or published a research paper.*

MISCELLANY

- ▶ *Little or nothing meaningful will be accomplished at a faculty committee meeting. The more frequently the committee has regularly scheduled meetings, the more I would be willing to bet on this one. Furthermore, the larger the committee, the less it will accomplish.*
- ▶ *New faculty members who get some formal training and/or mentorship will be better teachers and more successful researchers after two years than their counterparts who get the traditional amount of training and mentorship (none). More and more schools are choosing to bet my way by giving their new hires*

meaningful orientation and formal mentorship.

- ▶ *Departments that decide to give tenure and promotion to qualified faculty members who focus on teaching and educational scholarship will have stronger teaching programs than they had before, and their research productivity and quality will not suffer.*
- ▶ *A high school senior contemplating engineering will get a better education by avoiding schools where much of the administration and faculty think ABET is the enemy.*
- ▶ *Textbooks with CD supplements will soon be replaced by interactive DVDs that may or may not have text supplements, which will lead to improved learning. The present generation of faculty and students may find the adjustment difficult, but the next generation will have no trouble with it at all.*
- ▶ *Traditional campus-based departments will find it increasingly hard to compete with excellent distance programs for good applicants. An online course that includes user-friendly interactive tutorials, electronic interactions between students and instructors and among students, and individual conferencing with the professor and tutors, provides a better educational experience than a campus-based course that is mostly chalk and talk—and distance programs are getting better at those things all the time.*
- ▶ *More and more traditional engineering jobs will be handled by computers, technicians, and engineers in India and China (and Malaysia and Croatia and . . .). Graduates of schools that continue to focus on traditional content will have a harder and harder time finding and keeping jobs. Graduates of schools that focus more on entrepreneurship, critical and creative thinking, multidisciplinary project management, and global economics will do fine.*

I have undoubtedly tipped over some sacred cows here. Some of you will tell me that “Professor X dumbed his tests down and started to get great student evaluations,” or “Professor Y’s students burn her in effigy every year but as alumni they create multimillion-dollar endowments in her name,” or “I can *so* name an educational research journal!!!” You don’t have to send me an angry e-mail message about it—I’ll cheerfully concede right now that if I bet against Professor X or Y or against you I’ll lose. In Vegas the casinos lose thousands of gambles every hour. They make *many* thousands of gambles, though, and the odds are with them. In the long run, they always win. □

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

A FLEXIBLE PILOT-SCALE SETUP FOR REAL-TIME STUDIES IN PROCESS SYSTEMS ENGINEERING

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The inclusion of process control experiments in chemical engineering curriculums and the introduction of new process control experiments^[1,2,3] indicate recognition of the importance of real-time experiments in process systems engineering. The experiments allow an instructor to reinforce and demonstrate theoretical systems concepts presented in lectures. Laboratory systems experiments in an academic setting provide students with an invaluable opportunity to familiarize themselves with important practical issues (*i.e.*, nonideality of industrial processes), such as process-model mismatch, measurement noise, inadequate number of measurements, digital measurements, actuator saturation, unmeasured disturbances, and process nonlinearity—issues often neglected in computer simulations.

This manuscript describes a low-maintenance, low-safety-risk, flexible, 0.9-m × 1.5-m × 2.4-m, pilot-scale setup that can be used for training students and carrying out research in process systems engineering. It briefly states typical applications of the setup. Detailed specific sample applications of the setup, together with real-time results, will be presented in forthcoming paper(s). The setup was built in the Department of Chemical and Biological Engineering at Drexel University and is located in the Process Systems Engineering Laboratory. The setup allows one to study a variety of process-systems engineering concepts such as design feasibility, de-

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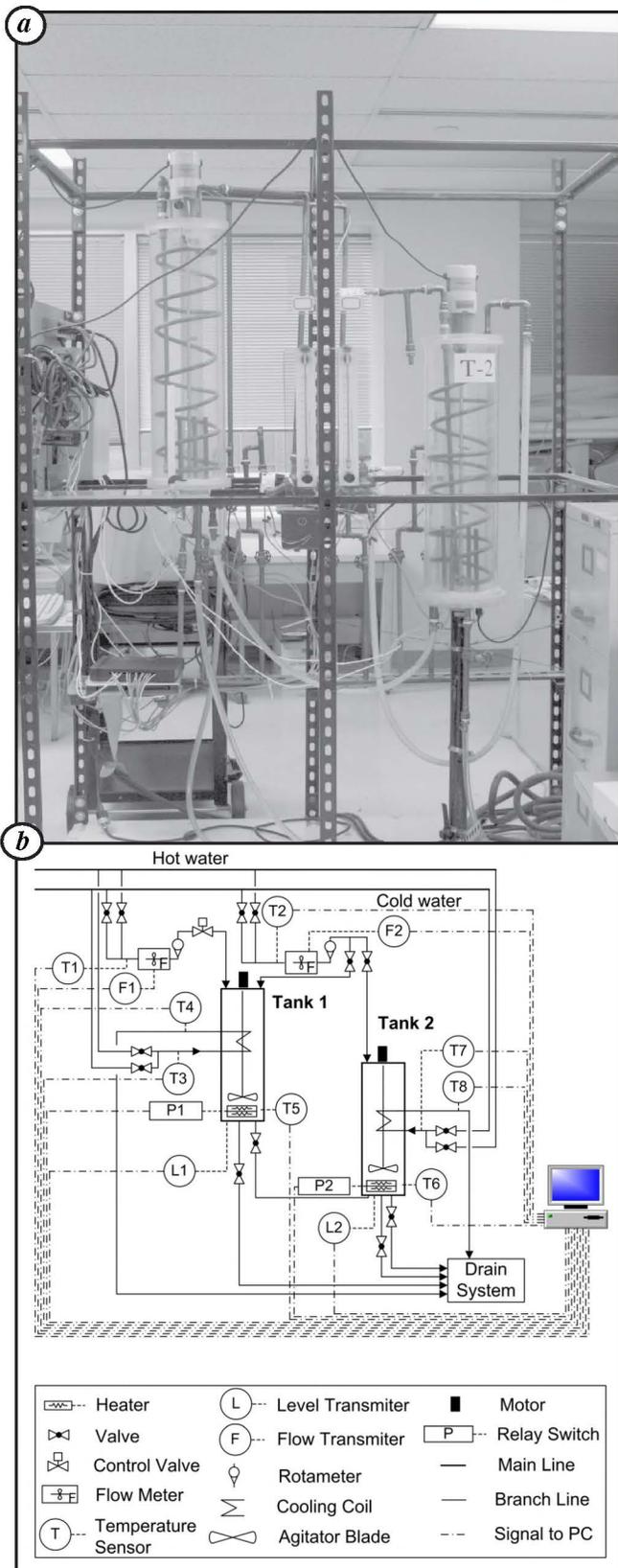


Figure 1. The pilot-scale setup, in photograph (a) and schematic (b).

sign flexibility, control configuration selection, parameter estimation, process and instrument fault detection and identification, controller design and implementation, instrument calibration, and process modeling. Notable features of the setup are its flexibility and low safety risk (because it uses water only). The setup can be single-variable or multivariable, mildly or strongly nonlinear, interacting or noninteracting, and/or single- or multi-tank. It has features of both apparatus # 4 and 10 described by Ang and Braatz^[1]; it can be configured to be the same as apparatus # 4 or 10, or a combination of apparatus # 4 and 10. The setup can be used in both undergraduate and graduate process control laboratories to reinforce, through hands-on experiments, the concepts taught in process control and process analysis lectures.

PILOT-SCALE SETUP

A picture of the 0.9-m × 1.5-m × 2.4-m pilot-scale setup is shown in Figure 1a, and a schematic in Figure 1b. The setup has two identical, clear-plastic, cylindrical tanks. Each tank has an outside diameter of 0.2 m and a height of 1.0 m. The tanks can be connected to each other (by easy-connect/disconnect flexible hoses) in several ways, which allows one to operate the setup as a system of a single tank, two parallel tanks, two interacting tanks in series, or two noninteracting tanks in series. The elevation of the second tank can be adjusted (via a jack) to alter the level of the interaction between the two tanks. Inside both tanks, there are helical copper tubes that can be used for heating or cooling, depending on the temperature of the water flowing into the copper tubes. One end of each copper tube is connected by a hose to a city water supply that is cold, hot, or a mixture of both—allowing adjustment of the inlet temperature of the water stream flowing into the copper tubes. Thermal energy can also be supplied to each tank by an electrical heater consisting of two heat cartridges inside the tank. Each tank has a variable-speed agitator.

The setup has eight resistance temperature detectors (RTDs), two flowrate sensors, two level sensors, and one control valve. The RTDs measure the temperature of the inlet and outlet streams of the tanks and the cooling/heating copper tubes. The level sensors measure the level of water in the tanks. The flowrates of two inlet streams are measured by the two online and two off-line (rotameter) flow meters. A control valve adjusts the flowrate of a water stream flowing into Tank 1.

ELECTRONIC HARDWARE

Analog Input Devices

Each of the sensors measures a process variable and generates a 4-20 mA analog signal, which is then sent to an analog input channel of a data acquisition board. The board then converts the analog signal to a digital signal. There are three

types of analog instruments in this setup

- **Pulse-Output Flow Meter.** The paddle flow meter generates a positive on/off pulse signal when its rotor is rotated by the fluid flow. The pulse signal is then converted to 4-20 mA signal proportional to the flowrate (0-5 gpm).
- **RTD Temperature Sensors.** The resistance temperature detectors are connected to a Wheatstone bridge circuit that uses a reference resistor of 100 ohms, which corresponds to 0 °Celsius.
- **Level Sensors.** The level sensors used in the setup are of the pressure-transducer type. The liquid static pressure in a tank presses on the diaphragm of the transducer, generating a proportional analog signal.

Analog Output Devices

The proportional control valve is an analog output device that receives an analog input signal (4-20 mA) and sets the flowrate proportionally. It is a fail-to-close control valve. The power of the heaters is adjusted by a solid-state relay (SSR), which is connected to a pulse-controller module (both from Omega Engineering, Inc.). The module allows simple conversion of the on/off SSR to a proportional power regulator. Therefore, the average power to the heater is proportional to the input 4-20 mA analog signal to the module. Each of the electrical heaters consists of two High Watt Density Cartridge Heaters (rated power of each: 1.5 kJ/s at 240 volts).

Data-Acquisition Board

A DAS-1701ST-DA data-acquisition board^[4, 5] and an EXP-1800 extension board^[6] (both from Keithley Instruments, Inc.) are used. The data-acquisition board has eight analog input channels. It receives and time-discretizes the incoming analog input signals. The expansion board allows one to expand each input channel of the data-acquisition board to eight input channels. Therefore, the data-acquisition system can support up to 64 analog input channels. It receives 12 analog signals from the eight temperature sensors, the two flow meters, and the two level sensors,

and sends one analog signal to the control valve and two binary signals to the two heaters. The data-acquisition board can communicate with the central processing unit via interface software, such as Visual Basic, Visual C++ (Microsoft Corp.), and LabVIEW (National Instruments Corp.). The software then analyzes the data. A graphical user interface (GUI) is then used to present the data. In this setup, the data-acquisition application is developed by using Visual Basic as the

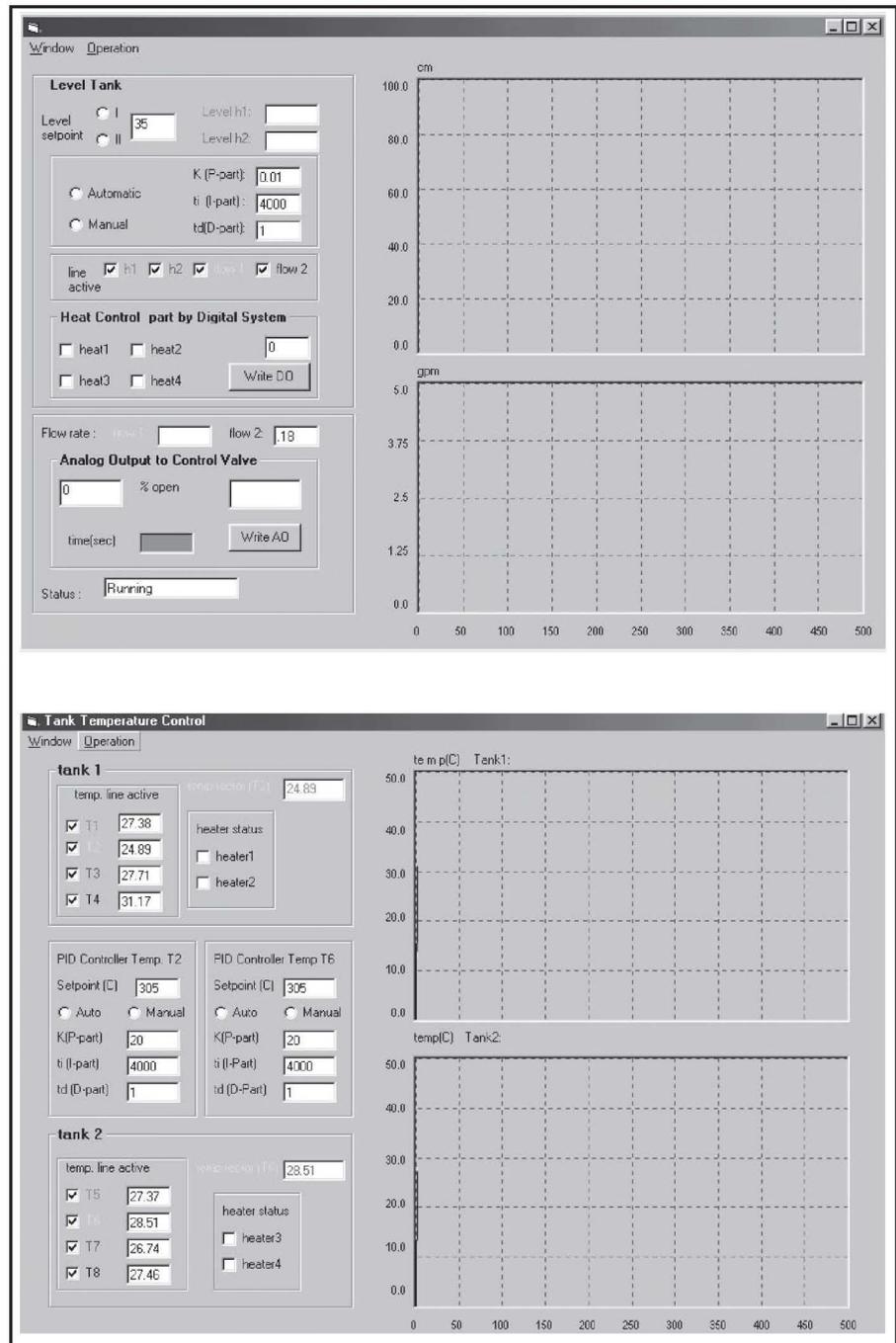


Figure 2. Front-end interface for the level control.

front end and C++ as the backbone. Visual Basic can be used to create a GUI easily, and C++ used to support Windows-based input/output operations. For this setup, front-end windows for temperature control, flow control, and data storage are developed. Two of the windows are shown in Figures 2 and 3. Data from the setup can be saved as Excel files and then be imported to Matlab (Mathworks, Inc.) easily.

TYPICAL APPLICATIONS OF THE PILOT-SCALE SETUP

With the flexibility to operate in various configurations, and its many sensors and actuators, the setup allows real-time study of a variety of process-systems engineering concepts. Figure 4 shows the variables that can be measured and/or adjusted in this setup. Below is a brief description of typical real-time studies that one can perform using the setup.

Process Modeling

Given the online measurements, models including first-principles, empirical (black box), or hybrid (first-principles/empirical)^[7] can be developed to describe water temperature and/or level in one or both tanks. In the case of empirical and hybrid modeling, the students can be taught model-parameter estimation as well. Hybrid model parameters include the resistances of the tank exit pipes as well as the overall heat transfer coefficients of the coiled copper tube banks. The model structure is obtained from mass and energy balances in the cases of first-principles and hybrid modeling, and from prior process knowledge (an assumption) in the case of empirical modeling. The empirical modeling can be off-line or

online. In the latter case, one must use a model identification method.^[7]

Process Design Analysis

The setup can be used to analyze the following process design aspects:

- ① **Feasibility.** Given desired steady-state values of temperature(s) and level(s), and nominal values of temperature and flowrate of the disturbance stream (inlet stream with no control valve), students are asked to evaluate theoretically and experimentally the feasibility of the design to operate at the desired steady state; that is, to check whether the design can provide heater power, water flowrate, and energy (through the heating/cooling coils) adequate to operate the process at the desired steady state.^[8] For example, a desired water temperature below the city water temperature is definitely infeasible.
- ① **Flexibility.** Flexibility is feasibility in the presence of uncertainties such as disturbances and parameter uncertainties/variations. In this analysis, the students are asked to evaluate the feasibility of the design to operate at a given steady state when the temperature and flowrate of the disturbance stream vary within a given range.^[8] Students can map theoretically the disturbance region in which the design is feasible and then verify the region experimentally.

