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If Kenneth R. Jolls were the main character in a novel, it would probably tell about a child who took a toaster apart and used its components to beat an intricate rhythm on the kitchen table. In real life, the young Kenneth did take a toaster apart (and couldn't put it back together), but his musical talent didn't surface until high school when he picked up a guitar his older brother had left behind. Still, science and music (specifically, chemical engineering and jazz) shaped Ken's novel life.

Ken started as a musician in his hometown of Raleigh, North Carolina, in the era of big bands and small combos. His first job, as a high school sophomore playing guitar in a quartet, paid $9 a night. Occasionally he worked with a vibrapharp player—a relatively new instrument that had its origins in vaudeville. "I was captivated by the sound and also by the sight of the mallets—usually two, sometimes four—racing over the bars, so I began teaching myself to play," Ken remembers. He would eventually captivate his own audiences with the mallets—sometimes five of them—dancing over the aluminum bars in complicated patterns. But that rushes the story.

In the tenth grade, Ken was certain music would be his career. At school he played the tuba and occasionally solo marimba; in professional country and commercial dance bands he played the guitar and the vibraharp. After graduation he enrolled at North Carolina State "because it was there." He chose nuclear engineering as his major (his father had encouraged him to "get into something more focused") but worked part-time as a rural high school band director and played in clubs on weekends. Then he won a scholarship to the highly regarded music school at Indiana University, choosing the tuba as his major and paying his bills by playing baritone horn in the marching band and writing music for football half-time shows. He soon switched to a music theory major with a percussion emphasis that included lessons on the marimba but not the vibraharp, although he owned one by that time.

But bulbar polio intervened, and instead of returning to Indiana in the fall of 1954, Ken found himself in an iron lung in a Raleigh hospital. As he recovered he began playing again. One of the groups he played with was the Duke Ambassadors, Duke University's popular big band, and that contact with Duke students encouraged him to enroll at Duke. He earned tuition fees by playing the university's carillon, writing music for half-time shows, playing with the Ambassadors, writing many of their arrangements, and, as a senior, leading the group.

Duke also whetted Ken's appetite for academics in general and science in particular. So, Duke music degree in hand, he went back to North Carolina State to earn a second bachelor's degree, this time in chemical engineering. Dance jobs and even a stint in a country-western band on a live weekly TV show paid his bills. During his five semesters at NC State, Ken also sampled the professional world of chemical engineering through summer jobs at DuPont and Sun Oil.

One of his favorite professors, Kenneth O. Beatty, suggested graduate school, and Ken was soon working for Thomas J. Hanratty at the University of Illinois. "Tom was one of the great formative people in my life, and I knew I had to get his opinion on what was best for Ken," Kenneth R. Jolls said. Ken was soon working for Thomas J. Hanratty at the University of Illinois. "Tom was one of the great formative people in my life, and I knew I had to get his opinion on what was best for Ken," Kenneth R. Jolls said. Ken was soon working for Thomas J. Hanratty at the University of Illinois.
life," Ken says, "but he wonders to this day how I 'kept the music hidden.' I didn't think I was hiding it," Ken says—he played frequently during those years, including once for Bob Hope. "I was playing the piano," Ken recalls, "and he asked if I could play Thanks for the Memory. My response was, 'What key?'

Ken was one of the first of Tom Hanratty's students to work on the now-famous diffusion-controlled electrode technique to measure mass-transfer rate and shear stress in flowing liquids. In Ken's case, the system was a packed bed. The apparatus was a glass column six feet tall and twelve inches in diameter, filled with 11,000 1-inch glass marbles. Most of their research involved electrochemical measurements, but they also did some visualization studies using dye to confirm the onset of turbulence. Their work became part of the basic packed-bed literature and is still cited.

The first year of graduate school was awful, Ken says. "There I was, a musician, in Harry Drickamer's class, of all places, competing with real chemical engineers. But when I passed the oral prelim, I realized I would get that PhD." He did, and a subsequent series of interview trips landed him a job at the Polytechnic Institute of Brooklyn.

When his new department head, Jim Conti, asked him what he wanted to teach, Ken replied, "Anything but thermodynamics." But Ken's first course assignments had him facing thirty-five New York City seniors three times a week to teach them—thermodynamics. "Fortunately, I had the second edition of Smith and Van Ness," Ken says, "but I was never more than two or three pages ahead of the students." John McFeeley, now a senior manager at Polaroid who considers Ken the "most significant influence in my professional career," recalls some of Ken's initial teaching devices: "Maxwellian demons, the Ideal Rubber Band Law, and even the little-publicized Zeroth Law of Thermodynamics."

A few useful revelations resulted from that year, Ken says: "I realized I didn't understand thermodynamics; if possible, my students understood even less about it; and even when I did understand it, I didn't know how to explain it."

Ken concluded that there had to be a better way to teach thermodynamics, but he didn't start pursuing it because he had added electronics and instrumentation courses to his academic repertoire. A flair for instruments and circuits, discovered in graduate school, led him to associate with chemist Howard Malmstadt who had been presenting 'Electronics for Scientists' courses at Illinois since the late 1950s. Ken went back to Illinois for several summers to teach with Malmstadt and also taught his own NSF summer electronics courses at Brooklyn Poly while writing a series on the subject for Chemical Engineering.

Ken also contributed a session on "Harmonic Oscillators" at Brooklyn Poly's annual Executive Technical Development Program. His after-dinner session, scheduled near the end of three weeks of intense continuing education courses on statistics, math, and semiconductors, sounded oppressive to the executives in the program. They were relieved, however, to discover that the oscillators were vibraharp bars, the harmonies were jazz "changes," and the lecture was on the history of jazz. "I didn't even mention Fourier," Ken says.

During his New York years, Ken also played the "wedding-Bar Mitzvah-Scandinavian circuit." At one memorable dinner-dance in New Jersey, many of the guests came with bodyguards, and at another job Ken was playing in the Grand Ballroom of the Waldorf Astoria while Robert Goulet sang in the room next door.

Ken, equally hard at work preparing a demonstration of the Joule-Thomson process (shown above with Ron Cotterman, John Prausnitz's grad student) or manipulating the mallets (right) for his own and others' enjoyment.

Winter 1994
But then he left the Big Apple for Iowa State University. "I was getting serious about teaching thermodynamics by this time," he says. "I didn't think we needed another textbook, but we did need better ways to explain fundamentally difficult concepts. We could demonstrate fluid flow in a pipe and do experiments showing heat and mass transfer, for example, but we couldn't demonstrate enthalpy or buy an entropy meter." For him the better way was visual: "I was convinced that many of the thermodynamic subtleties that usually bewilder students could be represented graphically, and that the phase diagram was the basic structure for doing this. I may not have been very sophisticated in thermodynamics," Ken recalls, "but I had discovered that textbook authors liked to draw pictures of thermodynamic surfaces.

In the early 1970s, Ken saw a thesis that used a 3-D plotting program to locate the minimum points of a function showing the economics of power-plant design, and the connection to using the computer for thermodynamic drawings became obvious to him. "I wanted to try 3-D pictures, and the PVT diagram was the simplest I could think of," he says. Over the next five years he and three students wrote computer programs to draw phase diagrams for pure fluids, using the geometrical operations associated with projecting 3-D images onto a 2-D plane. With steam-table data they drew a variety of thermodynamic functions and published several papers. They also tackled mixtures. Kenneth Starling at Oklahoma provided a program that generated mixture data, and two more students joined Ken to do the graphics.

Ken's drawings were more than just cosmetic; they were quantitative, and they were helpful in teaching. But they were still just "a picture of this, and a picture of that," he says. No conceptual links existed among the drawings until he discovered Thermodynamics and Its Applications, by Modell and Reid. The textbook changed the way he thought about and taught thermodynamics.

Modell and Reid described "a fundamental equation that sits at the top of the thermodynamic hierarchy and contains all the information about the variables," Ken explains. The Legendre transform connects the various fundamental forms, and the applied functions, such as PVT, heat capacity, and refrigeration diagrams, are derived from them. "To learn more about this connectivity, he went on leave in 1981 to work with John Prausnitz at Berkeley.

Meanwhile, Ken hadn't neglected his aural art. During his early years in Ames he played for Sonny and Cher and for Helen Reddy, as well as numerous area events. He played in shows such as Pippin and The Fantastiks, directed the orchestra for the musicals Hair and Jesus Christ Superstar, and occasionally played percussion with the Des Moines Symphony. At Berkeley he played a Noon Concert in Hertz Hall with two Bay area musicians.