Process Control

The setup can be used to carry out the following process control studies:

- ① **Measurement Selection.** Many control problems with one or more objectives can be posed, and students are

time	Temp_T1	Temp_T2	Temp_T3	Temp_T4	Temp_T5	Temp_T6	Temp_T7	Temp_T8	LevelT1	LevelT2	FlowrateT1	f
0	0	0	0	0	0	0	0	0	0	0	0	
1	6.56130	2.93279	11.09619	9.08538	6.69209	5.77131	6.73902	7.61479	5.21040	5.05750	1.7330	
2	6.56130	2.93279	11.09619	9.88538	6.69209	5.77131	8.73902	7.61479	5.21040	5.05750	1.7330	
3	27.45595	24.79294	27.64977	31.22095	27.22928	28.64874	26.77901	27.56280	30.3998	2.21104	1.7938	
4	27.45595	24.79294	27.64977	31.22095	27.22928	28.64874	26.77901	27.56280	30.3998	2.21104	1.7938	
5	27.57091	24.95282	27.73053	31.30678	27.26090	28.74178	26.89670	27.46193	30.5739	2.17960	1.7908	
6	27.57091	24.95282	27.73053	31.30678	27.26090	28.74178	26.89670	27.46193	30.5739	2.17960	1.7908	
7	27.57091	24.95282	27.73053	31.30678	27.26090	28.74178	26.89670	27.46193	30.5739	2.17960	1.7908	
8	27.37935	24.86715	27.59242	31.37452	27.15258	28.85218	26.66854	27.56584	30.9797	2.50564	1.7894	
9	27.37935	24.86715	27.59242	31.37452	27.15258	28.85218	26.66854	27.56584	30.9797	2.50564	1.7894	

Figure 3. Front-end interface for temperature control and data storage.

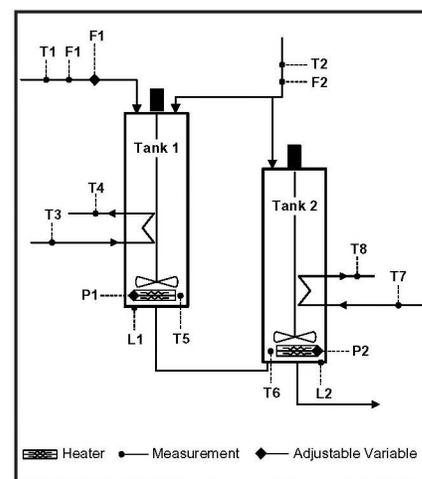


Figure 4. Adjustable and measured variables of the setup.

Laboratory systems experiments in an academic setting provide students with an invaluable opportunity to familiarize themselves with important practical issues (i.e., nonideality of industrial processes), such as process-model mismatch, measurement noise, inadequate number of measurements, digital measurements, actuator saturation, unmeasured disturbances, and process nonlinearity—issues often neglected in computer simulations.

then asked to list the measurements needed to achieve the control objective. These objectives include control of temperature and/or level in Tank 1, and/or control of temperature and/or level in Tank 2. For example, for control of temperature in Tank 1, at least, the temperature measurement T5 is needed.

- ❶ **Control Configuration Selection.** After choosing the necessary measurements, students can be asked to propose a set of manipulated inputs that can be used (adjusted) to realize the control objective(s). The controlled outputs should be controllable from the manipulated inputs. For example, temperatures in Tanks 1 and 2 are controllable from heater power P1 and P2. The state and/or output controllability^[7,9] of the control configuration can be tested.
- ❷ **Input-Output Pairing.** For multi-input, multi-output (MIMO) control problems, students can be asked to pair the inputs and outputs of the selected control configuration so that completely decentralized control can be implemented. To evaluate the level of interactions among the process variables, students can use tools such as the relative gain array,^[10] relative orders,^[11] and/or time delays to propose effective pairs.^[12]
- ❸ **Controller Selection.** One can select a feedback or a feedback/feedforward control system depending on what control system is desired: completely decentralized (set of single-input, single-output, or SISO, controllers) or centralized (multivariable). For example, one can use the flow measurement F2 and the temperature measurement T2 (measurements of disturbance inputs), to add feedforward loop(s) to feedback control of temperature and/or level control in Tank 1. Furthermore, the controller can be: (1) a conventional controller, such as a proportional (P), a proportional-integral (PI), or a proportional-integral-derivative (PID) controller; or (2) an advanced controller such as a model-based controller.^[7,10] The setup can be used to understand the limitations of decentralized control and implement decouplers in reducing the effect of interactions. Further, the model-based controller can be analytical (such as an input-output linearizing controller) or numerical (such as a model-predictive controller). Whether conventional or not, adaptive features can be

added to the controller.^[7,10] In real time, students can observe and compare the performance of different controllers, and evaluate the pros and cons of each.

Parameter Estimation

Given the flowrate, level, and temperature measurements, students can estimate the heater powers and the heating/cooling coil-tank overall heat-transfer coefficients. In the case of the heater powers, since the heater powers are set by the computer, the values of the heater powers are known. This allows one to evaluate the accuracy of the estimated heater powers by comparing them to the actual values.

A parameter estimator that can be implemented in real-time on this setup is described by Tatiraju and Soroush.^[13]

Fault Detection and Identification

The equipment can be used to demonstrate fault detection and identification.

- ❶ **Sensor Fault Detection and Identification.** The setup can be used to learn sensor fault detection and identification in real-time. Noise, drift, and/or bias are added to a sensor reading, and a sensor fault detection and identification method is then used to detect the fault in the sensor and identify the fault type (noise, drift, and/or bias). An example of such a study can be found in Mehranbod and Soroush,^[14] in which sensors L1, F1, and F2, and a PI controller to control the liquid level in Tank 1, were considered.
- ❷ **Process Fault Detection and Identification.** Partial or complete failure of one of the process actuators is an example of a process fault. A process fault detection and identification method can be used to detect an actuator failure and the type of the failure. An intentional fault can be introduced in any of the actuators, and it can be detected and identified in real time by using a process fault detection and identification method.

Instrument Calibration

The setup has three actuators and 12 sensors. For each actuator, a calibration curve is obtained by finding the relation between the raw digital signal (that the computer sends to the data-acquisition board) and the actual value of the corresponding physical variable. For example, the control-valve cali-

bration curve can be obtained by measuring the flowrate with the rotameter at different, constant, raw, digital signals set at the computer. For a sensor, a calibration curve is obtained by finding the relation between the raw digital signal that the computer receives from the data-acquisition board and the *actual* value of the corresponding physical variable. For example, an RTD is calibrated by placing it in beakers of water at different known temperatures and recording the value of the corresponding steady-state, raw, digital signal received by the computer. A typical calibration curve is presented in Figure 5. It shows how the flowrate of the water stream through the control valve depends on the raw digital signal.

Calorimetric Studies

The electrical heaters can be used to simulate heat of reactions. An exothermic reaction or set of exothermic reactions can be considered and simulated on the microcomputer, and the rate of heat production by the simulated reaction(s) is then sent to the heater to set the heater power to the calculated rate of heat generation. Material and energy balances for the tanks, considered with the temperature and flowrate measurements, can then be used to estimate the power to the heaters; that is, the rate of heat production by the simulated reactions.

CONCLUSIONS

This manuscript describes a low-maintenance, low-safety-risk, flexible, pilot-scale setup that can be used for training students and carrying out research in process systems engineering. It briefly states typical applications of the setup. Detailed specific sample applications of the setup together with real-time results will be presented in forthcoming paper(s). The setup allows one to study a variety of process-systems engineer-

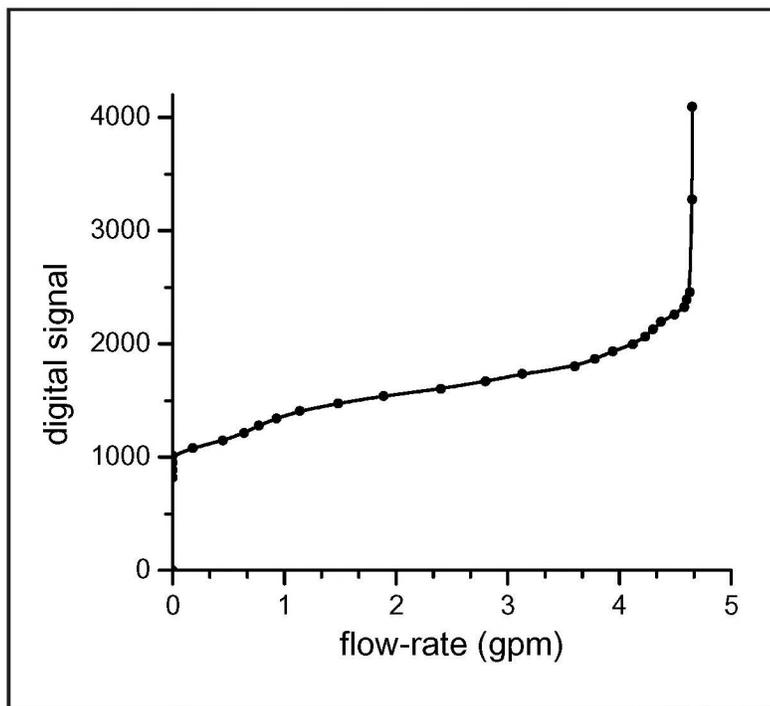


Figure 5. Calibration curve for the control valve.

ing concepts in real time. Among these concepts are design feasibility, design flexibility, control configuration selection, parameter estimation, process and instrument fault detection and identification, controller design and implementation, instrument calibration, and process modeling. The setup can be used to provide graduate and undergraduate students with hands-on experience and to carry out research in process systems engineering.

ACKNOWLEDGMENTS

The authors would like to thank Srinivas Tatiraju, Neeraj Zambare, and Roberto Pena for their input into the project, and Dan Lau for his essential role in assembling the setup. The authors would also like to thank the Department of Chemical and Biological Engineering at Drexel University for supporting this project.

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MECHANICAL TESTING OF COMMON-USE POLYMERIC MATERIALS WITH AN IN-HOUSE-BUILT APPARATUS

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The polymer production or transformation industries employ a very significant percentage of chemical engineers. This justifies the presence of a variety of polymer science and engineering subjects in the chemical engineering undergraduate curricula. Topics on solid polymer mechanics, in particular, are often quite useful for future engineers. They establish the basic tools for evaluating whether a material is appropriate for an intended use, or to tune its performance by acting on the synthesis/processing conditions. These subjects are present in general polymer textbooks (*e.g.*, References 1 and 2). Because ChE student laboratories are not traditionally equipped with the machinery used for mechanical testing, however, introductory courses on this subject often suffer from not having an appropriate *applied* component. Therefore, students don't gain a hands-on understanding of the phenomena involved.

One of the most commonly used mechanical tests in industry is tensile testing, in which the stress exerted by the material is measured at a constant strain rate. In addition to providing direct measurements of relevant properties, the stress-strain curves constitute "fingerprints" of a material's mechanical characteristics. The stress-strain curves are also often used for quality control of either raw materials or final products.

Most mechanical testing machines can perform several standardized tests (tensile, compression, flexural, etc.) by using appropriate accessories. Such machines are designed for heavy loads, however, and are significantly expensive. In addition, in order to use such a "heavy duty" machine, one has to prepare a test specimen that will exhibit a measurable stress-strain behavior. Furthermore, the specimens must be cut or cast into a standard shape and dimension, which might not be easy for many materials of interest. Standard-shape polymeric specimens of known composition and molecular weight are commercially available, but at a cost.

There is also equipment available for *low* stress/strain measurements—suitable for testing specimens of smaller dimensions, such as thin films—but these are also high-priced (about \$8,000 USD).

On the other hand, polymeric materials are readily available in the form of everyday-use items. Even informal observation of the behavior of these materials under mechanical solicitation may give the attentive student a wide variety of illustrations for important concepts in solid-polymer mechan-



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ics. An inspiring example was provided by J. Walker in the “Amateur Scientist” column of *Scientific American* magazine,^[3] in which the molecular phenomena involved in the stretching of a polyethylene film are illustrated and discussed in a simple and captivating fashion.

Our challenge was to build, on a very tight budget, a tensile-testing machine that chemical engineering undergraduate students could use freely in the lab for testing polymeric specimens gathered from common-use objects selected and prepared by them. Some of the design criteria we adopted for this project were:

- *Keep costs as low as possible, without compromising the quality of the machine’s measurements (i.e., reasonable accuracy and reproducibility).*
- *Keep in mind that the specimens should be easy to obtain and prepare. Using thin films for testing seemed to be a good idea. Many materials (plastic or otherwise) are commonly available in that form and can be easily cut into standard shapes. This option implies designing the machine for small loads and strains.*
- *Build a compact setup, so as to allow portability and use inside temperature-controlled chambers (e.g., refrigerators and ovens).*
- *Make it fully automated, allowing total control of its functionalities through a computer-based data-acquisition system.*
- *Make it operationally robust, safe, and intuitive, since students are supposed to operate it themselves.*

This paper describes the machine developed, as well as some of the experiments performed. This project has been successful in giving students a hands-on perspective on some key aspects of the mechanical behavior of polymeric materials.

SETUP OF THE TENSILE-TESTING MACHINE

The design of the testing machine comprised four key components: (1) a set of two grips, which firmly hold both ends of the test specimen; (2) a motor, which pulls one of the grips at a constant pre-set speed; (3) a force sensor, which measures continuously the force exerted on the material; and (4) a displacement sensor, which measures the distance traveled by the moving grip during the test. Figure 1 shows the original sketch of the machine’s layout, comprising these components. Further details are discussed below.

We intended to mostly test polymeric materials, such as polyethylene, in the form of thin films. We looked at some of the standardized tests used in industry to have an idea of the sizes and shapes of the test specimens used. According to ASTM D882-02,^[4] the plastic films being tested are cut into rectangular specimens (at least 150 mm in length and 5 to 25 mm in width). On the other hand, on ASTM D2370-98(2002),^[5] which applies to organic coatings (e.g., elasto-

meric paint films), the specimens are also rectangular in shape, but the length may be lower (at least 50 mm in length and 13 to 25 mm in width). We decided to use a short specimen length to minimize the maximum strain involved in the tests, and thus allow the use of a reasonably priced continuous-displacement transducer—and keep the machine’s size small. Therefore, we adopted the latter standard. (Note that we actually also tested paint films with this machine.) Some crude preliminary tests done with film strips cut from supermarket plastic bags gave us the basic information for the specifications for the load sensor, the motor, and the displacement transducer.

To provide linear motion to a lead screw, we chose a permanent magnet-stepper motor that employs a rotor with an internal thread. One end of the screw pulls one of the grips. The other end is attached to the moving lead of the LVDT-type displacement transducer. This transducer was the most expensive component in the setup (about 35% of the total cost). Cheaper alternatives are available, but an LVDT offers high accuracy and reproducibility, as well as wear-free and

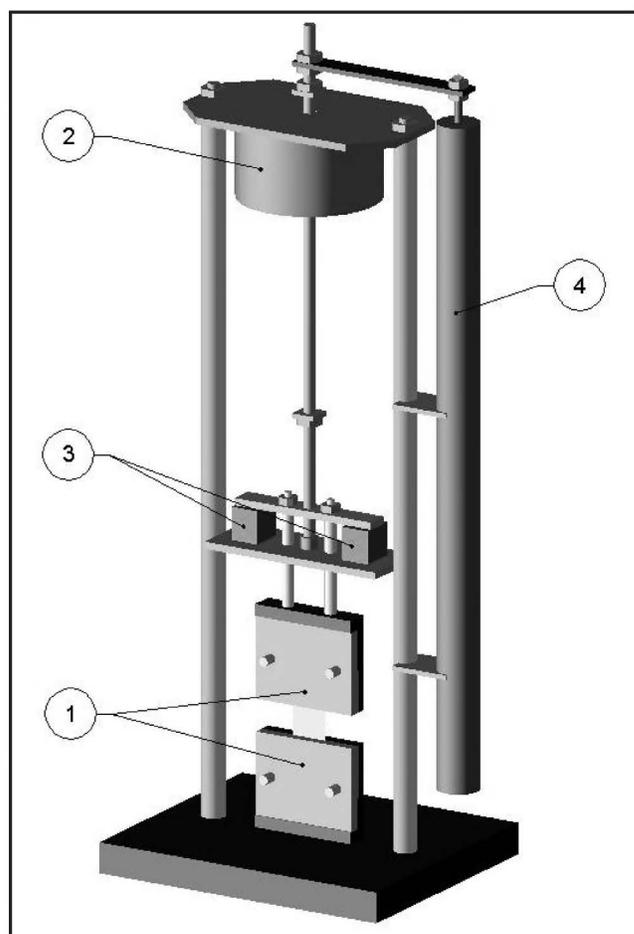


Figure 1. A 3-D sketch of the tensile-testing machine, showing the major components: (1) grips; (2) motor; (3) force sensors; (4) displacement sensor.

frictionless operation. Two force sensors, of piezoresistive type, are attached to the end of the lead screw. These sensors can measure only compression loads. The pulling grip is attached to a transversal bar that sits on top of the force sensors, thus transferring the tensile load, as is shown in Figure 1. Table 1 lists the main components and their costs. Figure 2 shows a photo of the actual unit, in its final working form.

The machine can measure loads up to 30 N. The maximum strain rate is 300 mm/min and the maximum linear displacement is approximately 140 mm, but this value can be increased by using a longer lead screw combined with longer lateral support bars. The machine is monitored and controlled with a desktop computer using a data-acquisition card (National Instruments PCI-6014). The program LabVIEW 7.1 (from National Instruments) was used to develop the software that fully controls the apparatus and analyzes the measured data. Figure 3 summarizes the information flow between the computer and the machine.

This machine was first implemented in an introductory course on solid polymer mechanics, which is an optional part of our chemical engineering undergraduate program. The students perform the tests themselves, on materials that they have gathered

according to the instructor's suggestions. They analyze the results both qualitatively and quantitatively, computing different parameters from the measured data.

Some representative tests and results are described in the ensuing text. For the sake of conciseness, the discussion in this paper is kept on a qualitative level.

TENSILE AND TEAR TESTING HDPE FILMS

Students are asked to prepare test specimens from plastic shopping bags obtained at their favorite supermarkets. These are commonly made of high-density polyethylene (HDPE). Students can easily identify the polymer by noting the recycling symbol that is typically printed on the bags.

The specimens to be used on the stress-strain tests are cut into 60 x 15 mm rectangles and reinforced with adhesive tape at their extremities, covering 20 mm on each end (see Figure 4a). The grips hold the specimens by grabbing on these reinforced ends.

Special care must be taken in cutting these specimens. The cut should be perfectly straight and without indentations; im-

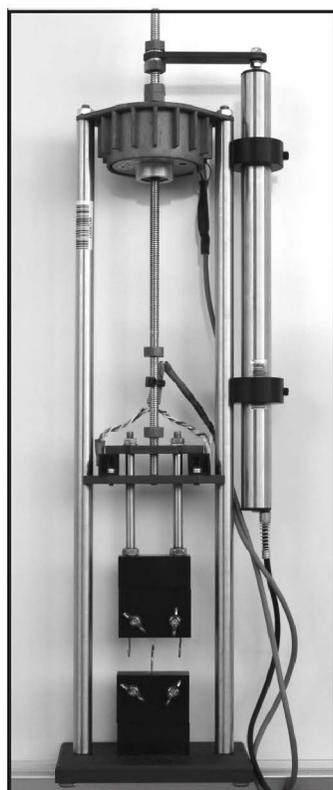


Figure 2. Photograph of the tensile-testing machine (showing the holders used for the three-point bending test).

TABLE 1
Tensile-Testing Machine Components
(Not Including Data-Acquisition Board and Computer)

Component	Maker and Model	Specifications	Price (pre-tax, USD)
Stepper motor + lead screw	McLennan L92411-P2	Max. linear force = 88 N	\$263
Driver board for stepper motor	Eurocard		\$48
Displacement transducer (LVDT)	Solartron DC50 920128	Range = ± 75 mm	\$463
Force sensors (2) (piezoresistive)	Honeywell FSG	Max. load p/sensor = 15 N	2 \times \$75
Power supplies (2)	EMS B811 and Astec LPS23	12 V	\$60 + \$53
Holding structure and grips (carbon steel + polyacetal)	Local workshop		\$250
Other components			\$33
TOTAL			\$1320

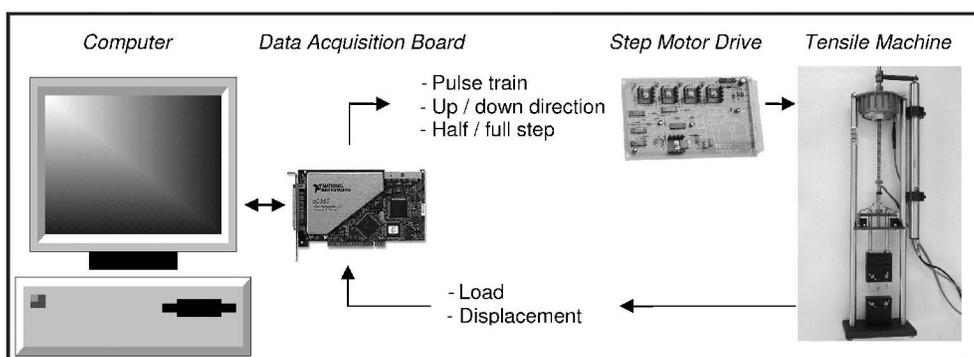


Figure 3. Schematic representation of digital and analog signal flow between the machine and the data-acquisition system.

perfections may cause the films to tear prematurely instead of reaching the ultimate rupture point. Sharp scissors or a fresh razor blade should be used. Students are asked to cut the specimens in two different ways: longitudinally and transversally in relation to the direction of the bags' "vertical" position (see Figure 5). Each specimen is labeled with a soft-tip marker so that the information on the specimen's cutting orientation is not lost.

Students also prepare specimens for tear-strength tests, which consist of 40 x 40 mm squares with an initial indentation (10 mm long) at the center of one of the sides (see Figure 4b). These indentations are done so that the tearing will propagate as intended: along the longitudinal or transversal directions mentioned before.

Before performing the stress-strain tests, students measure the thickness of each film, using a digital micrometer. This information is used to compute the initial cross-sectional area of the specimen, on which the loading stress will be based. Typical values are in the order of 10^{-2} mm.

Figure 6 shows representative results for two specimens cut along perpendicular directions as described before. The distinct behavior presented by the two is quite noticeable. The specimen cut along the bag's "longitudinal" direction (L

specimen) shows a rapid increase in stress, followed by a short plateau and afterwards a gentler increase, up to rupture. On the other hand, the T specimen (cut along the transversal direction), after a similar initial raise goes through a very well-defined maximum in stress and then stabilizes on an essentially constant value, almost up to the final rupture. The stress for this specimen is always significantly lower than for the L specimen.

Another fundamental difference can be observed when, prior to performing the tests, horizontal lines (perpendicular to the direction of elongation) are drawn with a soft-tip marker at different sections along the specimens. As the L specimen is elongated, one can see that the lines increase almost identically in thickness, up to rupture; this indicates that the material is being uniformly deformed. On the other hand, on the T specimen some lines become noticeably thicker as others remain almost unchanged; this indicates that the specimen is being stretched at the expense of deforming the material in limited regions. As elongation continues, the extent of the undrawn regions successively decreases until the entire specimen becomes uniformly stretched and rupture occurs. Some students recognize this as being an example of *cold drawing*—a phenomenon discussed in previous classes. It occurs on some semicrystalline polymers, like HDPE. The stress maximum corresponds to the yield point and the onset of necking.

But why is cold drawing not observed on the L specimen?

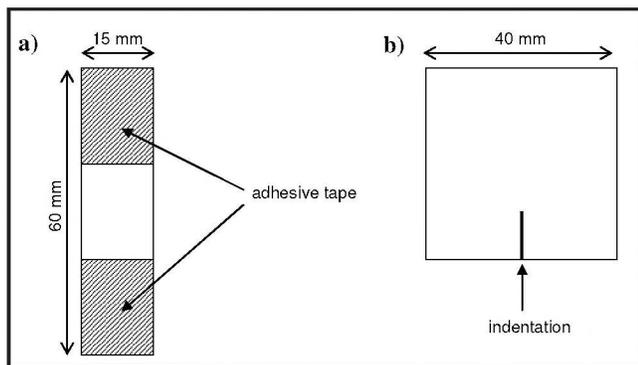


Figure 4. Specimen cut from plastic bag films: a) for stress-strain tests and b) for tear-strength tests.

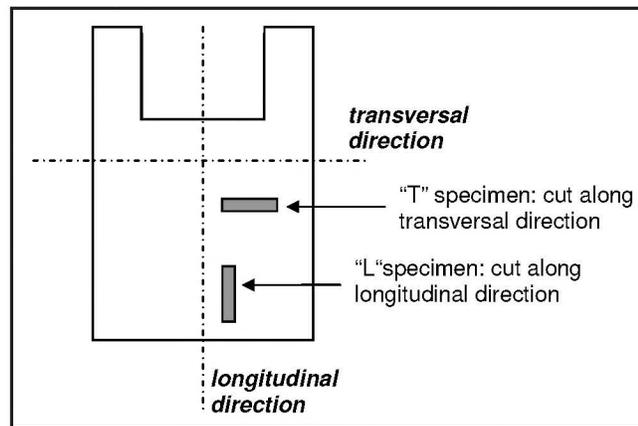


Figure 5. Definition of the longitudinal and transversal directions on a plastic bag.

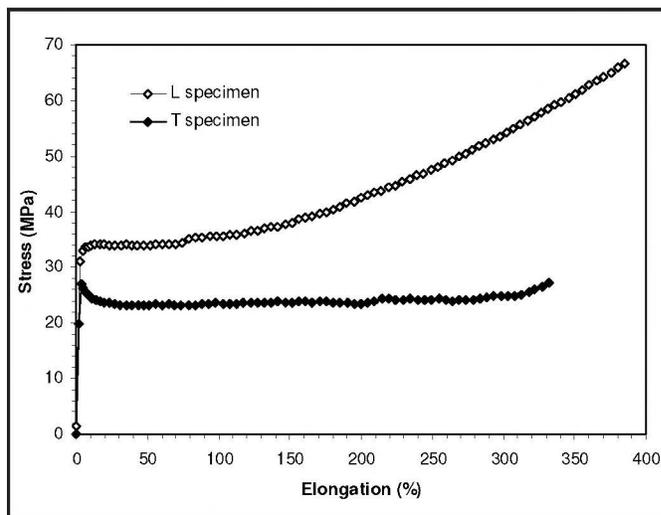


Figure 6. Typical stress-strain curves obtained for high-density polyethylene films from a plastic shopping bag. The two specimens were cut along two perpendicular directions (see description of L and T specimens in Figure 4). The end point on each curve corresponds to rupture of the film. Operating temperature = 20 °C; strain rate = 200 mm/min; original film thickness = 0.016 mm. Note that the stress indicated is the "conventional" or "engineering" stress, i.e., the measured load divided by the initial cross-section of the specimen. Decreases in cross-section along the test are disregarded.

This mechanical anisotropy is not usually expected by students, and they are encouraged to offer explanations. The tear-strength tests that are performed afterward supply extra material for the discussion.

The test is performed as schematized in Figure 7. The force exerted by the material is measured as the ends of the specimen are pulled at a constant rate and the tear propagates. Typical results from this test are shown in Figure 8.

When the tearing propagates along the longitudinal direction, the force is essentially constant and relatively low; in the end one observes that tearing originated a straight and clean cut. On the other hand, a much higher force is necessary to tear the specimen along the transversal direction; vi-

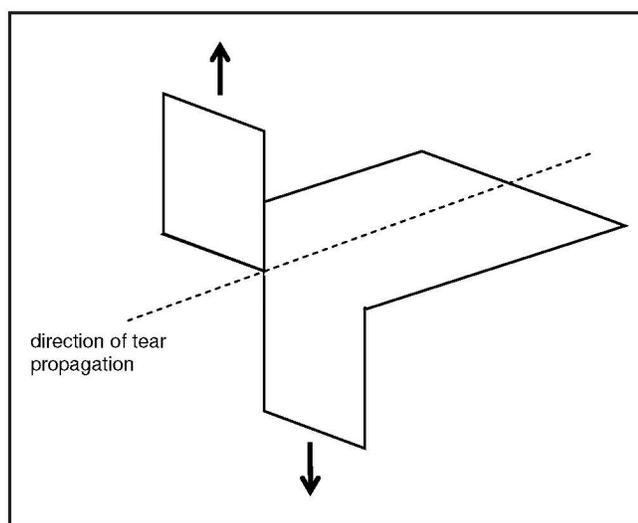


Figure 7. Schematic representation of a tear-strength test.

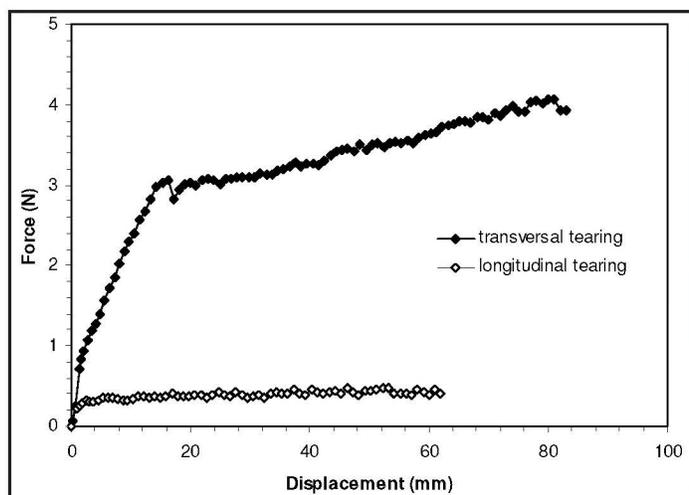


Figure 8. Typical tear-strength curves obtained for polyethylene films cut from a plastic shopping bag. Tearing propagates along perpendicular directions on the two specimens (see description of transversal and longitudinal directions on Figure 4); same operating conditions as in Figure 5.

sually one can see that the material is stretched and distorted during the test and the final cut shows permanent deformation of the material at the edges.

After analyzing this second set of results, students often suggest that this anisotropy is associated to a particular molecular orientation of the polyethylene chains in the shopping bag. It becomes clear that this is the correct hypothesis after the instructor describes the manufacture process for HDPE bags, commonly known as *blown-film extrusion*. This process is described in several processing handbooks.^[6, 7] It involves submitting the polymer to a sequence of transformations: melting, extrusion, blowing, drawing, cutting, and sealing. A continuously extruded thin-polymer tube is inflated by a jet of air blown into it. The blowup ratio (defined as the ratio between the diameters of the expanded film bubble and the die) controls the molecular orientation along the transversal direction. This ratio is usually 2 to 4. On the other hand, the drawdown ratio (the ratio between the speeds of the film at the nip rolls and at the die exit) determines the longitudinal orientation (called machine direction). A balance between these two parameters governs the final orientation within the film. Partial crystallization occurs as the material is cooled, thus conserving the molecular orientation imposed.

This flow-induced crystallization is actually a bit more complex than it would seem, due to the particular morphology that polymers exhibit upon crystallization. At a sufficiently high drawdown ratio, film-blown HDPE undergoes a so-called *row-nucleated crystallization*^[8]: Extended molecular chains oriented along the machine direction form fibrillar structures that act as nuclei for the crystallization of the bulk material, in the form of radially grown lamellae. Figure 9 schematically illustrates these structures.

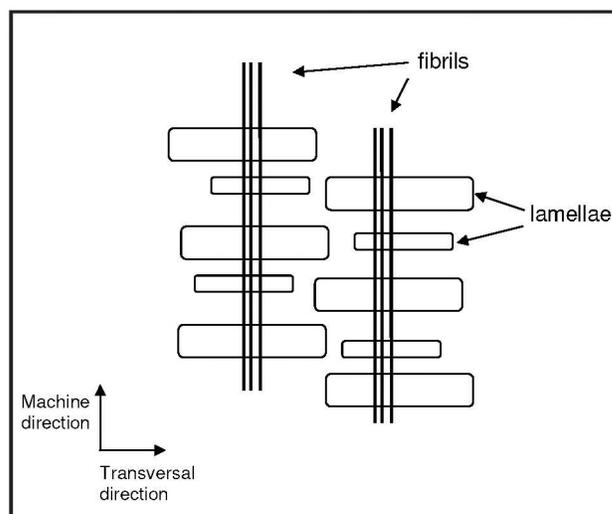


Figure 9. Row-nucleated morphology of film-blown HDPE. The fibrils oriented along the machine direction act as nuclei for the growth of the lamellae (chain-folded crystalline structures).

These long fibrils with perpendicular growths are often appropriately described as shish kebabs. They are responsible for the high tensile strength of the material along the machine direction (corresponding to the response of the L specimen in Figure 6).

Because, in the case of HDPE, there is no significant interconnection between the “kebabs” of adjacent fibrils, the tensile strength in the transversal direction is significantly lower. This transversal straining causes a noticeable yielding of the material, associated to local fibrillar reorientation toward the direction of the applied strain. The stress remains typically constant along this drawing process (see the curve for the T specimen in Figure 6). When the fibrillar rearrangement has extended throughout the entire material, the stress often rises slightly and rupture occurs shortly after. This cold-drawing phenomenon is characteristic of many semicrystalline polymers and is described in most polymer science textbooks. A recent paper by Zhang, *et al.*^[9] provides an interesting dis-

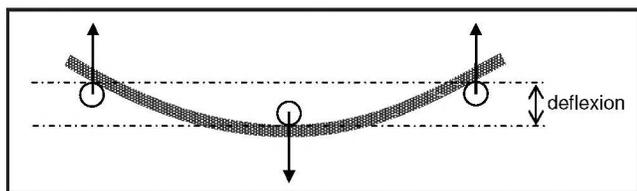


Figure 10. Schematic representation of a three-point bending test. The two holders at the extremities are connected to the machine's upper grip and move at a constant rate. The holder at the center is attached to the lower grip and remains stationary. The two holders at the extremities are 30 mm apart. The specimen length is about 50 mm.