A letter Ken received at Berkeley changed his approach to his visualization work. "When two minds separated by many years . . . arrive independently at the same conclusion (concerning the usefulness of graphical methods)," wrote North Carolina State chemistry professor Henry Bent, "perhaps . . . there is something compelling to that conclusion. Indeed, the time is probably ripe for someone with the proper gifts and interests and experience to go back over that ground covered by Gibbs, from the standpoint of the capabilities of modern computers. You may be precisely the right person for that project."

That message sent Ken to the library for J. Willard Gibbs' original accounts of his geometry-based formulation of thermodynamics. Gibbs' elaborate descriptions of lines, planes, and contours described intriguing rationales for the state of a system and for the tendency—through consideration of thermodynamic stability—for those states to change. For the first time, Ken says, someone had proposed a geometric art form to show the structure and logic of thermodynamics.

"Although Gibbs used very few drawings, he had an exact geometrical analogy for phase transitions," Ken says. "It was based on the energy-entropy-volume surface with its changing curvatures, and it used a plane rolling over the surface to reveal not only the property values but also the phase transitions associated with those changes. If you have the fundamental equation model for a particular system and the right kind of geometrical tools, you can roll that plane and determine precisely all the thermodynamic properties one normally tabulates. I found that idea fascinating and learned that other people found it fascinating, too, and had tried to model it." But their efforts, all done by hand, were imprecise—and as one-of-a-kind models, gave no hint of the connectivity Gibbs had described.

Ken was convinced that the Gibbsian approach could explain how thermodynamic functions are related and thus remove some of the abstraction that makes it such a difficult subject. "Gibbs postulated these connections more than a century before machines were invented to visualize them," he marvels. "It's a stroke of fortune that we now have the ideal scientific visualization tool—computer graphics."

After returning to Iowa State, Ken discovered that Keith Gubbins at Cornell shared some of his interests in graphics, so he spent a semester there teaching thermodynamics and working on the visualization processes. But he found that the facilities, good as they were, could not accomplish what he wanted to do.

"Gibbs postulated these connections more than a century before machines were invented to visualize them," [Ken] marvels. "It's a stroke of fortune that we now have the ideal scientific visualization tool—computer graphics."
By the time he returned to ISU, he was quite comfortable with the Modell and Reid approach to thermodynamics and the concept of using fundamental equations to reveal the various levels of stability and provide a logical flow of information for developing practical tools. Still, interest in using the geometric approach for teaching was limited. "I couldn't understand it," Ken says. "All the complicated things we talked about we could now see—all the interesting thermodynamic effects we deal with we could now visualize."

"Thermodynamic diagrams show many relationships that otherwise require verbal, numerical, 'left-brain' processing," Ken says. "I am utterly convinced, and enough others who understand thermodynamics agree, that this is the way, maybe the best way, to solve the long-standing teaching problem in this difficult subject." As physicist Herbert Callen wrote to Ken, "your elegant pictures" mean students will "have a more concrete view of a subject which has always been hampered by its abstract nature."

Of course, visualization skills are not distributed equally throughout the population. "I didn't realize when I started that people learn in different ways," Ken says. "Learning through visualization was natural for me, and twenty years ago I assumed it was natural for everyone else, too. Even though it isn't ideal for everyone, visual learning does work well for many people. But the pedagogical methods we use in engineering tend to ignore them."

In 1984, a computer engineering student, John Ries, added an interactive shell to one of Ken's PVT programs, allowing users to input data more easily. Computer equipment had also improved by this time, and color was available. Another undergraduate student, Dan Coy, created a PC version of the program, and these changes liberated the process of making the drawings and changing them to fit specific situations. Ken named the program "Equations of State," added tutorials and documentation, and began taking it to conferences and writing about it. Although some viewers didn't "get it," others thought it was marvelous, and thermodynamics teachers around the world (nearly fifty of them to date) bought it for use in their classes.

"I knew what was hard about thermodynamics, and I knew what would make the course better and help students learn," Ken reflects. "In this case, I needed the power of the computer, and I molded the tool to fit the subject. I think too often it happens the other way around: the computer looks like a neat tool and someone contrives a way to plug it into a course. Unfortunately, it may not add anything of substance; it may not be a genuine improvement in the course or in the way it's taught. The judicious use of technology to do something substantive in teaching can enhance a good textbook and even a good teacher," he adds. "Too often the computer is much ado about not very much. Students rave about 'Equations of State' because they can do things with the computer that they can't do any other way." As Imre Zwiebel at Arizona State puts it, Ken's program "makes students think before they plunge into a problem."

Students also rave about another program Ken developed. When he began teaching the separations course at ISU, he realized he couldn't assign some of the most interesting problems because the computations were too hard. "But with process simulators like FLOWTRAN or ASPEN to do the calculations, students could work on these more realistic examples in absorption, distillation, and extraction," he notes. Since those solutions almost always end up in graphical form as stagewise operating diagrams, it seemed obvious to Ken that he could use computer graphics for the drawings. One of his graduate students, Deepak Lumba, wrote a program to extract the numerical results from FLOWTRAN and produce the stagewise displays; another student, Michelle Nelson, wrote a program to let students run the simulator interactively. The combination produced "Simulation Graphics."

"I think it's an enormous advance in teaching separations processes," Ken says. "You can do complicated separations quickly, repetitively, and in different modes and then see the results graphically." Students agreed, and Dick Seagrave, Ken's department head during most of that development period, told him "Simulation Graphics" was the best thing he had produced.

And through it all was the music. Ken played at after...
The Chemical Engineering Department at S.U.N.Y. is undergoing great change. Some mirrors the change that the profession itself is experiencing, but more so it reflects the coming of a new generation to the department. Our founders succeeded remarkably well in building a strong teaching and research program, and now our generation bears the responsibility of continuing their tradition of excellence. The changes present new opportunities as well as new challenges.

HISTORY

The University of Buffalo (UB) was founded as a private institution in 1846, and Millard Fillmore served as its first Chancellor. It grew over the next century, and in 1962 it merged into the State University of New York (SUNY) system. Shortly thereafter, planning and construction began for a new campus to be located three miles north of the original UB site. Our department moved to this "North Campus" in 1977, and it now occupies many of Furnas Hall's ten stories.

The campus continues to expand, most recently with the dedication of an impressive 17,000-seat stadium, a student union, a retail complex, and two spacious, modern facilities for chemistry and fine arts. UB has the highest enrollment of any campus in the SUNY system and offers the widest range of academic programs of any public institution in New York and New England. The Buffalo campus remains the only one in SUNY to offer degrees in chemical engineering.

Later arrivals were also instrumental in the department's development. Eli Ruckenstein came from the University of Delaware after emigrating from Rumania in 1973. Ralph Yang arrived from Brookhaven National Labs in 1978, and Vladimir Hlavacek joined us in 1981 from Czechoslovakia. All three have made tremendous contributions to the profession and science of chemical engineering. Eli holds the rank of Distinguished Professor, and he has received broader recognition for his many achievements through election to the National Academy of Engineering.
Ralph's very active research program is all the more remarkable in light of the additional responsibilities he has assumed as department chair. These three, along with Tom and Ken, form the senior core of our faculty.

The long-term future of the department rests, of course, with the junior faculty. The most senior of these is Mike Ryan, with John Tsamopoulos and Carl Lund rounding out the ranks of Associate Professor. Following them are no fewer than five new hires over the past four years: Dave Kofke, Lakis Mountziaris, Scott Diamond, Johannes Nitsche, and Deborah Leckband. The eight junior faculty are establishing solid reputations in teaching and research: four are National Science Foundation PYI/NYI awardees, and other awards include an NIH First Award, a Whitaker Foundation Award, and a Hackerman Young Author Award. All have been successful in acquiring funds to conduct ambitious research programs in a wide array of fields.

The success of the junior faculty owes much to the selfless support and encouragement they receive from their senior colleagues, and indeed, many significant changes have been instituted at the behest of the newest arrivals. An atmosphere of cooperation and camaraderie has blossomed in this environment, and morale in the department is very high. Evidence is provided by two multi-investigator grants awarded to the department by NSF in the past two years; details follow below.

THE UNDERGRADUATE PROGRAM

The State of New York has an unusually strong commitment to providing accessible higher education to its citizens. In-state tuition remains very low, and consequently a large majority of our undergraduates are State residents. Freshmen arrive with 3.6/4.0 high school averages and SAT scores averaging 650/545 (M/V). Recent graduating classes have numbered approximately thirty, but it seems that future classes will see this figure more than double.

The chemical engineering curriculum at UB is typical of ABET-accredited schools, but some offerings are less common. Close relations with local industry allow our students to gain, as a three-credit elective, the practical experience of an internship. Each intern spends ten hours per week for one semester at an industrial site. Lakis Mountziaris and Mike Ryan have for several years offered undergraduate research projects on paper- and tire-recycling. Scott Diamond has taken this notion a step further by offering a university-wide elective entitled "Biotechnology and Society" which attempts to prepare the non-technical but educated person to make informed decisions about some of the complex issues facing society. The department can boast of ten local and national teaching awards, including four instances of the SUNY Chancellor's Award for Excellence in Teaching, the highest teaching award given by SUNY.