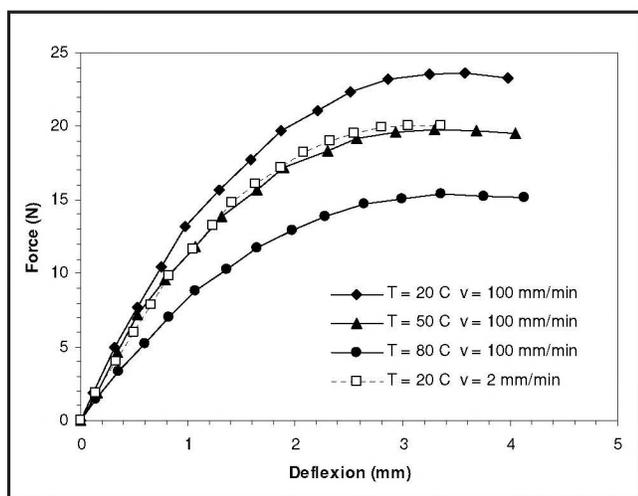


Figure 11. Typical force vs. deflexion curves obtained for polystyrene coffee stirrers. The labels indicate the specimens' temperature in Celsius (T) and the deflexion rate (v). The end point on each curve corresponds to rupture of the material.

ussion of the mechanical anisotropy and crystalline morphologies of different kinds of polyethylene-blown films.

From Figure 6 we see that the tensile strength (defined as the maximum stress measured during the test) is about 2.5 times higher when the material is strained along the direction that coincides with the fibrillar orientation (which we named the longitudinal direction). It makes a lot of sense that plastic bags are assembled so that normal use implies applying the stress along this direction.

The tear-strength test results (Figure 8) further confirm these findings. It is clear that it will be much easier to tear the material along the direction of the fibrils than along the transversal direction.

The “cherry on top” for this set of experiments comes when the instructor suggests that students take a piece of the plastic bag and heat it above a flame lighter (holding it with pincers and taking care to not actually burn the material). Immediately they see that the film starts to crumple and shrink. The temperature rise causes the gradual melting of the crystalline regions, loosening the mobility of the polymeric chains (the melting temperature of polyethylene is about 140 °C). This allows the originally extended chains to rearrange toward the more favorable coiled conformation. The result is the crumpling of the polyethylene film. Further heating would cause the total disappearance of the crystalline regions, resulting in a polymer melt.

FLEXURAL TESTING OF PS BARS

The machine is limited to tensile testing of thin films of relatively soft materials. Glassy polymers cannot be tested, since they involve much higher tensile stresses. Nonetheless, we have adapted the machine to perform a different kind of test on such materials: a three-point bending test at constant deflexion rate. We used polystyrene (PS) coffee stirrers, collected from a nearby vending machine, as test specimens. Figure 10 schematizes how the test is implemented: by using hard-wire hooks to attach the specimen to the grips. PS is glassy at room temperature (its glass-transition temperature, T_g , is about 100 °C).

Figure 11 shows some of the results obtained for different temperatures and deflexion rates. Since it is faster to place the rigid PS specimen on the support hooks than it was to attach a film to the grips, these tests did not involve placing the machine in a temperature-controlled chamber. Rather, the specimens were stabilized in an oven at the desired temperature. Prior to testing, each specimen was quickly transferred to the machine. The entire procedure (including performing the test) took no more than 30 seconds. In the figure one can see that the maximum deflexion is relatively low, as expected from a glassy polymer. For a deflexion rate of 100 mm/min, as the specimen temperature approaches the glass-transition temperature, its softness is significantly increased. Students

are asked to visually inspect the broken specimens. They notice that the ones tested at higher temperature show a visibly higher extension of *crazed* material (crazing, *i.e.*, the appearance of semi-opaque transversal bands in the neighborhood of the break surface, is a localized molecular-orientation phenomenon that occurs when some glassy polymers are close to rupture).

Note that the measured values of the deflexion at break are not reproducible and should not be considered. In the many tests performed, some discrepancies were obtained for this parameter. This was probably due to sample heterogeneity. The force-deflexion curves measured at lower deflexions were always quite reproducible.

When the test is repeated at room temperature, but at a lower deflexion rate (2 mm/min), the material's stiffness decreases, coincidentally giving a curve similar to the one previously obtained at 50 °C. This is a good illustration of time/temperature equivalence. In polymeric materials, molecular response is highly time and temperature dependent.

CONCLUSION

The in-house-built tensile-testing machine proved to be an economical tool for allowing students to test the mechanical behavior of different polymeric materials. The results can be analyzed both quantitatively and qualitatively. The fact that the test specimens can be obtained from everyday-use materials is not only an economic advantage but also an added factor of interest for students, since they can do the material selection and preparation themselves. The pedagogical benefits obtained from direct experimentation were confirmed by the interest and motivation shown by our students. Awareness that the machine was built in-house actually seemed to raise the students' curiosity toward comparing its components to the ones used in the commercial models.

The results shown here are representative of some important aspects of the mechanical behavior of solid polymers, such as the influence of processing conditions and the effects of temperature or strain rate. Students are encouraged to analyze their results and provide interpretations on a molecular level.

Other materials used successfully with this machine include rubber bands and films of elastomeric wall coating (EWC). The latter constitute a type of paint that, due its elastomeric character, is able to protect cracked walls from rain damage, since the film stretches to keep the gaps covered. It is an enriching exercise to analyze the mechanical response of EWC films under conditions such as low temperatures, aging (UV degradation), or water exposure (plasticization).

The tests performed with this device can be used either as an illustration of the concepts and phenomena previously discussed in class or, perhaps more interestingly, in a reversed approach. Indeed, the experimental observations are quite

thought-provoking and motivate students to ponder and hypothesize on the reasons for the results obtained—thus paving the way for a structured discussion led by the instructor.

It must be remarked that the tensile and tearing tests described here for polymeric films are actually similar to some of the standard industrial practices, both in terms of specimen dimensions and operation parameters. It can be noted, as an example, that a data sheet for blown film obtained from ExxonMobil's HDPE resin HTA 001HD^[10] (recommended for shopping bags, among other uses) reports an elongation at break of about 380% and a tensile strength (stress at break) of 56 MPa (it does not exhibit anisotropy for the particular processing conditions employed); this result is quite consistent with the values obtained with our shopping-bag material (of unknown origin).

In addition, a fairly good reproducibility is obtained with our in-house-built machine. The only problems are usually associated with discrepancies in the rupture points. For stress-strain tests, this is due to premature breaking caused by tears that initiated at imperfections in the specimen side cuttings, as mentioned before. These anomalous rupture behaviors can be easily detected visually and can be minimized by cutting the samples carefully. In the flexural tests, rupture discrepancies are probably associated to imperfections or inhomogeneities among samples.

Naturally, the machine presents limitations when compared to the models used industrially, namely in terms of measurement accuracies and limitations on load and strain ranges.

ACKNOWLEDGMENT

The authors would like to thank the Department of Chemical Engineering of the Faculty of Engineering of the University of Porto for the financial support provided for assembling this machine.

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Partnering With Industry

Continued from page 37

Instructor comment: I suspect the three students who rated this query as poor may have been reflecting on how valuable they felt their work was to Wacker and Air Products. This perception is expressed in the student comment #3 below.

Three students provided personal comments of the industry project on the evaluation form:

- ▲ **Comment #1:** *"I think the project would have gone better if we were able to run the equipment and take the samples ourselves."*
- ▲ **Comment #2:** *"It would be beneficial to our understanding of particle technology if we were allowed a more hands-on approach rather than analyzing given data."*

Instructor comment: I believe these two students were referring to collecting samples from the process, as all students were required to run the Beckman Coulter Counter.

- ▲ **Comment #3:** *"I thought it was neat to see an actual application of particles, but I didn't feel we actually accomplished anything."*

Comments from Industry Participants on evaluation results:

- ▲ *"I thought the feedback from the students was interesting and very candid. The students that rated the exercise as fair to poor shouldn't be viewed negatively, but rather that their engineering interests might lie in marketing, sales, or areas other than manufacturing."*
- ▲ *"Many students saw this project as a research study or 'make-work' study with no commercial application or contribution to a company's profit. When we started to connect the dots to commercial applications during the presentations and relate to benefits for the company, many students felt better about the project and started to appreciate their contributions."*

CONCLUSIONS AND RECOMMENDATIONS

It is obvious from the feedback that certain students were frustrated with the amount of contact they had with the process, and didn't perceive any benefit to the company from the projects.

Benefits weren't discussed until the end of the projects, in the presentation phase, which, in retrospect, was too late. In the future, it would be better to introduce benefits earlier in the execution of the projects. This might be best accomplished by having the industry personnel visit the classroom and introduce projects themselves, including potential benefits for the company. The students, however, should also be made to realize that these projects are chosen partially for the benefit of the industry, but the main driving force is to provide the students with a real-world learning experience.

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"It would be beneficial to our understanding of particle technology if we were allowed a more hands-on approach rather than analyzing given data."

— Student feedback

Two of the biggest challenges of this exercise were: (1) finding industry projects that could feasibly be completed by the students in the project time frame, and (2) finding three projects requiring a comparable quality of student experience. As is obvious from these three projects, one resulted in a better student experience than others. In Project 3, the students had more project participation since they were able to plan and run experiments using the Ro-Tap machine, as well as run the particle analyzer. Projects 1 and 2, on the other hand, were straightforward as far as obtaining samples, which were collected by industry personnel, and the students' only participation in data collection was running the particle analyzer on the samples. In the future, this deficiency could be overcome by suggesting students shadow the industry participants during procedures that they can't perform themselves due to safety and liability issues. Also, more pre-planning by the instructor to assure better equity of the project experience may be necessary (initiation of partnership occurred in July, with the course beginning in August).

By the very nature of the projects being based on unanswered questions about the process, however, it would be impossible to predict project results and effects in this scenario.

Overall, the majority of the students felt the industry project was beneficial to their careers and experience. The project accomplished the main goals of (1) exposing students to a real-life particle manufacturing process, (2) gaining hands-on experience running a state-of-the-art particle measuring device, and (3) applying the basic concepts presented in the course.

ACKNOWLEDGMENT

We wish to acknowledge the support given by Josh Brien, Wacker engineer, in assisting students with data collection.

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A NONLINEAR, MULTI-INPUT, MULTI-OUTPUT *Process Control Laboratory Experiment*

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The laboratory course in process control constitutes an important component of an undergraduate chemical engineer's education because it provides hands-on training in the application of process control to real processes. The laboratory course exposes the student to industrial process control hardware and the impact of measurement noise and unmeasured disturbances upon the control of real processes.

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In most university courses these laboratories are essentially linear single-input, single-output (SISO) unit operations. Until recently, the Department of Chemical and Petroleum Engineering at the University of Calgary was no exception. Yet such SISO control laboratories do not expose the student to the complexities of nonlinear or multi-input, multi-output (MIMO) processes.

A few laboratories in the literature^[1-4] have attempted to address these shortcomings. Rivera at Arizona State University^[1] describes a salt-mixing laboratory that examines the concentration dynamics at different tank levels using system identification techniques in a first process dynamics and control course. Fisher and Shah at the University of Alberta^[2] describe a complex three-tank-level plus temperature arrangement that allows MIMO processes and process nonlinearity to be studied at the senior undergraduate or first-year-graduate course level. Braatz, *et al.*, at the University of Illinois^[3,4] describe a nonlinear but SISO pH neutralization process and a quadruple-tank apparatus that illustrates time-varying dynamics for a senior undergraduate process control course.

In this paper we describe a relatively simple salt-mixing laboratory in the undergraduate chemical engineering process control course at the University of Calgary that allows students to study both MIMO behavior and nonlinearity.

THE UNIVERSITY OF CALGARY'S PROCESS CONTROL COURSE

The University of Calgary requires process dynamics and control as part of the degree requirements for undergraduate students in chemical engineering, in a course that pioneered the hands-on, real-time (time domain) approach to teaching process dynamics and control.^[5] Students in the class employ dynamic process simulation using a dynamic process simulator, such as HYSYS or Aspen Dynamics,^[6] to model chemi-

cal process plants and their control systems. The students then create “disturbances” in the plant, which may involve changes in feed composition, flow, system temperatures, and/or pressures. The simulator demonstrates in real time what the effects of these “disturbances” would be on the plant operation, and it allows the student to evaluate the strengths and weaknesses of a given process control scheme.

The course is accompanied by a textbook written by the course instructors, *A Real-Time Approach to Process Control*.^[7] The text has 10 chapters, each of which focuses on a given aspect of process dynamics and control, whether it be investigating the concepts of process gain, time constants, and deadtimes, studying control schemes for distillation columns, or examining plant-wide control. Associated with the chapters are eight workshops^[8] that are to be completed by the student using a dynamic simulator. Each individual workshop explores the concepts explained in the associated chapter, allowing students to assign meaning to the words.

Due to the electronic nature of the workshops, hands-on, real-time experiments on laboratory unit operations equipment were considered a necessity to further reinforce the practical approach of the textbook. As a consequence, there is a compulsory laboratory component to the course.

LABORATORY OVERVIEW

The laboratory component of the process dynamics and control course includes two traditional experiments: (1) a

three-tank cascade where simple process identification and level control are the objectives, and (2) a double-pipe heat exchanger with a variable deadtime leg which can be configured to investigate feedback, cascade, and feedforward control. While these experiments offer students the chance to experience the effects of process/measurement noise and unmeasured disturbances, the behavior of the experiments is essentially linear, and the control loop studied is SISO in structure.

SALT-MIXING LAB EXPERIMENT

The salt-mixing lab experiment that incorporates nonlinearity and MIMO behavior was designed in 2002 for immediate introduction into the curricula.

Figure 1 is a schematic of the laboratory process experiment. The following is a description of what occurs in the process:

A concentrated salt solution is mixed and stored in a large holding tank that was sized to give a five-hour or more run time. This solution is pumped into the conical mixing tank, passing through a magnetic flow meter and flow-control valve, which are used to regulate flow via a flow-control loop. Fresh water is supplied via building utilities; the water passes through a magnetic flow meter and control loop that are used in a flow-control loop to regulate the fresh-water flowrate. Upon entering the mixing tank the fresh- and saltwater streams are blended using a stirrer. The conical section of the mixing tank provides a strong process

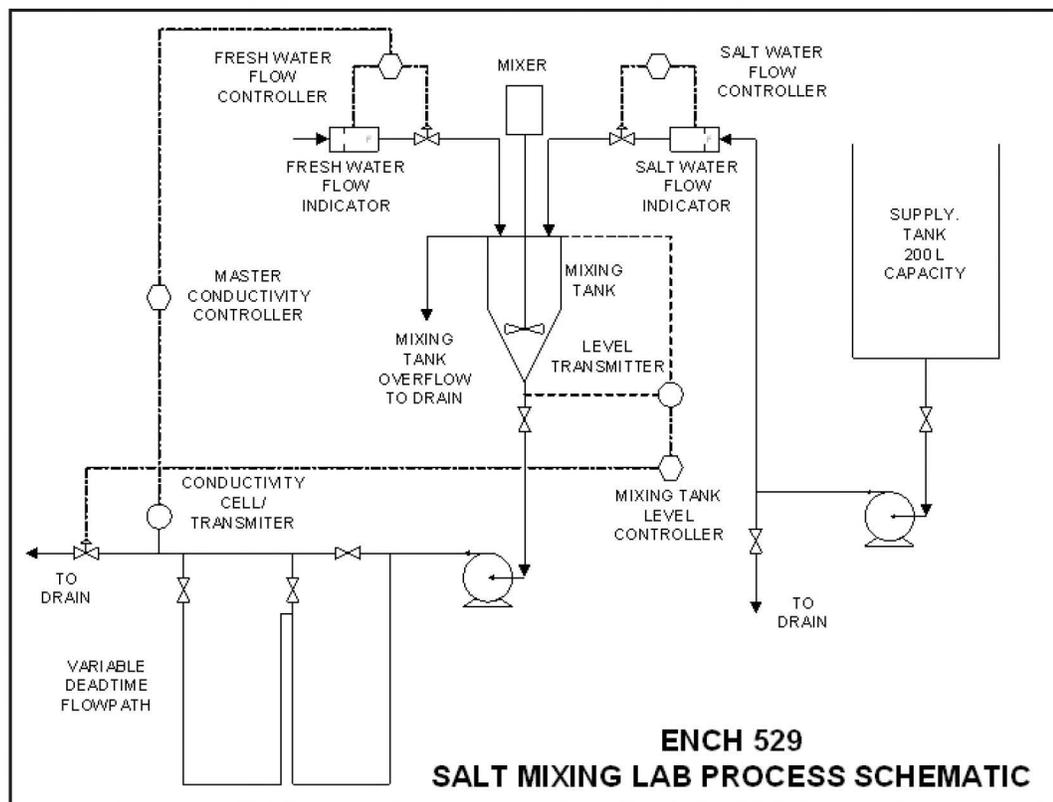


Figure 1. A schematic of the Salt-Mixing Laboratory Process.

nonlinearity. The level in the mixing tank is measured using a differential pressure cell. The blended solution enters a pump, is pressurized, and then moves to a pipe segment that allows for one of three flow paths of larger tube diameter to be selected. This setup allows one of three deadtimes to be examined. The stream will then pass through a conductivity cell/transmitter, which is used as the input to the master conductivity control loop. This loop's output is a cascaded setpoint to the slave fresh-water flow controller. Before going to drain, the stream passes through a control valve that is manipulated in order to regulate the level in the mixing tank. The flowrate, level, and conductivity inputs are all fed to the DCS system, as are the fresh-water, saltwater and level-control-valve-manipulated variables for this MIMO system. The input and manipulated variables are

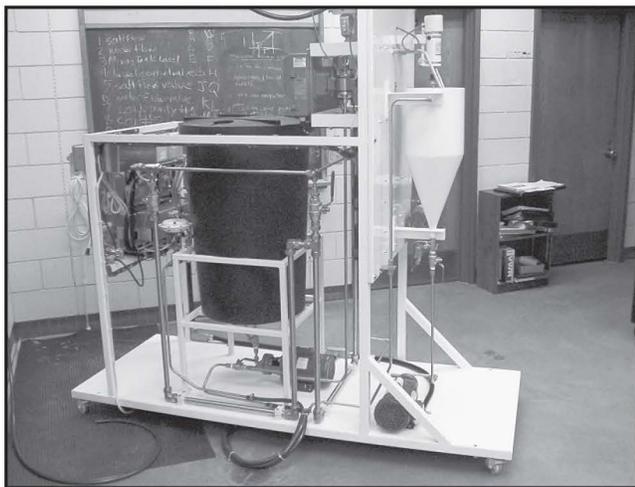


Figure 2. A photograph of the Salt-Mixing Laboratory.

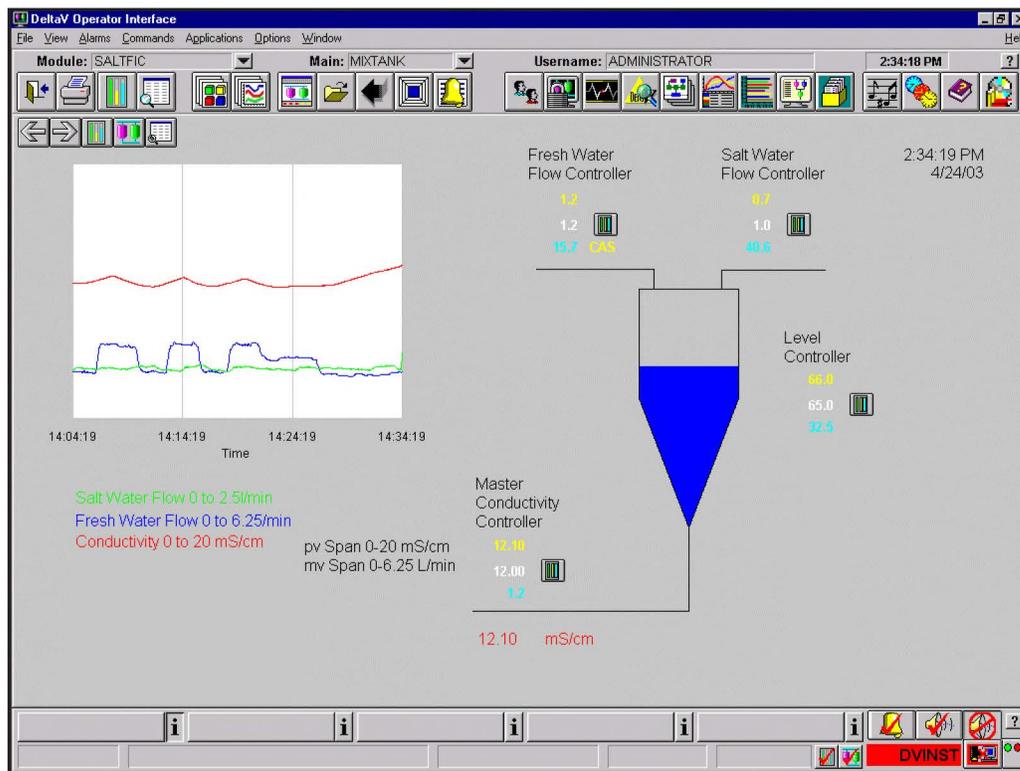
used within the DCS system with predefined function blocks to create the appropriate control loops.

Figure 2 shows the salt-mixing laboratory skid. The instrumentation, tank pumps, and additional parts were purchased from suppliers but the construction of the skid and commissioning of the equipment was completed in-house with the help of university support staff. This resulted in a compact unit that has capacity for expansion and is completely portable, allowing for more efficient use of laboratory space.

Figure 3 is a screen shot from the Emerson DeltaV distributed-control system (DCS) that is used for process data acquisition, monitoring, and control in the laboratory. The advantage of using a DCS is that they are common to modern industrial installations; as such, undergraduate engineering students should be taught what a DCS looks like as well as be provided with experience in controlling processes using such graphical interfaces.

Other laboratories in the literature^[1, 9-11] have also realized this necessity and addressed it in different ways. Rivera, *et al.*,^[1] also employed an industrial DCS (Honeywell, in that case), as did Skliar, *et al.*, at the University of Utah^[9] in a graduate course also open to seniors (Opto 22, in the latter work). The approach of Bequette, *et al.*, at Rensselaer Polytechnic Institute^[10] was perhaps the more typical use of Matlab/Simulink block diagrams as an interface to simulated experiments. Braatz, *et al.*,^[11] employed the Hewlett Packard Visual Engineering Environment (HPVEE) to construct their student-operator interfaces to have a similar look and feel to an industrial DCS.

Figure 3. A screen-shot from the DeltaV DCS.



The overall mass and species balance equations that describe the dynamics of the system are included in Table 1, and the system nonlinearities are delineated and linearized in Table 2 so that the nonlinearities are clearer to non-control experts who have been assigned to teach process control. Figure 4 gives a time-domain plot from the DCS showing sys-

tem response to saltwater flowrate changes from 0 to 0.5 then to 1.0 L/min (plus a few more). The effective tank-time constant varies with the flow.

LABORATORY TASKS

Myriad tasks can be done with the aforementioned apparatus. The purpose of this laboratory portion of the course is to allow students the opportunity to evaluate a variety of control schemes. To initiate this with the mixing-tank experiment, students set a tank level and then perform three step tests, where each step test is either an increase or a decrease from a nominal value. Tuning parameters (PI) are then calculated from the resulting process-reaction curves, using the students' choice of method (Cohen-Coon, Ziegler-Nichols, or IMC open-loop rules). The calculated tuning parameters are then compared with the tuning parameters obtained using the DeltaV automated tuning program (DeltaV tune), and both sets are tested by making setpoint changes or disturbances in the saltwater flowrate. The "best" set of tuning parameters is then chosen based on visual observations of the system response, including time to steady state, for each set of tuning parameters. With the best

TABLE 1 Overall Mass and Species Balance Equations	
Overall Mass Balance Equation (Assuming constant density and isothermal)	$F_{\text{Fresh Water}} + F_{\text{Saltwater}} - F_{\text{Product}} = \frac{dV}{dt}$
Salt Species Balance Equation (Assuming constant density and isothermal)	$F_{\text{Saltwater}} \cdot x - F_{\text{Product}} \cdot y = \frac{d(Vy)}{dt}$

TABLE 2 System Nonlinearities		
Nonlinearity	Nonlinear Characteristic	Linearized Characteristic
Volume change with level in the conical section	$V = \frac{1}{3} \tan^2 \theta \cdot h^3$	$V = \tan^2 \theta \cdot h_{\text{op}}^2 \cdot h$
Product flowrate change with the level due to the valve	$F_{\text{product}} = K_v \sqrt{h}$	$F_{\text{product}} = \frac{K_v}{2\sqrt{h_{\text{op}}}} h$
Multiplicative nonlinearity between the volume and the salt concentration	$\frac{d(Vy)}{dt}$	$V \frac{dy}{dt} + y \frac{dV}{dt}$

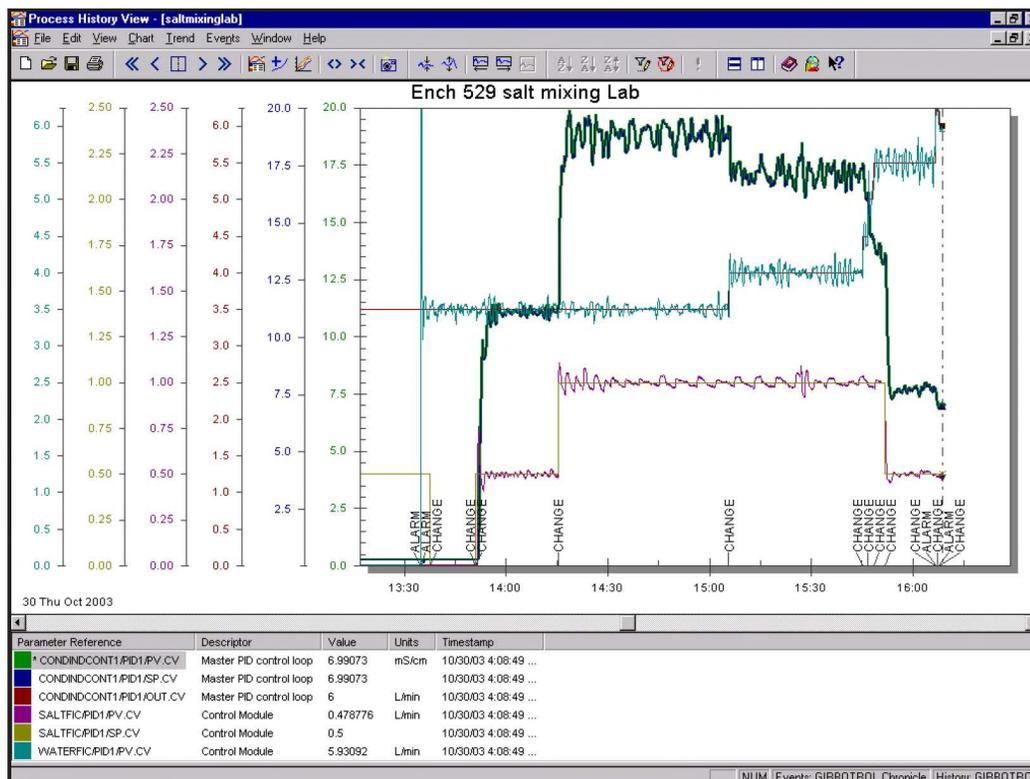


Figure 4. A time-domain plot from the DCS demonstrating the system response to saltwater flowrate changes from 0 to 0.5 then to 1.0 L/min (plus a few more).

The simulator demonstrates in real time what the effects of . . . “disturbances” would be on the plant operation, and it allows the student to evaluate the strengths and weaknesses of a given process control scheme.

tuning parameters entered into the system, the level in the mixing tank is then changed significantly, for example from 65% to 35%, which would mean moving from the cylindrical (linear) to the conical (nonlinear) section of the mixing tank or vice versa. Setpoint change(s) are then made in order to allow students to examine the process response.

The students are then asked to perform a full analysis of the process behavior in both open and closed loop, including comments on linearity, order of response, and possible better control strategies for the apparatus. As well, the students are given an additional open-ended problem: to calculate the amount of salt initially added to the storage tank. The information given to the students to complete these tasks includes printouts of process data (*e.g.*, flowrates, conductivity) and the initial height of water in the storage tank. Students are also able to measure the tank dimensions if they so desire.

EVALUATION

Along with an analysis of the process behavior, the students were asked to provide some general comments on the laboratory. Overall, the laboratory was found to provide good exposure to the latest process equipment, along with demonstrating different tuning methods (including those done using the built-in autotuner). Students were able to recognize the nonlinearity in the system and provide an explanation, as well as provide explanations for the changes in time constant and deadtime with different flowrates. System noise was well demonstrated in this laboratory and its effect on the graphical method for calculating tuning parameters was noted. As well, the effect of capacity was seen. Many students also attempted the open-ended problem—to calculate the initial mass of salt—and used a number of approaches in attempts to solve it. General student comments and laboratory reports indicated that students enjoyed working with the new laboratory experiment, and that it was helpful to see a real process that could provide them with a feel for what types of disturbances can be made in a plant. (Whereas, in the simulation workshops, unrealistic disturbances are quite possible and it is sometimes difficult to measure the actual time effect a disturbance would have.)

Because it was a real process, the students did find the experiment was a little long, as it usually ran slightly in excess of four hours (the time period scheduled for the experiment). A smaller process could be considered, but long time constants are a reality of industrial plants and this is an important fact for students to realize that is often somewhat overlooked in their process control education.

In general, it was felt that the laboratory was well received by students, and that it provided them with good exposure to state-of-the-art control hardware. The students were also exposed to instrumentation they had not seen before, such as magnetic flow meters and conductivity cells. The experiment also effectively displayed the difference between a simulation and a real process, in that it took up to 30 minutes to achieve steady state in closed loop, depending on the tuning parameters and the setpoint change made. Some ways in which this “down” time could be used more effectively include:

- ❑ *Quizzes*
- ❑ *Lab discussions*
- ❑ *Tutorial support*
- ❑ *Additional reading material*
- ❑ *Increased time to explain the apparatus*

These options could be used to keep the students focused on the experiment since it is felt that what was actually going on in the process was often overlooked due to other distractions during the time lags. Despite this, students did seem to take note of some pitfalls that can be encountered when tuning controllers, such as the errors associated with the graphical methods and the importance of proper input design.

The experiment also reaffirmed the value of a DCS in the teaching environment. Unit operations laboratories had previously had DCS systems integrated into them, but the DCS was not used in a control context and students did not need to make use of all of the data-collection and

handling capabilities of the system. This experiment also showed a practical application of cascade control as the fresh-water supply pressure was not regulated—therefore changes in the water system would propagate through the system but would be quickly compensated for by the slave fresh-water flow-control loop that is manipulated by the master-conductivity control loop. It was felt that the bonus question worked well and that it should be made mandatory for future labs. It was also convenient for the teaching assistants that the lab could be run differently for each group by simply changing the initial salt concentration or flowrates. As well, this changeability provided the teaching assistants with an opportunity to learn more about process control.

Overall, it was thought the lab performed very well and showed much promise as well as many other areas of potential use. For instance, it would be useful in a more advanced process control course where it could be used to demonstrate system identification and model predictive control in a practical setting.

CONCLUSIONS

The introduction of this new lab was successful from the students' point of view. They enjoyed working with the latest process control instrumentation. They also gained a new appreciation of the problems associated with real plants, in the form of noise and unexpected disturbances. The comparison of conventional open-loop tuning methods and an automated tuning package was appreciated, as was the chance to show their creativity in the solution of the open-ended bonus question.

From the instructors' point of view, the laboratory was considered successful. The only real concerns with the lab were based on the length of time it took to complete. This will be addressed in coming years with the introduction of quizzes and discussion while waiting for the process to reach steady state. Despite these concerns the lab provided an effective demonstration of a nonlinear and MIMO system. Most importantly, it was felt the students were better able to understand process behavior by being able to see many of the classroom concepts on an actual process. The department also gained a valuable tool for additional process control courses due to this lab's ability to have the control configuration changed, the ease in which it can be upgraded or modified, and its extensive data-collection and data-handling capabilities.

ACKNOWLEDGMENTS

Financial support from the Calgary Engineering Endowment fund is gratefully acknowledged for the purchase of the laboratory hardware. Bernie Then is thanked for the assembly of and assistance in commissioning the laboratory hardware.

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General student comments and laboratory reports indicated that students enjoyed working with the new laboratory experiment, and that it was helpful to see a real process that could provide them with a feel for what types of disturbances can be made in a plant.

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.

DATA ANALYSIS MADE EASY WITH DATAFIT

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Shortly after starting as an assistant professor, I realized that quite a few of our students were unable to analyze laboratory data at a level consistent with that expected when I had worked in industry. Having been put in charge of the Florida Institute of Technology's introductory chemical engineering course and its materials science and engineering laboratory course, I decided that a strong emphasis on data analysis would be added to each of these courses in order to satisfy ABET's requirement regarding the ability of students to analyze data.

Most departments emphasize spreadsheet calculations and plotting of data in Microsoft Excel as part of their introductory chemical engineering course. Experience in our department has shown that unless sufficient time is spent on data analysis instruction such that spreadsheet calculations, plotting, and curve fitting become second nature, such skills are either forgotten or are never learned properly.

We have incorporated DataFit from Oakdale Engineering^[1] throughout the entire curriculum at Florida Tech, beginning with CHE 1102, an eight-week, one-day-per-week, two-hour, one-credit-hour, second-semester Introduction to Chemical Engineering course in a hands-on computer classroom. The syllabus for CHE 1102 is shown in Table 1. The examples

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chosen, shown in parentheses, are selected so as to be consistent with concepts that students learn concurrently in other courses. DataFit also has become commonly used in our Physical Chemistry Lab and Materials Science and Engineering Lab courses, as well as in several courses in other engineering departments. Our experience at Florida Tech is that

students retain data analysis concepts best when such concepts are formally taught to them in this short course and then periodically reinforced throughout their academic careers. Several examples covered in weeks three through eight will be discussed here.

An introduction to basic statistics is included in nearly all introductory ChE courses and will not be discussed in this ar-

Experience in our department has shown that unless sufficient time is spent on data analysis instruction such that spreadsheet calculations, plotting, and curve fitting become second nature, such skills are either forgotten or are never learned properly.