The department is now embarking on an ambitious, col-

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In and Around S.U.N.Y.

Left: World-famous Niagara Falls attracts locals as well as honeymooners from far and wide.

Right: The area's pastoral beauty is typified by this scene from UB's south campus.

Below: The Albright-Knox gallery, home of many treasures of modern art.
laborative project to advance the use of computers in chemical engineering instruction. Seven faculty co-investigators have been awarded funding under the very competitive Leadership in Laboratory Development program in NSF's Division of Undergraduate Education. The goal of the project is to develop a Chemical Engineering Simulation Laboratory (CESL) that will greatly expand the role of simulation as a supplement to the laboratory and classroom experiences.

CESL will be an interactive simulation package that instills in students an intuitive feel for chemical processes. The simulation modules will provide virtual laboratory experiences—the student being presented with "equipment" to be characterized by "experiments" of their design. More interesting will be situations in which the student operates a simulated process, drawing on acquired intuition to respond quickly to unexpected changes. We seek eventually to incorporate design elements in which the student must assemble a process to accomplish a particular task.

GRADUATE PROGRAM

We are very proud of the stature our department has acquired for research in the short period of its existence. Each year the department secures new external funding at a level of about $1 million, graduates roughly ten PhD and eight MS students, and publishes nearly a hundred articles in refereed journals. The graduate program displays a healthy balance between experimental and theoretical research, and between fundamental and applied studies.

Catalysis and Reaction Engineering

Research in catalysis and reaction engineering is performed by Yang, Lund, Ruckenstein, Mountziaris, and Hlavacek. The efforts of Mountziaris and Hlavacek are materials-oriented, and both of them rely on an unusually well-balanced combination of theory, computer simulation, and experiments to tackle their research problems. Vladimir Hlavacek holds the C.C. Furnas Chair and is Director of the Laboratory for Ceramic and Reaction Engineering, which was established in 1987 with the goal of bridging the gap between chemical engineering and materials science. One of the Laboratory's finest achievements is the development of combustion synthesis methods to produce superhard ceramic materials—nitrides, borides, carbides and the like. In this technology, the reaction precursors are "ignited" to initiate a self-propagating but controlled reaction which yields a very pure, sinterable product without any additional energy input. Hlavacek's group is also very active in studying the dynamics of nonlinear reacting systems.

Hlavacek and Lakis Mountziaris both have research interests in chemical vapor deposition (CVD). CVD delicately balances transport processes with both gas- and surface-phase kinetics to produce solid films from reactive gases. Hlavacek uses CVD to make non-oxide ceramic fibers and thick films, while Mountziaris is studying metalorganic CVD as a means to produce thin films of compound semiconductors for advanced electronic and optical devices. There are many novelties in Mountziaris' research, not the least of which is a counterflow jet reactor for studying the decomposition kinetics of CVD precursor gases.

Mountziaris is also applying CVD to grow diamond films from hydrocarbons at low pressure. The value of such a product is obvious, but Mountziaris takes it a step further—by inserting dopant atoms in the growing film, he is attempting to produce diamond-based semiconductors; diamond's electronic and heat transfer properties would make such a material very useful in electronic devices.

The reaction engineering performed by Ralph Yang and Carl Lund has a different flavor: it is oriented toward the catalyst and the catalytic processes. Yang, the holder of the Praxair Endowed Chair, is studying catalytic reduction of NO for pollution control from power-plant emissions. Presently this task is accomplished by selective reduction of NO with ammonia over a V2O5 catalyst. Yang has found that pillared clays are better catalysts and, moreover, he has developed a new sorbent-catalyst approach to NO reduction without a reducing gas. Also, his work on carbon-gasification reactions continues to be at the forefront of that field.

Lund is enhancing commercial reactions by applying a strategy perfected long ago by biological systems: selective removal of reaction intermediates via transport across a membrane. Selective removal of reaction products increases reactor yield by exploiting chemical thermodynamics; this notion is well established and is routinely exploited. Lund's new approach exploits the kinetic features of the process instead: timely removal of reaction intermediates prevents them from participating in additional, undesired reactions that degrade the product. The net result is an increased yield.

In one of several other projects, Lund is performing transient kinetic experiments with isotopically labeled reactants to identify the pathways of coke formation in acid catalysts. The enormous network of microscopic pores which endow these catalysts with many wonderful properties also make them susceptible to deactivation by coking. Lund's research is needed to develop strategies that will minimize these coking reactions, and thereby extend catalyst life.

The efforts of Eli Ruckenstein round out the department's research in catalysis and materials. His research program is remarkable for its astounding degree of diversity and novelty. Eli has major thrusts in materials, colloids, separations, catalysis, and bioengineering, and in his career he has made significant contributions in transport phenomena and thermodynamics as well. His encyclopedic knowledge of the literature forms the intellectual timber for the inspired works that have earned him such acclaim. Eli's grasp of world history and politics is equally amazing, but that is a story (actually many stories, best told over lunch) in itself.

Ruckenstein's present work in catalysis reflects the diver-
sity of his entire research program. He is building theories for the activity and selectivity of catalytic reactions on supported-metal systems by combining sophisticated experimental techniques with new concepts concerning the active sites. In other work, he has developed biaxial-promoted magnesium-oxide catalysts that are proving effective in many reactions of industrial importance, including the conversion of methane to ethylene, toluene to styrene, and acetonitrile to acrylonitrile.

In the area of materials, Ruckenstein has had several breakthroughs in developing composite polymers with useful properties, such as electrical conductivity or great hardness. Another project has produced a new membrane that is highly permeactive yet possesses good mechanical properties. In still another project, he has combined the Debye model of a crystal with a Langevin model for diffusion to generate a new, unified theory for mass transport in solids. His work with colloidal systems continues, and is now directed to the study of the properties of foams, focusing on film drainage and Voronoi analysis of foam structure.

**Transport Phenomena**

The bulk of the department's research in transport phenomena is done by Mountziaris, Nitsche, Ryan, and Tsamopoulos. Mountziaris supplements his reaction-engineering research with computational studies of multiphase flows which display a rich variety of nonlinear phenomena. Also, he—together with Lund—played a major role in initiating the undergraduate simulation lab project described above; before that he served as PI of a collaborative proposal that led to the purchase of a state-of-the-art graphics system for visualizing complex modeling calculations. Mountziaris, perhaps more than anyone, personifies the spirit of cooperation that has overtaken this department.

The behavior of drops and bubbles represents the essential fluid mechanics underlying many multiphase phenomena of interest to the chemical industry. John Tsamopoulos is applying asymptotic theories and boundary- and finite-element calculations to understand the behavior of these very complex dynamical systems. His work can be used to describe the coalescence of bubbles suspended in liquids and thereby aid in preparing or destabilizing emulsions and dispersions. The dynamics become particularly interesting when a solid surface is introduced: fluids flowing rapidly near the surface experience a local decrease in pressure, which causes the formation of cavitation bubbles; subsequent collapse of these bubbles contributes to erosion of the surface.

Tsamopoulos shares an interest with Mike Ryan in problems that concern the processing of polymers. Tsamopoulos' focus is the fundamental fluid mechanics and finite-element modeling, while Ryan concentrates on the process engineering. Ryan's experiments with injection molding and thermoforming processes will help manufacturers predict the ultimate properties of a finished part, knowing only the polymer's material properties and details of the forming process. In another area, they are working to develop software that can simulate the various stages of a blow-molding cycle. Of interest here is the ability to predict the final wall thickness of the product (such as a plastic cup): walls that are too thin may fail, while overly thick walls waste material. Ryan is also Director of the Business-Industry Affiliates Program of the New York State Center for Hazardous Waste Management, where he oversees research on the reduction of hazardous waste generation at the source. Specific interests include recycling and reuse of post-consumer scrap rubber and plastics, biodegradable polymers, and the use of additives to enhance the degradability of a polymer material.

Arguably the busiest man in the department, Johannes Nitsche has not let his enormous dedication to teaching detract from his research program. He has great expertise on Brownian transport in confined spaces, and he brings to bear a wide range of mathematical and computational tools to examine these problems in the context of catalysis and separations technology. In diffusion of nonspherical particles in pores, the confining walls couple strongly with particle hydrodynamics to produce unexpected behavior, such as anomalous density distributions. Rotational diffusion is a concept that is relatively unappreciated by many engineers, yet it plays a key role in reactions in porous media. The phenomenon is especially relevant to proteins and other macromolecules that are reactive on only a small portion of their surface. Nitsche is embarking on several experimental investigations to guide and corroborate his calculations.