TABLE 1
Data Analysis Curriculum

- 1) Statistics and Confidence Intervals
- 2) Introduction to Plotting and Calculations in Excel
- 3) $y = ax + b$ Fitting in DataFit (Pressure Transducer Calibration)
- 4) $y = ax$ Requires User-Defined Models (Hygrometer Calibration)
- 5) Semi-Log Functions (First-Order Rate Laws - Felder and Rousseau 2.34)
- 6) Plotting and Curve Fitting of Power-Law Functions (Crystal Growth - Felder and Rousseau 2.37)
- 7) Nonlinear Functions (Vapor Pressures)
- 8) Curve-Fitting in 3-D (Rate Laws With Two Reactants)

ticle. Students in CHE 1102 cover basic statistics during the first week of the course and get constant reinforcement of these concepts through the use of DataFit.^[1] The second half of CHE 1102 consists of problems that require Polymath- or Excel-based solutions to either sets of linear and nonlinear algebraic equations or numeric integration, as suggested by Clough.^[2]

All Excel and DataFit files are available at <<http://my.fit.edu/~jbrenner/dataanalysispaper1.zip>>.

SOLVING PROBLEMS WITH DATAFIT

Problem 1. Calibration of a Pressure Transducer

Following the introduction to basic statistics, the first problem that I assign students is the calibration of a 0-250 psig Span Instruments' NTT-204 (now Millipore) pressure transducer against a 0-1000 psia Paroscientific pressure transmitter. In addition to being useful for teaching students how to make plots with error bars and determine the difference between

absolute and gauge pressures, it provides a relatively simple problem for studying linear regression with DataFit. The repeatability and lack of drift of Paroscientific pressure transmitters is even superior to that of a deadweight tester that was calibrated at NIST.^[3] The repeatability of the quartz oscillator that the Paroscientific pressure transmitters use is certainly within the quoted 0.01% of full-scale precision (*i.e.*, 0.1 psia fixed error for a 1000-psia transmitter). Span Instruments' pressure transducers output a signal that ranges from 4-20 milliamps to within 0.08 milliamps.

After having the students prepare a plot of the data shown in Figure 1, including error bars, I ask the stu-

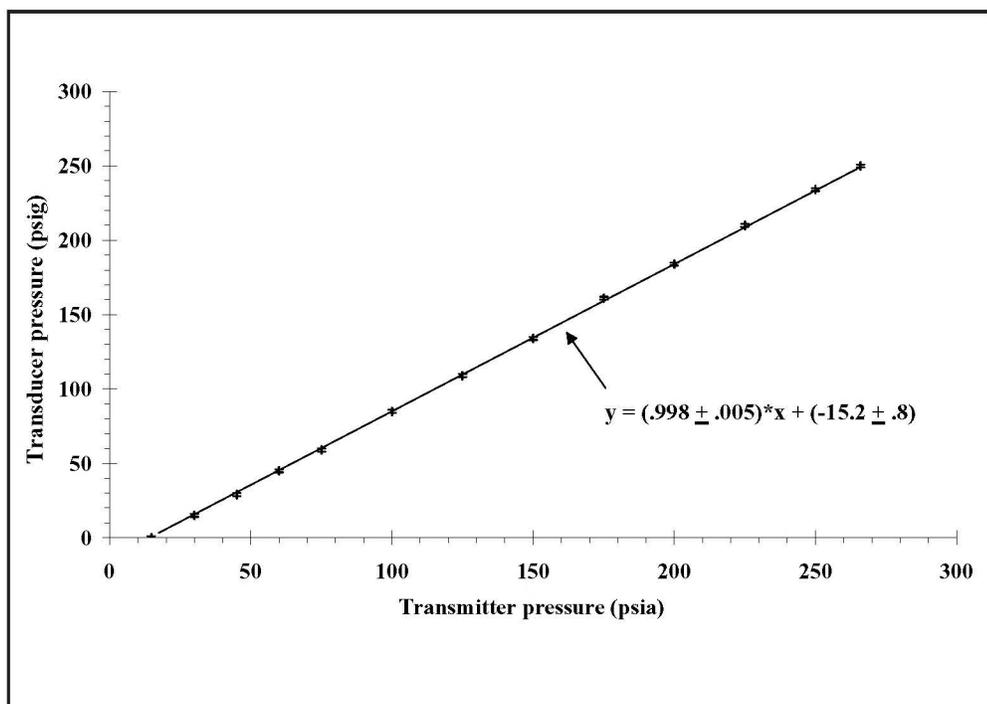


Figure 1. Calibration of a Span Instruments' pressure transducer against an NIST-traceable Paroscientific pressure transmitter.

dents to copy and paste the data into DataFit, click on the Solve Regression option, click on OK, select the $y = ax + b$ option, and let DataFit do the work for them. By clicking on Results Detailed, the Fit Information output is obtained (Table 2). Included in the output are the residual sum of squares (RSS), which is the sum of the squares of the differences between the calculated values of Y, the pressure in psig as determined by the pressure transducer, and the corresponding experimental values. Also evaluated are the commonly seen R² correlation parameter as well as several more-advanced goodness-of-fit parameters. Most importantly, the 68%, 90%, 95%, and 99% confidence intervals are conveniently tabulated. This is an excellent opportunity to reinforce basic statistics, most notably the Gaussian distribution, which is typically taught at the beginning of CHE 1102.

Problem 2. Calibration of a Hygrometer

The second problem that I assign is Problem 2.32 from Felder and Rousseau's textbook.^[4] This problem involves the correlation of a signal from a hygrometer versus the mass fraction of water in the inlet stream to the hygrometer. For this problem, first ask students to do the $y = ax + b$ fit as described in the previous section. The 95% confidence intervals on the slope, a, and the intercept, b, are as follows: $a = 470 \pm 20$; $b = 0 \pm 2$, at the appropriate number of significant figures (proper use of significant figures is an extremely difficult concept to get students to consistently apply). Then ask them whether the intercept, b, is mathematically significant (*i.e.*, nonzero within the 95% confidence interval). They should answer that b is not mathematically significant at the 95% confidence level. Out of a sample of 100 students asked over the last five years as part of an in-class exercise, only 50% have answered correctly to this question; 25% of students replied "don't know." This is a surprisingly difficult concept to master that requires consistent reinforcement throughout CHE 1102. Yet, of the same sample of students,

98% replied correctly to a similar question during hourly and final exams.

Once the students have realized that b is unnecessary, it is time to teach them how to create a user-defined model in DataFit, as $y = ax$ is not one of the built-in models (one of DataFit's few shortcomings). This can be done by returning to DataFit's main menu and clicking on the Define User Model option under the Solve menu. The user defines a Model ID, (which I defined as "Linear, no intercept," in this case). The user also inputs the Model Definition, in this case $Y = a*x$. Mathematical functions in DataFit, such as multiplication and exponentiation, work in the same way as Excel.

In many cases, including this one and all cases where the fitting is of a linear function, initial estimates are unneces-

TABLE 2
Fit Information for Pressure Transducer Calibration

DataFit version 6.1.10		Sum of Residuals = 4.08562073062058E-14			
Results from project		Average Residual = 3.14278517740044E-15			
"F:\brenner\datafit\pcalib.dft"		Residual Sum of Squares (Absolute) = 5.20799168906741			
Equation ID: a*x+b		Residual Sum of Squares (Relative) = 5.20799168906741			
Number of observations = 13		Standard Error of the Estimate = 0.688079784556427			
Number of missing observations = 0		Coefficient of Multiple Determination (R ²) = 0.99994096			
Solver type: Nonlinear		Proportion of Variance Explained = 99.994096%			
Nonlinear iteration limit = 2000		Adjusted coefficient of multiple determination (Ra ²) = 0.9999355927			
Diverging nonlinear iteration limit = 10		Durbin-Watson statistic = 2.88469613789683			
Number of nonlinear iterations performed = 1					
Residual tolerance = 0.000000001					
Regression Variable Results					
Variable	Value	Standard Error	t-ratio	Prob(t)	
a	0.998001779	0.002312177		431.6287071 0	
b	-15.1762779	0.359917526		-42.1659876 0	
68% Confidence Intervals					
Variable	Value	68% (+/-)	Lower Limit	Upper Limit	
a	0.998001779	0.002408132	0.995593648	1.000409911	
b	-15.1762779	0.374854103	-15.551132	-14.8014238	
90% Confidence Intervals					
Variable	Value	90% (+/-)	Lower Limit	Upper Limit	
a	0.998001779	0.004152438	0.993849342	1.002154217	
b	-15.1762779	0.646375884	-15.8226538	-14.529902	
95% Confidence Intervals					
Variable	Value	95% (+/-)	Lower Limit	Upper Limit	
a	0.998001779	0.005089101	0.992912679	1.00309088	
b	-15.1762779	0.792178474	-15.9684564	-14.3840995	
99% Confidence Intervals					
Variable	Value	99% (+/-)	Lower Limit	Upper Limit	
a	0.998001779	0.007181158	0.990820622	1.005182937	
b	-15.1762779	1.117831851	-16.2941098	-14.0584461	
Variance Analysis					
Source	DF	Sum of Square	Mean Square	F Ratio	Prob(F)
Regression	1	88206.02278	88206.02278	186303.3408	0
Error	11	5.207991689	0.47345379		
Total	12	88211.23077			

sary, but they become critical when doing some nonlinear fitting. The default values of each of the curve-fit parameters are unity in all cases. I look at this as one of DataFit's very few design flaws. When one goes through a Taylor series expansion, terms involving higher-order parameters are supposed to be corrections to the previous terms, meaning that the *product* of the curve-fit coefficient multiplying a high-order term and that higher-order term (*i.e.*, d^*x^3) should be less than those of previous terms. Without some exceptional physical justification, it would be difficult to throw out constant, linear, or quadratic terms and keep a cubic term.

After manually assigning initial estimates and/or constraints on the curve-fit coefficients, clicking OK, clicking Solve Regression, and OK again, the user will need to locate his or her user-defined model in the list of models. After locating your recently defined model, click on Solve, click OK, and then click on Results Detailed to return to the Fit Information screen once again. The models are ranked by the RSS, and so the Fit Information that pops up first is the one with the lowest RSS, not the one for the most recent fit. By clicking on the uppermost dialog box to locate the user-defined model, one will get the Fit Information associated with the user-defined model, "Linear, no intercept." Interestingly, scrolling down to the 95% confidence interval shows that the confidence interval for the one-parameter model ($a = 473 \pm 8$) is narrower than the slope from the two-parameter model ($a = 470 \pm 20$).

Problem 3. Fitting Water Vapor Pressures to the Clausius-Clapeyron and Antoine Equations

Fitting water vapor-pressure data to the Clausius-Clapeyron equation is challenging for underclassmen, but usually can be done successfully if the previous examples have been worked out in class or for homework. This problem, along with the follow-up fitting of the same data to the Antoine equation, typically is either the final in-class or homework problem that students are asked to solve during CHE 1102. Data for the vapor pressure of water is tabulated in Appendix B.3 of Felder and Rousseau.^[4] The Clausius-Clapeyron equation is as follows, and requires conversion of temperatures into Kelvin:

$$\log_{10} P = A - \frac{B}{T} \quad (1)$$

At this point in the course, the students know that they should plot pressure on a logarithmic scale on the y-axis and reciprocal temperature on the x-axis. Students are asked to plot $1000/T$ so that the values on the x-axis are between a more aesthetically pleasing 0 and 10, to estimate the slope ($-B$) and the intercept (A) graphically, to use DataFit to determine A and B , and finally to superimpose the curve fit (the solid line) on top of the experimental points (Figure 2).

The Clausius-Clapeyron equation is a reasonably good fit

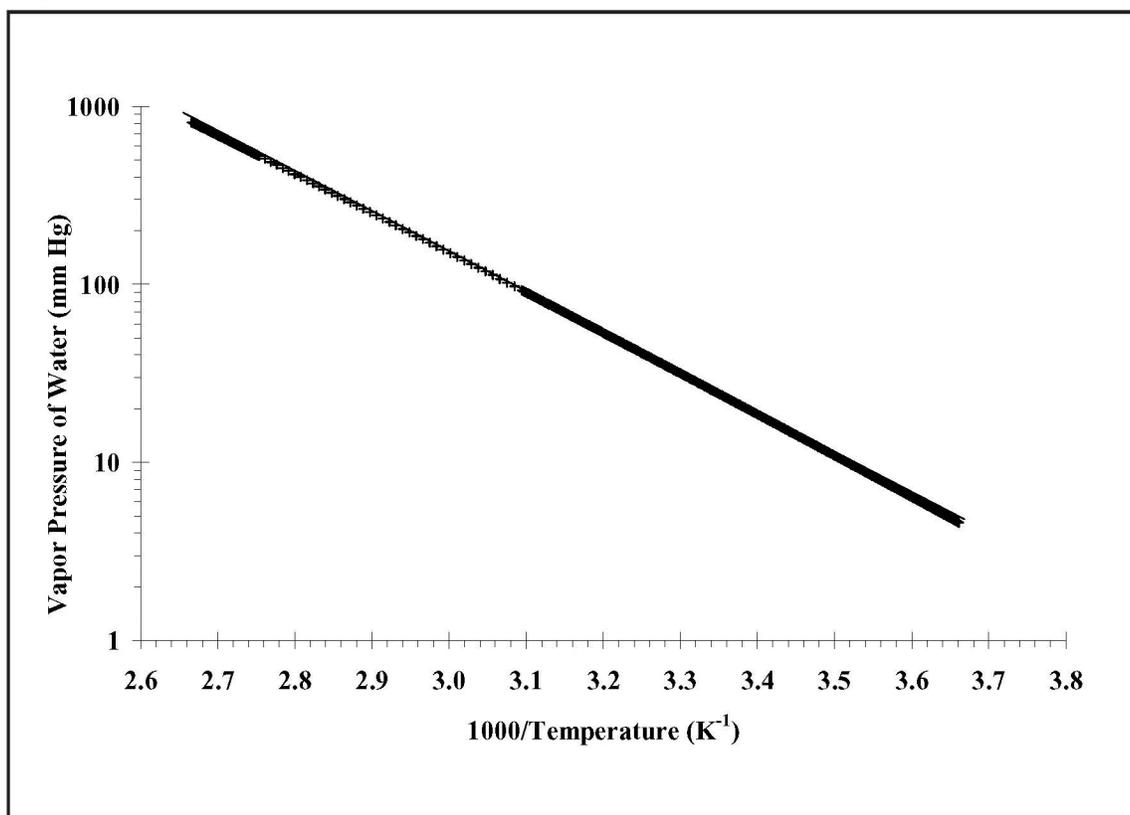


Figure 2. Clausius-Clapeyron plot for water vapor pressures.^[4]

of the vapor pressure of water data from 0 to 60 °C, but one can see that there is a systematic deviation from linearity at low temperature and pressure. By graphically extrapolating a straight line through the portion of the data that appears to be linear, one can estimate the slope (-B) as -2200 and the intercept (A) as 109 from Figure 2. Interestingly, there are slight differences in the DataFit estimates of the curve fit parameters, depending on whether the logarithm of the pressure data and the inversion of the temperature data are taken before curve fitting in DataFit or not (Table 3). In the case where the data are not so linearized before entry into DataFit and then a nonlinear model is generated in DataFit, the points at low vapor pressures are de-emphasized relative to the other points.

If one tries to fit the Antoine equation for water vapor pres-

ures either below 60 °C or above 60 °C, in either case if one does not manually change the default parameter guesses of unity, DataFit's "solution" will require more iterations than the default number of iterations, which is 250.

$$\log_{10} P = A - \frac{B}{(T+C)} \quad (2)$$

This problem can be changed using Edit Preferences. I have changed the default number of iterations permanently to 2,000.

The problem with using the results for A and B from the Clausius-Clapeyron equation as initial guesses for A and B for the Antoine equation fit is that the Antoine equation requires temperatures to be in degrees Celsius instead of in Kelvin. In fact, if one uses the Clausius-Clapeyron equation constants to fit the water-vapor pressures above 60°C and lets DataFit set the default value of C to 1, then even after having made the appropriate conversion of the data from Kelvin into Celsius, DataFit will erroneously return a "successful" result after only one iteration that contains errors larger than the values of the parameters themselves. The Antoine equation *cannot be solved* for temperature ranges in which the denominator, (T+C), switches from negative to positive *over the range of temperatures*. If one uses the values of A and B from the Clausius-Clapeyron equation and an initial guess for C of 273.15, then the Antoine equation does converge properly to the answers below in Table 4 in the "Proper Convergence" column.

This discrepancy proved a difficult challenge for even the best students. At a minimum, the number of significant figures reported for Antoine equation constants in the literature^[4,5] is grossly overstated, and, for some molecules, is just not quite right (see Table 5).

ASSESSMENT

In the first class exposed to this curriculum, 17 of 20 students successfully completed both the Clausius-Clapeyron and Antoine problems. Two of the three students who failed to make a proper plot and a proper fit in DataFit attended class less than one-third of the time, and the other student, although in good attendance, turned in less than half of the homework assignments and had significant language problems. The past four years of classes have had similar results.