Nitsche possesses several unique and en­viable gifts, not the least of which is his muse, Elroy Hutch. Nitsche has been generous enough to share his "musings" with Elroy with his students—graduate and undergradu­ate—and his colleagues here at UB and, in fact, worldwide [see Fluid Phase Equil., 78, 157 (1992)]. Elroy's antics have delighted our students in unit operations for several years now and have taught them several lessons of how chemical engineering should not be done.

**Biochemical Engineering**

The department has recently initiated a major concentration in biochemical engineering. Scott Diamond and Deborah Leckband are the principals in the endeavor, along with Eli Ruckenstein and another faculty member who will be re-
crutied soon. The facility assembled for this work is impres­
sive by any standard. Bioengineering occupies the entire
ninth floor (6000 ft²) of Furnas Hall, and it features seven
fully equipped laboratories: molecular biology, microbial
engineering, cell culture, separations, analytical surface sci­
ence, and video microscopy. Additional facilities, including
three environmental chambers, support these labs.

Mammalian cells exposed to laminar shear stresses (as are,
for example, the cells lining blood vessels) behave differ­
ently than do cells removed from such an environment.
The response of living cells to mechanical forces is distinct
from the relatively well-understood phenomenon of recep­
tor-mediated signaling. **Scott Diamond** measures intracellu­
lar concentrations of key biomolecules and is assembling his
findings into a theory for the mechano-biological response.
The relevance of this work to the treatment and prevention
of coronary and vascular disease has been recognized tangi­
bly by the American Heart Association. The research is also
proving useful in the design and operation of bioreactors. In
other work, Diamond is examining the transport and kinetics
of proteolytic enzymes in entangled, cross-linked protein
gels, such as fibrin and collagen. While the work has several
direct applications, Diamond's primary interest relates to the
design of blood-clot dissolving agents and the design of
thrombolytic therapies.

**Deborah Leckband**'s presence strengthens and expands
the department's reputation in colloids and interfaces. She
uses the surface forces apparatus in concert with sophisti­
cated biochemical and surface analytic techniques to probe
the nature of cell- and biopolymer-surface interactions. In
one application, Leckband examines the forces that govern
molecular recognition to guide her development of very
sensitive and localized biomolecular sensors. In another, she
uses her surface-forces measurements to improve protein-
separation techniques, both by chromatography and by partition­ing
in aqueous solution. She also performs studies of
adhesion at the cellular level, with application to wound
healing, cancer cell metastasis, tissue engineering, and floc­
culation in bioreactors.

**Separations**

Much of the department's work in separations has been
discussed above, but it would be conspicuously incomplete
without highlighting the significant achievements of **Ralph
Yang**. He complements his work in catalysis with both
fundamental and applied studies of adsorption and adsorbent
materials. The author of *Gas Separation by Adsorption Pro­
cesses*, Yang is acknowledged as a leading expert in adsorp­
tion and its use as a separation technique. He is now studying
the molecular design and synthesis of new sorbents.

**Molecular Thermodynamics**

Finally, we come to **David Kofke** who, when he isn't
woodworking or speaking about himself in the third person,
conducts research in molecular thermodynamics. Com­
puter simulation is regarded by many as the third leg—
along with theory and experiment—upon which we build
our understanding of nature. Most of Kofke's group is busy
developing and applying Monte Carlo and molecular
dynamics simulation techniques—"experiments" on model
molecular systems. Much of their focus is on methods
for evaluating phase equilibria; other topics occupying
Kofke's attention include thermodynamics and transport
in anisotropic systems (such as liquid crystals) and theories to
predict properties of mixtures from data for the respective
pure components.

**BUFFALO AND ENVIRONS**

A local business official recently complained of two major
problems with operating in Buffalo—the number 2 problem
is getting people to relocate here, and the number 1 problem,
he said, is getting them to leave. Buffalo is New York's
second-largest city and is, according to recent rankings, its
"most livable." Housing is inexpensive, the roads are
uncongested, air travel is hassle-free, and (believe it or not)
the climate is moderate—temperatures below 15 or above
90°F are rare. We are also just north of the famed snow belt
beloved by skiers.

The city is rich in culture: the Albright-Knox gallery pos­s­
poses one of the world's finest collections of 20th century
art; the Buffalo Philharmonic consistently ranks as one of
the nation's top orchestras; the theatre district, developed as
part of a recent renaissance of the downtown area, provides
opportunities to enjoy the best works of local and national
theater companies. If that's not enough, Toronto, one of the
world’s premier cultural centers, is less than two hours away.

But Buffalo's biggest secret is its architecture: the region
boasts of a remarkable number of architectural masterpieces,
including five Prairie houses by Frank Lloyd Wright and
major works by Sullivan, Richardson, and others of similar
stature. Buffalo also possesses a beautiful system of parks
designed by Frederick Law Olmsted. Outdoor recreation
may be found in the waters of Lakes Erie and Ontario, or in
the many splendid woodland areas nearby. And, of course,
one of the world's greatest natural wonders—Niagara Falls—
is a mere twenty minutes from the campus.

**THE FUTURE**

The enthusiasm and optimism of the faculty, together with
their substantive accomplishments in both teaching and re­
search, paint a bright future for the department. This article,
we hope, has provided a convincing portrayal of the exciting
developments here. We urge any who are contemplating
their own future, either as a graduate student or an academic,
to give serious consideration to SUNY Buffalo and to the
opportunities that await you here. ☞
**EDUCATOR: Ken Jolls**

*Continued from page 5.*

concert dinners for three major orchestras (Philadelphia, Baltimore, Leningrad). He has played "Jazz in July" concerts in Des Moines each summer, a public TV special with a Des Moines personality, and numerous club dates. He hosted a reception for jazz vibes player Gary Burton, hosted a visit by pianist and radio personality Marian McPartland, conducted honors courses on jazz and improvisation, and presented pre-concert programs about the Modern Jazz Quartet and Marian McPartland.

And he kept thinking about Gibbs and his geometrical formulation of thermodynamics, but those drawings were harder to do. They needed more sophisticated equipment, for one thing, and in 1986 Ken got it: an NSF grant provided a Silicon Graphics IRIS 3030—the first advanced graphics workstation at ISU. On it, graduate student Michael Schmitz generated the first Gibbs surface—the Helmholtz energy function for a pure fluid—using Movie.BYU software.

Later, graduate student Day Coy produced the complete set of four pure-fluid images based on the Peng-Robinson equation for ethylene. "Those first Gibbs images represented a fixed amount of mass, but that isn't necessary in thermodynamics," Ken says. "The mathematical description of a thermodynamic system can be scaled in a variety of ways, depending on the ultimate use of the results. Dan later worked out schemes so that drawings could be made according to all scalings possible. To some people they seem almost like a circular set of representations of the same thing through the power of the Legendre transform. But these are necessary redundancies that give us more useful forms.

"Dan was able to generalize both the thermodynamics and the graphics schemes for producing the surfaces. He was able to comprehend the three major aspects of the project: the thermodynamic connectivity, the computer programming, and the visualization. His dissertation is a masterful piece of work," Ken says. "This is the first time these drawings have been presented in any connected, quantitative, knowing— even artistic—way. We thought about color, lighting, perspective—what we needed to make the contours convincing." Ken calls the drawings "the art of thermodynamics."

"If you take the time, you can look at every function in Modell and Reid and see that 'this comes from that and with good reason,'" Ken says. "Sometimes those reasons are pretty subtle, but they're all rooted in the structure of classical thermodynamics and in stability theory. That's what makes it all work. If it weren't for thermodynamic stability, the world would be a single-phase blah," he adds. "Stability theory says that we have preferred states—things boil, condense, freeze, form crystals. Dan's dissertation has drawings that show those ideas."

But it hasn't always been easy. "Funds are hard to get," Ken notes, "and funds for teaching improvements—especially for teaching improvements that don't involve laboratories—are even harder to come by." Ken has had NSF funding and grants from the Dreyfus Foundation and Union Carbide. "I was warned against doing this work," he recalls, "and I wouldn't advise a new faculty member trying to get tenure to do it either. To do this stuff right takes a lot of time. And you can't work in a vacuum; you need support from the department and the department head, plus release time. It doesn't work very well as an add-on."

Academic software needs to be documented, it needs to be used, and it needs to be reviewed, just like other scholarly efforts, Ken says. If the work is done right, the intellectual effort to develop teaching software is no different than the intellectual effort to do research. "That's not a popular opinion," he adds, "but it's the truth."

"I also have a good ear. A friend in music school once said I could 'hear around corners,'" Ken recalls. "That basic ability to detect harmonies is crucial. I was born with the nerve endings that create a good ear and a mathematical mind," he adds. "Seeing those traits reproduced in my son removes any doubt about the genetics," Michael Jolls works as a programmer analyst in St. Louis, plays guitar and piano, and does magic.

"I call it a quantitative ear," Ken explains. "I hear harmonies, realize exactly what creates them, and can reproduce them; I can connect what I hear—or even just what I think about—to the way to play it. Because of my formal training in theory, I can also talk about it, and often do—but it's still easier just to play it."

Jazz on the vibraharp is geometrical, too. "There's no magic," Ken says. "You just spread the two, four, or five mallets and turn them so as to connect pairs of points with straight lines." One of the things that keeps him playing is that he can. Even though he doesn't practice very much, he can shift into music mode very quickly. "Sometimes I feel like I won't be able to find middle C," he groans, "but once I get the mechanical thing going, I can do about 80% of the rest off the top of my head."

In jazz, a composer writes chord structures to fit a melody, and an improviser plays a line of notes that fits those chords but is different from the melody. That requires a willingness to take risks, to deviate from the formula, to step out of the mold and try something new, Ken says. Of course, that's what he's done in thermodynamics with his quantitative eye—with his work to express scientific ideas visually. "There must be a connection," Ken says, "or a very strange coincidence." Well, truth is often more novel than fiction.
SEPARATIONS
What to Teach Undergraduates

P. C. WANKAT, R. P. HESKETH,¹
K. H. SCHULZ,² C. S. SLATER³
Purdue University
West Lafayette, IN 47907

Separations (also known as mass transfer or unit operations) have always been an important area in chemical engineering, but recently separations have become a critical concern.¹⁻⁴ This concern arises because separations are typically between 50% and 90% of the plant cost and because the subject is so important in "hot" areas such as biotechnology and the environment.

A workshop at the ASEE Chemical Engineering Division Summer School in Bozeman, Montana, in August of 1992, wrestled with the problem of what separations should be taught to undergraduate chemical engineers. The workshop consisted of an overview of separations, a short presentation on educational ideas and educational philosophy, and small work groups discussing their curricula and the question of what to teach.

OVERVIEW OF SEPARATIONS

The general consensus of the workshop participants was that undergraduate students should be introduced to a broad overview of separations. One way to present this overview in a concise format is to use the classification shown in Figure 1.¹⁵ Some of the working groups found this scheme to be useful for organizing their thoughts—the scheme should also be useful to undergraduates, particularly global thinkers. If this or a similar classification scheme is shown, then each of the separations categories must be discussed. Several concrete examples from each separation category should be presented to the students. Within the category of equilibrium separation processes, the concept of a separating agent is useful.

Two other concepts which are useful for an overview of separations are the relationship between feed concentration and selling price⁶⁻⁷ and the wide range of production rates for different separations (see Figure 2). The Sherwood plots⁶⁻⁷ can be used to make the point that more concentrated feeds are easier to separate. Also, the point can be made that not all raw material sources are equal. Product rates for separations vary enormously, as shown in Figure 2.¹⁵ The type of separation used often depends on product rates. This can easily be illustrated for oxygen production at different product rates. For very small units membrane permeation and pressure swing adsorption compete, for medium-size units pressure and vacuum swing adsorption units seem to be favored, and for very large units cryogenic distillation is least expensive.

Our experience is that these concepts are easily understood by undergraduates. The concepts help the students obtain a perspective on separations and to understand the similarities and differences between separations. It is useful to present Figure 1 both at the very beginning of the semester to illustrate the course structure and at the very end to help review the material. Figure 1 also helps the students realize that there are many other separations in addition to those they studied. If one goal is to produce innovative

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Phil Wankat received his BSCHE from Purdue and his PhD from Princeton and is currently a professor of chemical engineering at Purdue University. He is interested in teaching and counseling, has won several teaching awards at Purdue, and is Head of Freshman Engineering. His research interests are in the area of separation processes, with particular emphasis on cyclic separations, adsorption, preparative chromatography, simultaneous fermentation, and separation.

Robert P. Hesketh is an assistant professor at the University of Tulsa. He received his BS (1982) at the University of Illinois Urbana, and his PhD (1987) from the University of Delaware. He teaches undergraduate mass transfer and chemical reactor design, and graduate reaction kinetics, multiphase reactor design, and combustion. His research interests include incineration, combustion, and multiphase flows.

Kirk H. Schulz is an assistant professor at the University of North Dakota. He received his BSCHE and PhD in chemical engineering from Virginia Polytechnic Institute and State University in 1986 and 1991, respectively. His research interests include surface science and catalysis, with teaching interests in mass transfer, chemical kinetics, and physical chemistry laboratories.

C. Stewart Slater is a professor of chemical engineering at Manhattan College. He received his PhD, MPhil, MS, and BS degrees in chemical engineering from Rutgers University. His research and teaching interests are in separation and purification technology, membrane processes, and biotechnology.
MECHANICAL
- Centrifuge
- Cyclone
- Decanter
- Demister
- Electrostatic Separator
- Emulsion Separator
- Expression
- Filtration
- Flotation
- High-Gradient Magnetic
- Impingement Separator
- Magnetic
- Sedimentation
- Scrubber
- Sink-Float

DIFFUSIONAL
- D.L. Isomer Sep.
- Ester Production

CHEMICAL MODIFICATIONS

HETEROGENEOUS
- Mass Spectrometer
- Pressure Diffusion
- Thermal Diffusion
- Ultracentrifuge
- Electrophoresis

HOMOGENEOUS
- Isoelectrical Focusing
- Isotachophoresis

NON-EQUILIBRIUM
- Electrostatic Separator
- Emulsion Separator
- Mass Spectrometer
- Pressurization Diffusion
- Ultracentrifuge
- High-Gradient Magnetic
- Electrophoresis

EQUILIBRIUM
- Membrane or barrier
- Non-membrane
- Ultracentrifuge
- Electrically Focusing
- Magnetic


Figure 2 (Left). Product rates for various Separation Processes.[21] Reproduced by permission of the American Institute of Chemical Engineering from G.E. Keller, III, AIChE Monograph Series, 83 (17), 1987. Copyright 1987, AIChE. All rights reserved.

Engineers, then Figure 1 coupled with Figure 3[22] are useful. Figure 3 is also useful in design classes to help explain the strong preference of many companies for well-known technology. The Sherwood-type plot[6,7] can be included in the course when the economics of separations are covered, or as part of the overview when Figure 1 is discussed. Figure 2 can also be part of the course overview, or it can be profitably employed when discussing the use of competing methods for the same separation problem.

EDUCATIONAL IDEAS AND PHILOSOPHY

The choices of what to teach and how to teach it are heavily influenced both by which educational methods work and by our philosophy of chemical engineering education. These topics were briefly covered in the workshop to give all of the working groups a common basis.

Inductive reasoning starts with specific cases and is followed by the develop-
opment of general rules, while deductive reasoning starts with a general theory and derives specifics from the general theory. Both methods are useful and are powerful reasoning methods; but inductive reasoning is the natural mode for learning completely new areas. Thus, when the students are exposed to separations for the first time, the use of inductive reasoning will be more effective. In elective and graduate student courses where the students are seeing some of the material for a second time, deductive reasoning may be a more efficient way to teach.

Four concepts of educational philosophy were presented and discussed at the workshop. The first three of them were extracted from Hougen's principles:\[^{10}\]

1. The undergraduate program should be practical and conservative, whereas the graduate program should be imaginative and exploratory.
2. There should be a smooth flow of information from graduate research to graduate teaching to undergraduate teaching.
3. If you can't find relevant problems to give the student, then you shouldn't be teaching the material to students.

The fourth statement of educational philosophy was added by the lecturer, Phil Wankat:

4. Different departments should do different things.

In the discussion following the presentation there was general agreement with these four statements of educational philosophy. The practical result of the first and third concepts is that only separations currently used in industry were included in the proposed undergraduate courses. The application of the fourth concept led to a lack of consensus on what to teach.

**WORKSHOP GROUPS**

Five working groups, with six or seven professors in each group, began the workshop portion by introducing themselves and discussing their current course structure in separations. Separations courses included courses with titles such as Separations, Mass Transfer, or Unit Operations, among others. In addition, the separations parts of laboratory and design classes were included in the discussion. Each group developed an undergraduate curriculum in separations subject to the constraint of no increase in the credit hours. A reporter recorded the group's comments, made a presentation to the large group, and if desired became a coauthor of this paper.