A similar problem, for butane vapor pressures, has been assigned to sophomores and graduate students, using data from the NIST Chemistry WebBook.^[12]

TABLE 3
Clausius-Clapeyron Constants for Vapor Pressure of Water from 0 to 60 °C

Clausius-Clapeyron Constants	Linear Fit of Linearized Data	Nonlinear Fit of Raw Data
A	9.091 ± 0.004	9.003 ± 0.004
B	2301 ± 1	2274 ± 1

TABLE 4
Antoine Curve Fitting of Vapor Pressure of Water from 0 to 60 °C

Constants	250 iterations	Proper Convergence	Literature Data ^[4,5]
A	6.95 ± 0.08	8.124 ± 0.002	8.10765
B	1180 ± 40	1759.8 ± 0.6	1750.286
C	186 ± 4	235.8 ± 0.1	235.000

TABLE 5
Clausius-Clapeyron Equation Parameters*

Molecule	A ^L	B ^L	A ^N	B ^N
Carbon Dioxide	7.58 ± 0.02	865 ± 4	7.58 ± 0.01	864 ± 3
Ethane	7.37 ± 0.05	837 ± 9	7.127 ± 0.008	785 ± 2
Propane	7.71 ± 0.08	1130 ± 14	7.191 ± 0.007	1128 ± 3
Isobutane	7.69 ± 0.07	1274 ± 16	7.198 ± 0.007	996 ± 2
Butane	7.61 ± 0.06	1306 ± 7	7.256 ± 0.009	1193 ± 4

*Pressures in mm Hg and temperatures in Kelvin
^LLogarithm of pressure taken first
^NLogarithm of pressure not taken first

All but one of 12 sampled students who came to Florida Tech from other countries for ChE graduate school sought me out for help. None of the eight students that went to Florida Tech for both bachelor's and master's degrees needed help. Ninety percent of sophomore students who took CHE 1102 as freshmen were also able to solve the butane problem successfully.

With the default guesses, DataFit failed to converge because it cannot handle the denominator changing from negative to positive, depending on temperature. When the second term exceeds A, the solution also diverges. Under some sets of initial estimates, DataFit "converges" to a flat line! When the initial estimates are reasonably close to what DataFit reports as the correct answer ($A = 7.44 \pm 0.04$; $B = 1330 \pm 30$; $C = 294 \pm 4$), the solution converges to what is shown in Figure 3. *Even this is clearly incorrect*, as the low vapor pressure data is de-emphasized, because the magnitude of the error in such a small quantity is dwarfed by a small percentage error in the high vapor pressure points. This kind of error is not unique to DataFit. I have seen it in Polymath curve fits as well.

CONCLUSIONS

Of the international graduate students asked to fit vapor-pressure data for the previous problem, none had previous exposure to either Polymath or DataFit. While each of them also learned how to use Polymath in graduate school, 11 of

the 12 polled said that they found DataFit easier to use. The reason that I downloaded DataFit in the first place was not because of its excellent curve-fitting capabilities, but because when I first started using it in industry in 1998, DataFit was the only program that did proper 3-D scientific plotting for less than \$500. In 1999, when Florida Tech bought a site license for DataFit version 6.1, it cost only \$750 for the entire campus (albeit a relatively small campus), whereas a single copy cost \$100. Moreover, the site license allowed for students and faculty to use DataFit at home as long as they were doing academic work. A comprehensive set of solutions to similar problems can be found at <<http://my.fit.edu/~jbrenner/dataanalysispaper1.zip>>.

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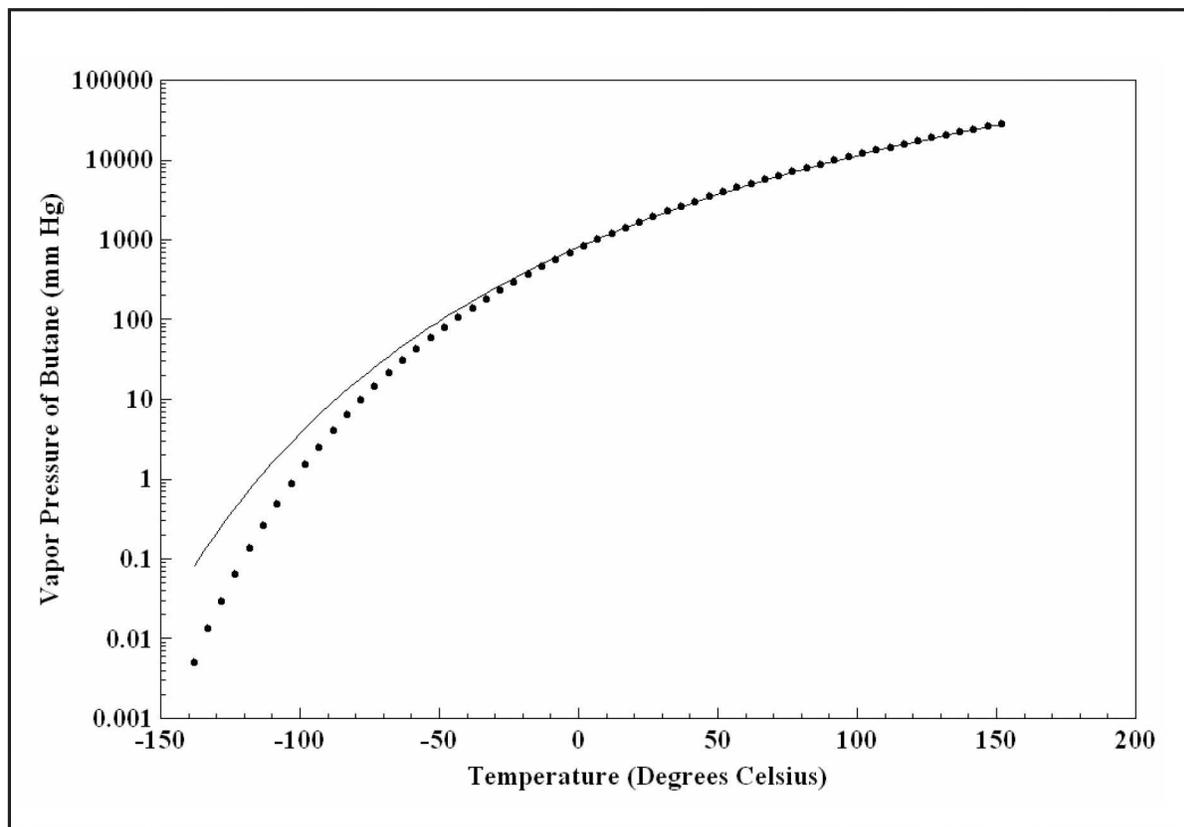


Figure 3. Antoine fit of butane vapor pressure data clearly shows bias against low vapor pressure points.

ENGINEERING ANALYSIS IN THE CHEM-E-CAR COMPETITION

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Since 1999, Chemical Engineering undergraduate students have had the opportunity to participate in the Chem-E-Car Competition at the regional and national level under the direction of the American Institute of Chemical Engineers (AIChE). The competition was initiated by AIChE members to (1) provide an opportunity for students to participate in a team competition at the national level, (2) encourage professional society interaction, and (3) increase the awareness of chemical engineering in the public.^[1] Examples of national competitions in other engineering disciplines include the concrete canoe race (civil engineering), mini-baja race (mechanical engineering), and International AIAA/ONR Design, Build, Fly contest (aerospace engineering).

The Chem-E-Car competition involves the design and construction of a chemically powered car that has to travel a specified distance (50-100 ft) while carrying a certain amount of water (0-500 ml). The car must fit into a box no larger than 40 cm × 30 cm × 18 cm and the team must be composed of members from at least two undergraduate classes. Additional rules are applicable to the competition.^[1] The objectives of the competition are applicable to numerous ABET educational outcomes including “an ability to design a system, component, or process to meet desired needs,” “an ability to function on multidisciplinary teams,” and “an ability to communicate effectively.”^[2]

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To promote the competition among Oklahoma State University (OSU) chemical engineering students and to provide an additional design experience in the undergraduate curriculum, the competition was implemented in 2000-2001 as part of a spring sophomore course (Introduction to Chemical Process Engineering) and a spring junior course (Chemical Reaction Engineering). The juniors initially worked on designing the cars and were eventually joined by the sophomores who primarily helped with the calibration, poster, and safety aspects. The teams (six-eight students) currently compete in the middle of the spring semester for the opportunity to represent OSU at the AIChE Regional Chem-E-Car Competition.

The evolution of the competition at OSU was recently presented.^[3] In brief, funding for the OSU competition was initially provided by the department, but ChevronPhillips now provides funding for equipment costs, T-shirts, the awards banquet, and travel to regional and national competitions. Further, ChevronPhillips personnel provide extensive safety reviews on students' reports. Liquid effluent

The Chem-E-Car competition involves the design and construction of a chemically powered car that has to travel a specified distance while carrying a certain amount of water.

was allowed to discharge from the car in 2001, only water was allowed in 2002, and no liquid discharge has been allowed since 2003.

In 2003, an additional fall junior course (Thermodynamics) was included in the competition to enable the students to spend more time working on their cars.

As part of the integrated sophomore and junior team, the students are required to write a safety and environmental report, provide a detailed sketch of the car, build a prototype, provide preliminary and final calibrations, provide an engineering analysis, give a poster presentation, and participate in the department competition. The engineering analysis is performed solely by the junior students, although they have traditionally provided a vague analysis such as using empirical equations, providing detailed equations without any solutions, and identifying fundamental equations that may not be applicable.

Engineering analysis is not required at the national competition and is often not applied. Rather, students rely on calibration data and trial and error to predict the distance traveled by their cars.

To demonstrate and encourage the use of detailed engineering analysis among the students in predicting the distance traveled by a car, a model was developed for a car (previously used in the competition) in which pressure generated by a chemical reaction resulted in car movement via the discharge of water. This work presents the model for predicting the travel distance based on the initial pressure and various car parameters.

Although discharged water must now be contained such that the model may not be applicable to current car designs, this work provides an example of how students can effectively apply engineering analysis. An advantage to engineering analysis is that it allows students an opportunity to determine the effects of design components (*e.g.*, vessel size, car weight, liquid volume, nozzle size, for this example) on the distance the car travels.

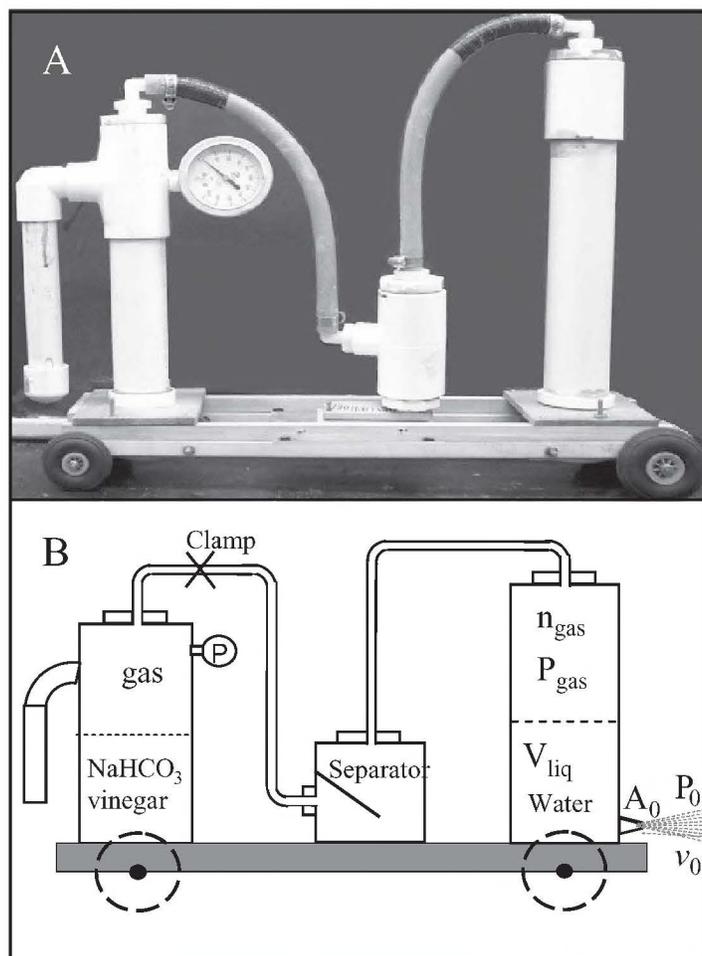


Figure 1. Picture (A) and diagram (B) of the Chem-E-Car. The left chamber was used to generate gas from a sodium bicarbonate (NaHCO_3) and vinegar reaction. The right chamber contained water that was forced from the chamber following the removal of the clamp. The expelled water propelled the car forward. The parameters and values are shown in Table 1.

MATERIALS AND METHODS

Car Design and Experimental Runs • The car, shown in Figure 1, was designed and built by Ali Moshfeghian, Christ Schulte, and Kyle Sharon (junior chemical engineering students at the time) and was used in the 2002 competition at OSU. The key car param-

eters are provided in Table 1. The left chamber, shown in Figure 1B, was initially filled with 125 ml of a saturated aqueous solution of sodium bicarbonate (NaHCO_3). Glacial acetic acid (vinegar) was then added to the solution, causing a chemical reaction to form CO_2 that increased the chamber

pressure. The acetic acid was added according to the amounts shown in Table 1 and, when necessary, additional water was added so that the acetic acid/water addition equaled 10 ml. Although acetic acid and sodium bicarbonate were used to generate the gas pressure, any pressure-generating chemical

TABLE 1
Parameters and Values Used in Engineering Analysis

<i>Run #</i>	<i>Acetic Acid (ml)</i>	<i>Initial gas pressure (atm)</i>	<i>Adjusted initial pressure (atm)</i>	<i>Distance (feet)</i>
1	2.5	4.39	2.78	4.3
2	5.0	8.14	4.76	19.3
3	7.5	11.20	6.37	32.6
4	10.0	13.24	7.43	41.7

<i>Parameter</i>	<i>Description</i>	<i>Value</i>	<i>Units</i>	<i>Note</i>
A_c	Area of water chamber	11.4	cm^2	Constant
A_0	Nozzle area	0.087	cm^2	Constant
C	Head loss coefficient	0 to 0.2	unitless	
g	Gravitational constant	9.81	cm/s^2	Constant
h_i	Water height above nozzle			
h_0	Nozzle height			
m	Mass of water	374	g	Initial value
m_{car}	Mass of car	2470	g	Initial value
n_{gas}	Moles of gas			
P_{gas}	Adjusted initial pressure	See above	atm	Initial value
P_0	Atmospheric pressure	1.0	atm	Constant
R	Gas constant	82.06	$\text{cm}^3\text{atm/molK}$	Constant
T	Temperature	298	K	Constant
v_{car}	Car velocity	0	cm/s	Initial value
V_{gas}	Gas volume	390	cm^3	Initial value
V_{liq}	Water volume	375	cm^3	Initial value
V_{tot}	Gas and initial water volume	765	cm^3	Constant
v_0	Water velocity	Eq. (8)	cm/s	Variable
x_{car}	Car distance	0	feet	Initial value
ρ_{liq}	Water density	0.997	g/cm^3	Constant
μ_k	Friction coefficient	0.07	unitless	Figure 4

reaction would be sufficient for operation of the car. It is important to note that the generated pressure should not exceed the pressure limits of the materials to prevent material failure. A clamp was used to keep the gas pressure in the left chamber until the pressure reached equilibrium. The right chamber was filled with 400 ml of water (V_{liq}). Following pressure equilibration, the clamp was removed and the rear nozzle opened. The pressure above the water (P_{gas}), related to the moles of gas (n_{gas}), forced the water to exit the rear nozzle (cross sectional area of A_0) at a given velocity (v_0). P_0 represents the atmospheric pressure. The separator was added to minimize foam, generated in the left chamber, from entering the water chamber. The exiting velocity produced a thrust that moved the car forward. When the water ran out, the car

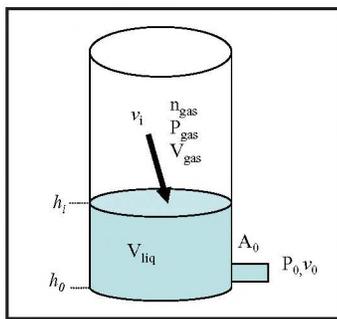


Figure 2. Diagram of model used for the engineering analysis. The model represents the chamber that contains the water. The parameters and values are shown in Table 1.

distance. Figure 2 shows a representation of the water chamber that was used for the model. V_{liq} is the water volume, h_0 is the height of the nozzle (assigned a value of zero), h_i is the height of the water above the nozzle, v_i is the surface velocity of the water at h_i , A_0 is the nozzle cross-sectional area, v_0 is the water velocity leaving the chamber, and P_0 is the pressure of the surrounding atmosphere. P_{gas} , V_{gas} , and n_{gas} represent the pressure, volume, and moles of the gas above the water, respectively.

A material balance on the total mass of the car (m_{car}), which is equivalent to a constant mass plus the mass of the water in the chamber (m), shows that the mass changes with time according to

$$\frac{dm_{car}}{dt} = \frac{dm}{dt} = -\rho_{liq} v_0 A_0 \quad (1)$$

where ρ_{liq} is the liquid density. The right term represents the mass flowrate of water leaving the water chamber (and the car). Since $m = V_{liq} \rho_{liq}$, and if ρ_{liq} is assumed constant, the water material balance shows how V_{liq} changes with time ac-

ording to

$$\frac{dV_{liq}}{dt} = -v_0 A_0 = -\frac{dV_{gas}}{dt} \quad (2)$$

The change in V_{gas} is also shown with time in Eq. (2) since any water volume decrease results in the same increase in the gas volume (*i.e.*, the total volume, V_{tot} , is constant and equal to $V_{gas} + V_{liq}$).

To assess how the gas pressure (P_{gas}) changes with time, the ideal gas law was assumed where $P_{gas} V_{gas} = P_{gas} (V_{tot} - V_{liq}) = n_{gas} RT$. Since V_{tot} is constant and $n_{gas} RT$ is constant as the water is leaving the nozzle (assuming negligible temperature change and no new gas is generated once the experiment starts), the time derivative of the ideal gas law gives

$$\frac{dP_{gas}}{dt} = \frac{P_{gas}}{(V_{tot} - V_{liq})} \frac{dV_{liq}}{dt} = \frac{-v_0 A_0}{(V_{tot} - V_{liq})} P_{gas} \quad (3)$$

Eq. (2) was substituted into the middle term of Equation 3 to obtain the term on the right.

The velocity of the car with time was predicted from a momentum balance on the car. The momentum balance states that the change of momentum (mass of the car, m_{car} , times the velocity of the car, v_{car}) is equal to the sum of the forces acting upon the car:

$$\frac{d(m_{car} v_{car})}{dt} = m_{car} \frac{dv_{car}}{dt} + v_{car} \frac{dm_{car}}{dt} = \rho_{liq} v_0^2 A_0 - \mu_k m_{car} g \quad (4)$$

The first term on the far right side of Eq. (4) represents the thrust force that pushes the car forward.^[4] Only thrust occurring when water leaves the chamber was considered. Once the water runs out, residual gas pressure greater than atmospheric pressure will cause some thrust but the thrust is likely negligible since the gas density is small compared to liquid. The second term on the far right side represents the friction force between the car and the ground, with μ_k as the friction coefficient.^[4] The negative sign signifies a force that decreases the car velocity. The drag force between air and the car was neglected. Substitution of Eq. (1) into Eq. (4) gives

$$\frac{dv_{car}}{dt} = \frac{\rho_{liq} v_0 A_0 (v_0 + v_{car})}{m_{car}} - \mu_k g \quad (5)$$

Once the water runs out of the chamber, the first term on the right side is zero and the velocity of the car will decrease as a result of friction until the car stops. The distance (x_{car}) at which the car stops was predicted from the definition of velocity,

$$\frac{dx_{car}}{dt} = v_{car} \quad (6)$$

To predict the velocity of water leaving the car (v_0) for ap-

plication in Eqs. (1)-(5), the mechanical energy balance,^[5] with the inclusion of frictional head loss due to the exit nozzle, was utilized such that

$$\frac{C}{2}v_0^2 + \frac{1}{2}(v_0^2 - v_i^2) = g(h_i - h_0) + \frac{(P_i - P_0)}{\rho_{\text{liq}}} \quad (7)$$

The subscripts *i* and *0* refer to the values at the gas-liquid interface and the nozzle exit, respectively. *C* is the head loss constant. Since $P_i = P_{\text{gas}}$, $(h_i - h_0) = V_{\text{liq}}/A_c$ (where A_c is the cross-sectional area of the water chamber), and if $v_i \ll v_0$ (the liquid velocity leaving the chamber is much faster than the velocity of the water surface at the gas-liquid interface) then

$$v_0 = \sqrt{\frac{2}{(1+C)} \left[g \frac{V_{\text{liq}}}{A_c} + \frac{(P_{\text{gas}} - P_0)}{\rho_{\text{liq}}} \right]} \quad (8)$$

Eqs. (7) and (8) are only valid when water is present in the chamber. Thus, once the water completely runs out of the chamber, Eqs. (7) and (8) no longer apply and v_0 is zero in Eqs. (1)-(5).

Eqs. (1)-(3), (5), and (6) [with the definition of Eq. (8)] were numerically integrated using Polymath^[6] to obtain values of the integrated parameters as a function of time. When

the model results showed that the water ran out ($V_{\text{liq}} = 0$), v_0 was set to zero for reasons stated above. At this point, only Eqs. (5) and (6) were numerically integrated.

The initial values for solving the model were $m_{\text{car}} = 2470$ g, $V_{\text{liq}} = 375$ cm³, $v_{\text{car}} = 0$, and $x_{\text{car}} = 0$. For the water volume, the volume initially added to the chamber was 400 ml. Since 25 ml was below the nozzle and did not leave the chamber, the initial water volume was modeled with a value of 375 ml. The values of P_{gas} for the four experimental runs are shown in Table 1. Since the initial gas pressure (P_{init}), as shown in Table 1, was measured prior to opening the clamp, the adjusted initial pressure was determined by $P_{\text{gas}} = (205/390) * P_{\text{init}} + (185/390) * 1 \text{ atm}$. The adjustment was based on the assumption that the pressure above the water chamber (with a volume of 185 ml) was 1 atm and that the initially measured pressure (with a volume of 205 ml) equilibrated (in the total volume of 390 ml) after the clamp was opened and prior to the opening of the rear nozzle. A value of $C=0.1$ is consistent with fluid leaving a large reservoir and entering a small rounded-edge entrance (*i.e.*, similar to liquid leaving the chamber and entering the nozzle).^[5] Table 1 summarizes the model parameters with their associated values. Unit consistency was ensured when solving the equations.

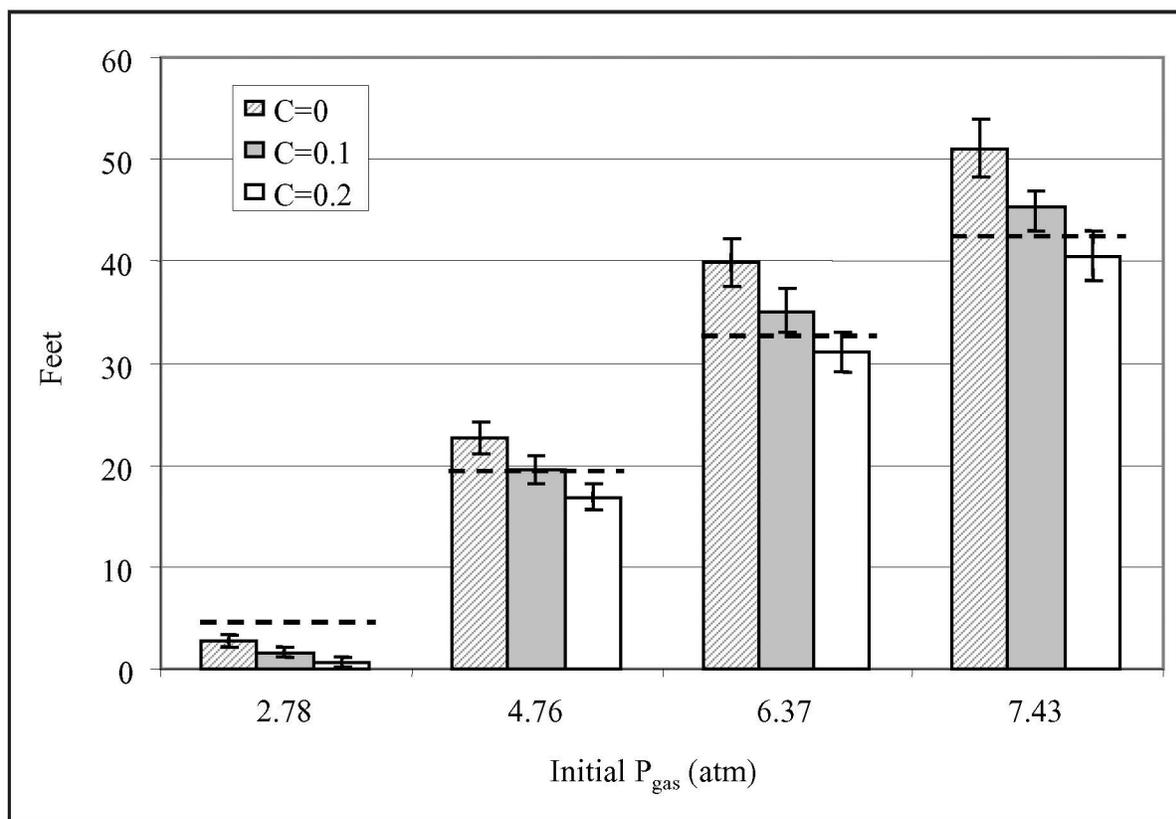


Figure 3. Measured (dashed lines) and predicted distance (bars with $\mu_k = 0.069$) traveled by the car as a function of initial gas pressure (P_{gas}) above the water. The error bars show the predicted range with $0.066 \leq \mu_k \leq 0.072$.

Friction Factor Analysis • The friction coefficient (μ_k) shown in Eq. (5) was needed for solving the system of differential equations. The coefficient is dependent upon the type of surface and the type of wheels contacting the surface. Thus, the coefficient can vary and must be measured for each surface upon which a car is tested. For this work, the friction coefficient was measured by pushing the car by hand, measuring the initial car velocity ($v_{car,0}$), and then measuring the final distance (x_f) at which the car stopped from the point at which the initial velocity was measured. The initial velocity was measured a short distance from where the car was pushed to ensure that the car was decelerating during the analysis. A ruler was placed at the initial velocity measuring point while a video camera recorded the time for the car to travel a given distance of the ruler (5-13 inches). An average initial velocity was obtained by dividing the distance by the time.

Since there was no thrust between the initial velocity point and when the car stopped, Eq. (5) states that $dv_{car}/dt = -\mu_k g$. Integration of Eqs. (5) and (6) gives

$$\int_{v_{car,0}}^{v_{car}} dv_{car} = \int_0^t -\mu_k g dt \Rightarrow v_{car} = v_{car,0} - \mu_k g t \quad (9)$$

$$\int_0^{x_f} dx_{car} = \int_0^{t_f} (v_{car,0} - \mu_k g t) dt \Rightarrow x_f = v_{car,0} t_f - \frac{\mu_k g t_f^2}{2} \quad (10)$$

Since $v_{car} = 0$ at t_f (the time for the car to travel the entire distance), $t_f = v_{car,0}/(\mu_k g)$ according to Eq. (9). Substitution into Eq. (10) gives

$$x_f = \frac{1}{\mu_k} \frac{v_{car,0}^2}{2g} \quad (11)$$

Thus, a plot of x_f versus $v_{car,0}^2/2g$ gives an inverse slope of the friction coefficient.

RESULTS AND DISCUSSION

Experimental Runs • The distances the car traveled during the four experiments are shown in Figure 3 with the dashed lines. The furthest distance traveled was 41.7 feet at an adjusted pressure of 7.43 atm as shown in Table 1. The traveled distance increased with initial pressure as expected.

Friction Factor • The results of the friction factor experiments are shown in Figure 4. Six experiments were performed such that the distance traveled varied between 10 and 30 feet. The wide range of distances allowed for a more complete analysis of the friction coefficient. The plot of x_f versus $v_{car,0}^2/2g$ yielded a straight line, which is in agreement with Eq. (11). Regression analysis resulted in an inverse slope of $\mu_k = 0.069 \pm 0.003$ (95% confidence) for the friction coefficient.

Model Predictions and Comparison • Figure 3 shows the model predictions based on $\mu_k = 0.069$ and a head loss coefficient (C) ranging from 0 to 0.2. The error bars show the range of model predictions when μ_k ranges from 0.066 to 0.072 (the

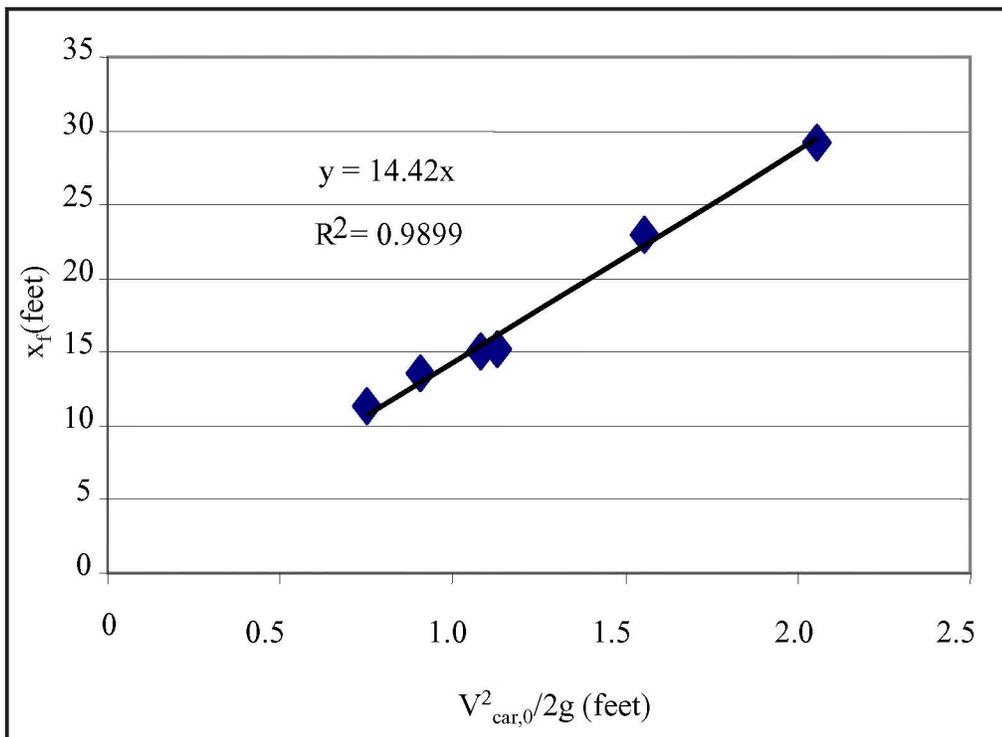


Figure 4. Friction coefficient analysis as described by Eq. (11). The inverse of the slope represents the friction coefficient. The distance traveled (x_f) is shown as a function of the initial car velocity ($v_{car,0}$).

***As part of the integrated sophomore and junior team,
the students are required to write a safety and
environmental report, provide a detailed sketch of the car,
build a prototype, provide preliminary and final calibrations,
provide an engineering analysis, give a poster presentation,
and participate in the department competition.***

95% confidence interval). As shown in Figure 3, the model predictions were in good agreement with the experimental results when $C=0.1$. With $C=0$, the model predictions were much higher than experimental measurements for the three highest initial pressures. However, $C=0$ is unreasonable since head loss occurs as a result of the nozzle. Model predictions with $C=0.2$ are lower than experimental measurements for the three highest initial pressures. The model predictions with a range of C values are shown to demonstrate the effect of C on model predictions.

With $C=0.1$, the predictions had a difference of 1.0%, 7.3%, and 8.6% from experimental values at initial pressures of 4.76, 6.37, and 7.43 atm, respectively. It must be remembered, however, that the only fitted parameter in the model was the friction coefficient, and the coefficient was measured via a different experiment than the experiment for which the model was used. All other parameters were car dimensions, the initial starting pressure, or the value of C . Thus, considering all of the model assumptions, the model did a reasonable job in predicting the traveled distance.

There are several possibilities as to why the model had some disagreement. The first possibility was that the initial starting pressure was lower than the adjusted initial pressure used in the model. In the future, the measurement of the initial pressure following the removal of the clamp would be beneficial. A second possibility was a potential gas leak, such that the contributing pressure to the thrust of the car would be lower. No noticeable gas leaks were observed when running the car, however. A third possibility is a change in the value of the friction coefficient, μ_k , during the course of experiments due to wind conditions and axle friction (since μ_k was a function of the experimental conditions). No noticeable wind changes were observed and the distances utilized in the evaluation of μ_k were similar to the experimental runs. The effects of changing μ_k , however, are noticeable by the error bars in Figure 3. The validity of assumptions is an area that could be further explored.

With the successful demonstration of the model predictions with the experimental results, the impact of car parameters on the traveled distance can be explored. For instance, the effects of varying the rear nozzle diameter, water volume, initial pressure, or friction coefficient (representing an increase

or decrease in friction due to changing the type of wheels or the type of surface on which the car travels) can be assessed with regard to distance traveled. This type of exercise allows a student to have a better understanding of how engineering design can affect the function of the car, without the need for numerous experimental designs.

CONCLUSIONS

This work describes the effective utilization of engineering principles in a model to predict the distance traveled by a Chem-E-Car using the acetic acid/baking soda reaction.

Although the model is specific for one type of car-propulsion system, this work demonstrates how engineering analysis is applicable to the Chem-E-Car competition.

One could extend the engineering analysis to include calculation of the theoretical pressure build-up in the reactor, and correlate the theoretical pressure to the experimentally observed pressure in the chamber. Similar analysis could be performed for hydrogen peroxide-catalase reaction systems that generate pressure. Engineering analysis is also applicable to other Chem-E-Car models, such as the iodide clock reaction used to stop a car via breaking an electronic circuitry. For example, the kinetics of the reaction could be incorporated with the momentum equation to predict the time at which the reaction stops the circuitry and the distance at which the car stops. In conclusion, engineering analysis concepts introduced through the Chem-E-Car competition not only provide an opportunity to reinforce theoretical concepts but also provide a tool for the design of the cars.

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