One of the functions of the working groups was to share information about the wide variety of coverage on separations topics, both in the U.S. and the Canadian schools. Schools reported from one to four lecture-type courses covering separations topics. There appeared to be approximately an equal distribution between stand-alone separations courses and mass transfer courses with a major separations compo-

![Figure 3. Technological and Use Maturities of Separation Processes.](image)

nent. In addition, all schools apparently include separations in laboratory and/or design courses.

At a few schools a significant portion of separations material was included in the capstone design course. Textbooks mentioned included: Bennett and Myers; Fousta, et al.; Geankoplis; Henley and Seader; Hines and Maddox; King; McCabe, et al.; Skelland; Treybal; Wankat; and notes by Rousseau and by Tiller. This list of texts is similar to the bibliography in the latest AIChE mass-transfer survey.\[^{9}\] Most schools supplement the textbooks with computer programs, often in design classes. Computer programs mentioned included Aspen, Aspen Plus, Flowtran, HYSIM, and various spreadsheets for doing McCabe-Thiele calculations. The working groups discussions showed a healthy diversity in both the material presented and the method of presentation.

**WORKING GROUP RESULTS**

None of the groups reached a consensus on what should be taught (except that all groups agreed that there was too much material to teach in the available time). This lack of consensus apparently occurred because of the large variety of offerings in separations and because everyone was explicitly encouraged to retain diversity. Despite the lack of an overall consensus, however, there were areas with substantial agreement—as well as an interesting split of opinions.

There was a general opinion that newer separations are under represented in the current curriculum. These processes include membrane separations (reverse osmosis, ultrafiltration, gas permeation, and pervaporation), adsorption including pressure swing adsorption, and chromatography. Since hybrid applications coupling two or more types of separations are becoming increasingly important in industry, stu-
dents should be made aware of these applications—perhaps in a design course.

In addition to the underrepresented new separations, a number of important existing mechanical separations (see Figure 1) involving particulates have almost disappeared from the curriculum at many, but not all, schools. Since separation operations with particulates are extremely important industrially, some way needs to be found to either retain or reinstall them into an already crowded curriculum.

One of the chemical engineering laboratory courses was proposed as a convenient place to cover those separations that don't conveniently fit into existing courses. Examples include mechanical separations such as filtration, centrifugation, or flotation. Many schools already have these experiments and membrane separations can easily be included in curriculum at many, but not all, schools. Since新技术 might increase the rate at which the students learned this material. Of course, there would be a strong temptation to use the same amount of time and have the students learn the material more thoroughly. Since writing educational software is extremely time-consuming, this approach is efficient if, and only if, the programs can be widely shared. Some participants also felt strongly that their schools had too much coverage of liquid-liquid extraction.

Although there were a few strong dissenters, most participants felt their current curriculum was too heavy in distillation. At the same time, there was an intriguing 50/50 split among participants as to whether or not to retain the use of Ponchon-Savarit diagrams in distillation. Paradoxically, many professors wanted less coverage of distillation, but wanted to retain use of Ponchon-Savarit diagrams. It was thought that some room might be made in the curriculum by using computer-aided instruction programs for helping the students to visualize McCabe-Thiele and Ponchon-Savarit diagrams and for doing “what-if?” calculations. This method might increase the rate at which the students learned this material. Of course, there would be a strong temptation to use the same amount of time and have the students learn the material more thoroughly. Since writing educational software is extremely time-consuming, this approach is efficient if, and only if, the programs can be widely shared. Some participants also felt strongly that their schools had too much coverage of liquid-liquid extraction.

As an illustration, the coverage at the authors' four schools is shown in Table 1. The order of topics in the table is not necessarily the order of presentation in the course. One can analyze the four required courses (not including Req'd. 2) in Table 1 for the lowest common denominator of course topics that is acceptable. The results are: Introduction (1), VLE (1), Flash distillation (1), McCabe-Thiele (8), Batch distillation (1), Short-cut distillation (1), Multicomponent distillation plus computer (5), Absorption/striping (3), Extraction (3), Packed design (1), and Examinations (3). Thus, 28 of the 46 class periods (or 61%) are common to all four courses. The remaining 39% could be up to the discretion of the instructor. Obviously, this allows significant opportunity to teach different material.

An elective course in bioseparations, particulate separation, or rate separations was

**TABLE 1**
Course Outlines at Authors' Schools

<table>
<thead>
<tr>
<th>Topic</th>
<th>Manhattan</th>
<th>N. Dakota</th>
<th>Purdue</th>
<th>Tulsa</th>
</tr>
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<tr>
<td>Introduction</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
<td>Costs &amp; Types of Separations</td>
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<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>VLE</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>1</td>
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<tr>
<td>Flash Distillation</td>
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<td>3</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Distillation: McCabe-Thiele</td>
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<td>12</td>
<td>9</td>
<td>12</td>
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<tr>
<td>Batch Distillation</td>
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<td>3</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Short-Cut Distillation Design</td>
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<td>3</td>
<td>2</td>
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<tr>
<td>Computer Methods</td>
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<td>3</td>
<td>1</td>
<td>-</td>
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<tr>
<td>Multi-Component Distillation</td>
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<td>3</td>
<td>7</td>
<td>5</td>
</tr>
<tr>
<td>Adsorption/Stripping</td>
<td>4</td>
<td>3</td>
<td>3</td>
<td>5</td>
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<tr>
<td>Extraction</td>
<td>-</td>
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<td>5</td>
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<tr>
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<td>-</td>
<td>2</td>
<td>-</td>
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<tr>
<td>Packed Column Design</td>
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<td>3</td>
<td>1</td>
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<td>Humidification</td>
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<td>-</td>
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<td>Ion Exchange</td>
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<td>3</td>
</tr>
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<td>4</td>
<td>7</td>
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<td>46</td>
<td>46</td>
<td>46</td>
</tr>
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</table>

**Textbook**

|---------|-------------------|--------------------|-------------|-------------|-------------------|-------------|

Winter 1994
considered to be a good method for allowing students to study additional separations without clogging the curriculum. These electives can be dual-level courses and might allow some faculty to teach in the area of their research. Unfortunately, when the details of an elective course were looked at there was considerable disagreement on the depth versus the breadth of the course. The compromise of covering a few topics in depth while other topics are only surveyed might be acceptable; but there was a strong feeling that the course had to be integrated (perhaps using Figures 1 to 3) and not be a series of unconnected topics. The coverage in an elective and a required advanced course at the authors' schools is shown in Table I.

**SUMMARY**

Like many other areas of chemical engineering, knowledge and application of new separation technologies are expanding at a rapid rate. The problem of how to introduce new separations into the curriculum is exacerbated by the neglect of particulate separations. Modest adjustments in current courses can probably be made by reducing the coverage of distillation and by adding new or neglected separations to the current course and in design and laboratory courses. One or more elective courses in separations are also highly desirable.

**ACKNOWLEDGMENT**

The authors thank all of the workshop attendees for their enthusiastic participation during the workshop. In particular, comments by recorders Alan Foss and Bonnie Tyler were helpful in writing this paper. We also thank the industrial supporters and the National Science Foundation for making the Summer School possible.

**CITED MASS TRANSFER AND SEPARATIONS TEXTS**


**REFERENCES**

characterized by reaction rates following the law of mass action and by the third step which is cubic and autocatalytic. This feature of the model provides the feedback mechanism which produces instability and oscillations. In the different chapters, the autocatalator is analyzed in detail by considering some of its meaningful modifications and several reactor configurations. This kinetic scheme has been chosen because it exhibits all kinds of typical complex nonlinear behavior, while it is simple enough to allow for much exact analysis.

In Chapters 2 through 5, the closed homogeneous reactor is considered. In Chapters 2 and 3, the isothermal case is analyzed, first by determining the pseudo-stationary states of the system. These are obtained by assuming that the reactant concentration, \( e.g. \), the concentration of \( P \), is constant. Then, the concept of steady-state stability is introduced and a linear stability analysis is performed to determine stability conditions on the parameters of the model. It is shown that under the assumption of no reactant depletion, the autocatalator exhibits oscillatory behavior (\( e.g. \), limit cycles) for the values of parameters where the steady-state is unstable. The importance of casting the model equations in dimensionless form is strongly emphasized and this technique is applied throughout the book. Finally, the complete model, accounting for reactant consumption, is studied, thus proving that its behavior can be understood and predicted by exploiting the previous analysis based on the pseudo-stationary states and their stability.

Chapters 4 and 5 deal with thermokinetic oscillations in a homogeneous reactor which exchanges heat with the surroundings but is closed to mass transfer. In this case the kinetic scheme simply consists of two consecutive first-order reactions: \( P \rightarrow A \) and \( A \rightarrow B \). Here the feedback mechanism is provided by the thermal effect due to the exothermicity of only the second reaction. Performing the same analysis (\( e.g. \), first determining the pseudo-stationary states and their stability and then describing the reactant consumption) yields similar results as in the isothermal case. In order to account for the temperature dependence of the model, the following approach is used throughout the entire book. First the Arrhenius law is approximated by a simple exponential expression, allowing one to obtain several analytical results. Then the exact Arrhenius law is used and the results are compared. In Chapter 5, the Hopf bifurcation analysis and techniques for the quantitative analysis of relaxation oscillations are described and applied to the thermokinetic oscillation model.

Chapters 6 through 8 deal with CSTRs. In Chapter 6, the isothermal case is considered and steady-state multiplicity patterns for kinetic schemes of increasing complexity are determined. The effects of residence time and of the reversibility of reactions are analyzed. The non-isothermal CSTR is studied in Chapter 7 with first-order kinetics and Arrhenius temperature dependence. Both adiabatic and non-adiabatic reactors are considered. Here, the strong analogies with the cubic autocatalytic kinetics in the isothermal CSTR are illustrated. Also in the chapter, singularity theory and its applications are introduced. In order to demonstrate its power, some results about isothermal cubic autocatalysis and non-isothermal CSTR are obtained again by applying singularity theory methods.

Chapter 8 deals with the stability of stationary states in the isothermal autocatalytic CSTR. In particular, the response to transient perturbations is analyzed, illustrating the exponential relaxation to stable states and the exponential growth from unstable states. The onset of oscillations when the stationary state loses its stability is studied, with particular reference to conditions for emerging stable or unstable limit cycles.

Chapters 9 through 11 are concerned with spatially distributed systems where molecular diffusion and thermal conduction processes play a fundamental role. First, reaction-diffusion cells are introduced, and spatially distributed systems where molecular diffusion and thermal conduction processes play a fundamental role.
A FIELD GUIDE TO THE EXCESS FUNCTIONS


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Over the past thirty-five years, a substantial data base has become available for the principal "energetic" excess properties (g_E, h_E, and c_E) of binary liquid mixtures. A major use of these numbers is for incorporation into group-contribution techniques (e.g., ASOG, UNIFAC) for estimating liquid-phase activity coefficients. The application here is quantitative; the ultimate goal is to predict the composition and temperature dependence of the activity coefficient, \( \gamma \), in binary and multicomponent mixtures.

The excess-property data can also serve another, more qualitative, purpose. Because they reflect differences between energetic and structural effects in a solution relative to those in the unmixed components, the excess properties serve as probes for elucidating phenomena at the molecular level. The signs and relative magnitudes of the excess properties can therefore, with judicious interpretation, be used to support or disqualify molecular theories. The desired generalizations, however, must be based on a large number of experimentally based results.

This "explanatory" role of the excess properties demands that the most rational and communicative way of organizing the data base be found. What simple ways exist to display g_E, h_E, and c_E which could highlight patterns and trends? How best can we use these plots as aids for modeling and as props for qualitative discussions of phase equilibria? Are there patterns and trends that suggest important generalizations connected to the chemical natures of the species involved?

Early work suggests that there is at least a qualified "yes" answer to these questions. Malesinski proposed classifications based on the signs of g_E, h_E, and c_E; it is this simple idea that all subsequent schemes share. Kauer, Bittrich, and Krug used a plot of g_E vs. T s_E to display the then small g_E/h_E data base; they also proposed classifications and generalizations based on signs and mixture type. Gaube and coworkers employed a plot of g_E vs. h_E and also a modified diagram in which g_E is replaced by g_E + T s_E, where s_E is the combinatorial excess entropy. In these later efforts, the g_E/h_E data base comprised about 200 points.

Most recently, Shukla, Chialvo, and Haile studied the h_E vs. g_E and h_E/RT vs. g_E/RT diagrams. While no data were displayed, the authors discussed the classical-thermodynamic features of these plots for miscible and immiscible systems and also noted how molecular theory with different size and energy ratios for the intermolecular potentials can lead to various diagrams.

Since 1983, when the paper of Kohler and Gaube first became known to us, we have explored the use of excess-property diagrams for organizing data and for discussing observed property and phase behavior. The diagrams are particularly helpful as visual aids in the classroom. In fact, early experiences with them were so positive that they subsequently became vehicles for two comprehensive classroom projects in which students scoured the literature for excess-property data and then participated in the posing of explanations and generalizations based on the results of their searches. Thus, most of the coauthors of this paper are former Rensselaer students who participated in these exercises, and many of the data reported herein were gleaned by them.

Michael M. Abbott and John P. O'Connell are Professors of chemical engineering at, respectively, Rensselaer Polytechnic Institute and The University of Virginia. They share interests in thermodynamics and in chemical-engineering education. Their twenty co-authors are former BS, MS, and/or PhD students from Rensselaer who participated in the collection, evaluation, and organization of the data upon which this paper is based.

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Chemical Engineering Education
EXCESS-PROPERTY DIAGRAMS

At modest pressures, the excess properties of liquid mixtures depend only on composition and temperature. Isothermal data allow separation of these effects; many data are reported at 298 K. At this temperature, comparison among systems may be most representative at equimolar composition (the choice we make), but the way to display data still must be chosen.

The excess Gibbs energy, excess enthalpy, and excess entropy are related by

\[
g^E = h^E - T s^E
\]  

(1)

The experimentally accessible quantities are \(g^E\) (via activity coefficients from vapor-liquid equilibria) and \(h^E\) (from calorimetry and temperature variations of \(g^E\)). When these are measured or estimated at the same conditions, a value for \(s^E\) can be found at the same conditions (there is no entropy meter!). Equation (1) shows that only two of these properties are independent, so any pair from the set \(\{g^E, h^E, s^E\}\) can be used as the coordinates. The three types of diagrams \((g^E\) vs. \(h^E\), \(g^E\) vs. \(s^E\), and \(h^E\) vs. \(s^E\)) convey exactly the same information.

Equivalent to Eq. (1), we may write

\[
g^E_{RT} = h^E_{RT} - s^E_{R}
\]  

(2)

which suggests choices from the set \(\{g^E_{RT}, h^E_{RT}, s^E_{R}\}\) as alternatives with exactly the same information.

We favor dimensionless ("scaled") coordinates \((i.e., \text{pairs from the second of the above sets})\) for the following reasons:

- The quantity \(g^E_{RT}\) is the most natural dependent variable for phase-equilibrium applications, because \(\gamma^E_{RT}\) is a partial molar property with respect to \(g^E_{RT}\).
- The quantity \(h^E_{RT}\) is cleanly related to \(g^E_{RT}\) via the Gibbs-Helmholtz equation

\[
h^E_{RT} = -T \left( \frac{\partial (g^E_{RT})}{\partial T} \right)_{P, x}
\]  

(3)

- One can establish temperature-independent upper bounds for \(g^E_{RT}\) of a stable liquid mixture.
- By scaling, values for \(g^E\) and/or \(h^E\) at different temperatures are put on a more comparable basis.
- Experience shows that important generalizations and rules-of-thumb are more easily grasped and retained when expressed in dimensionless terms.

Again, which scaled coordinates should be used? For everyday work, we favor the first \((g^E_{RT} \text{ vs. } h^E_{RT})\) and the last \((h^E_{RT} \text{ vs. } s^E_{R})\), which we call "engineering" and "modeling" coordinates, respectively. Engineering coordinates represent experimental quantities; they facilitate discussion of phase equilibria, especially liquid/liquid equilibria (see Shukla et al.\cite{Shukla}). Modeling coordinates represent directly the enthalpic and entropic contributions to \(g^E_{RT}\); they facilitate explanations of system-to-system trends in \(g^E_{RT}\). Our goal in this paper is to present the data base we have accumulated and demonstrate the engineering patterns it shows. Thus, we will focus on the \(g^E_{RT}\) vs. \(h^E_{RT}\) diagram.

For convenience, we introduce the following notation for equimolar binaries:

\[
\begin{align*}
g &= g^E_{RT} \\
h &= h^E_{RT} \\
s &= s^E_{R} \\
c &= c^E_{R}
\end{align*}
\]

At \(x_1 = x_2 = 0.5\)

\[
\begin{align*}
g &= g^{E}_{RT} \\
h &= h^{E}_{RT} \\
s &= s^{E}_{R} \\
c &= c^{E}_{R}
\end{align*}
\]

Equations (2) and (3) then become

\[
\begin{align*}
\frac{\partial g}{\partial T} &= h - s \\
\frac{\partial s}{\partial T} &= -h \\
\frac{\partial c}{\partial T} &= c
\end{align*}
\]

(4)  

(5)

We also have, from classical thermodynamics,

\[
\frac{\partial h}{\partial T} = \frac{\partial s}{\partial T} = \frac{c}{T}
\]

(6)

and thus, by Eqs. (4) through (6), we have

\[
\frac{\partial h}{\partial T} = \frac{\partial s}{\partial T} = \frac{c}{T}
\]

(7)

Equations (4) through (7) are useful for analyzing the features of the \(g\) vs. \(h\) diagram.

According to Eq. (4), there are just six possible combinations of sign for \(\delta, h,\) and \(\bar{s}\). These are listed in Table 1. Each sign combination defines a region on the \(g\) vs. \(h\) diagram (see Table 1 and Figure 1). We number the regions from I (counterclockwise) to VI.

The diagonal line on Figure 1 corresponds to \(\bar{s} = 0\). In regions to the right of the diagonal (V, VI, Table 1: Definition of Regions on the \(\bar{g}\) vs. \(\bar{h}\) Diagram

<table>
<thead>
<tr>
<th>Region</th>
<th>Sign (\bar{g})</th>
<th>Sign (\bar{h})</th>
<th>Sign (\bar{s})</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>+</td>
<td>+</td>
<td>+</td>
</tr>
<tr>
<td>II</td>
<td>+</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>III</td>
<td>+</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>IV</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>V</td>
<td>-</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>VI</td>
<td>-</td>
<td>+</td>
<td>+</td>
</tr>
</tbody>
</table>

Figure 1. The \(\bar{g}\) vs. \(\bar{h}\) diagram.

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and I), \( \hat{s} \) is positive, and for regions to the left of the diagonal (II, III, and IV), \( \hat{s} \) is negative. Lines of constant (nonzero) \( \hat{s} \) are parallel to the \( \hat{s} = 0 \) diagonal.

In Regions II and V the signs of \( \hat{g} \) are predetermined by the signs of \( \hat{h} \) and \( \hat{s} \) according to Eq. (4). This is not so for the rest of the diagram. Consider Region I where \( \hat{g} \), \( \hat{h} \), and \( \hat{s} \) are all positive. According to Eq. (4), the sign of \( \hat{g} \) is ambiguous, but the definitions actually require that in Region I enthalpy dominates since \( \hat{h} \) must be greater than \( \hat{s} \). Similar arguments show that enthalpy also dominates in Region IV, while entropy dominates in Regions III and VI. (This pretty line of reasoning, used by Malesinski,[11] is purely classical and model-independent.)

So far, we have said nothing about magnitudes. How large is large? We begin with \( \hat{g} \), defining a "large" \( \hat{g} \) as one for which phase-splitting (here, LLE) is likely. In the simplest approximation (with \( g/RT = A x_2 x_3 \)), \( \hat{g} = 1/2 \) yields LLE; this model-dependent result constitutes a practical lower bound on \( \hat{g} \) for phase-splitting. A greatest upper bound for stability obtains for \( \hat{g} = x_2 = 0.6931 \ldots \), corresponding to the Gibbs energy change of mixing \( \Delta g \) being zero for an equimolar binary mixture. Values in the range \( 0.50 < \hat{g} < 0.69 \) are thus "large," with \( \hat{g} = x_2 = 0.69 \) chosen as the concrete limit on "largeness."

What of \( \hat{h} \) and \( \hat{s} \)? Suppose that \( \hat{h} = 0 \), as for an "athermal" solution. According to Eq. (4), if \( \hat{g}_{ab} = x_2 = 0.69 \), then \( \hat{s}_{ab} = -0.8 \). Thus \( \hat{s} < -x_2 \) is an "large" negative \( \hat{s} \). In fact, if \( \hat{s} < -x_2 \), \( \hat{s} \) must be negative to produce a stable liquid mixture. (Notice that the entropy change of mixing \( \Delta s \) is negative for \( \hat{s} < -x_2 \). This perhaps counterintuitive, but occasionally observed, behavior suggests "unusual" phenomena in action.)

Suppose that \( \hat{s} = 0 \), as for a "regular" solution. According to Eq. (4), if \( \hat{g}_{eq} = x_2 = 0.69 \), then \( \hat{h}_{eq} = x_2 = 0.69 \). Hence \( \hat{h} = x_2 \) is a "large" positive \( \hat{h} \); if \( \hat{h} > x_2 \), \( \hat{s} \) must be positive to produce a stable liquid mixture.

We thus establish \( \hat{g} > x_2 \), \( \hat{s} < -x_2 \), and \( \hat{h} > x_2 \) as criteria of "largeness"; this is about as far as purely classical reasoning can take us. The missing bounds (practical lower bounds on \( \hat{g} \) and \( \hat{h} \), and a practical upper bound on \( \hat{s} \)), if they exist, must be supplied by Nature.

The temperature dependence of the excess properties for a given mixture defines a trajectory on the \( \hat{g} vs. \hat{h} \) diagram. Figure 2 shows a few examples. Some kinds of trajectories are forbidden. For example, Eq. (5) requires that \( \hat{g} \) increase with \( T \) in Regions III, IV, and V (where \( \hat{h} \) is negative), and that \( \hat{g} \) decrease with \( T \) in Regions VI, I, and II (where \( \hat{h} \) is positive).

From Eq. (6), the sign of \( \partial \hat{s}/\partial T \) is determined solely by the sign of \( \hat{c} \). On the other hand, Eq. (7) shows that both \( \hat{c} \) and \( \hat{h} \) contribute to \( \partial \hat{h}/\partial T \). (We will show later that negative \( \hat{h} \) usually implies positive \( \hat{c} \), so both \( \hat{s} \) and \( \hat{h} \) normally increase with \( T \) for systems in Regions III, IV, and V.)

In any case, \( \hat{c} \) is important in the analysis and prediction of trends with \( T \) on the \( \hat{g} vs. \hat{h} \) diagram. Thus, we seek effective ways of graphically displaying data for \( \hat{c} \). (We will show later that a plot of \( \hat{c} \) vs. \( \hat{h} \) has advantages as an organizational and explanatory aid.)

**MIXTURE TYPES AND DATA BASE**

For organizing and discussing the data base, we (like many others) find it convenient to classify mixtures by "type." We use a coarse classification based on separate identification of the components as nonpolar (NP), polar but nonassociating (NA), or polar and associating (A). Here, "association" means association only by hydrogen-bonding—though other association mechanisms exist. Hence, by our convention, acetone/titrate/n-hexane is an NA/NP mixture, whereas ethanol/n-hexane is an A/NP mixture. Notice that this scheme gives us the same number of binary mixture types (six) as there are regions on the \( \hat{g} vs. \hat{h} \) diagram. (This handy six-
by-six mnemonic has no special thermodynamic significance.)

Data were collected in two separate sweeps of the literature. In the first effort we sought systems for which both $g_E$ and $h_E$ had been measured (or could be estimated) at or near to 298 K. In the second search, we also looked for $c_p$ data. Both primary and secondary sources were consulted.

Table 2 summarizes the makeup of our $g_E/h_E$ data; the data themselves are in an Appendix that is available from the senior authors (Abbott and O'Connell). In addition to the approximately four hundred organic and aqueous/organic mixtures classified in Table 2, equimolar $g_E/h_E$ data were found for twenty-two cryogenic mixtures at temperatures ranging from 0.9 K (helium-3/helium-4) to 184 K (ethylene/nitrous oxide and nitrous oxide/xenon). These data are also available and can be obtained by writing the authors.

Although the $c_p$ data base is reasonably large (ca. 350 different mixtures), the overlap of systems with the $g_E/h_E$ data base is relatively modest. In many cases, however, the sign of $c_p$ (if not the magnitude) can be unequivocally fixed by interpolation, by analogy, or by inspection of the temperature variation of the data for $h_E$. For example, available data show that $c_p$ is always positive for 1-alkanol/n-alkane systems at 298 K. Similarly, $c_p$ is always positive for solvating NA/NA mixtures. (Here, "solvation" means that strong unlike attractions occur even though association may not be found for one or both of the unmixed components.) Thus, we can define an "extended" $g_E/h_E/c_p$ data base comprising about 150 systems for which $g_E$, $h_E$, and either $c_p$ or its sign are known; it is summarized in Tables 3 and 4.

Before presenting our findings, we offer a few words of caution:

- **First**: We make no claims of completeness. This collection is largely the result of two classroom (i.e., time- and resource-limited) searches of the mostly post-1960 literature.

- **Second**: Our ground rules were to include only miscible mixtures of nonelectrolytes at temperatures near to 298 K. This delimits and biases the data base. Partially-miscible mixtures are, of course, of great concern to designers of separation processes, yet our collection excludes such systems.

- **Third**: Although the relative proportions of data for the various mixture types should reflect the relative numbers of available $g_E/h_E$ sets for these types, one must recognize that the kinds of systems reported actually reflect the individual and collective biases of thermodynamic experimentalists and their customers. As a result, some classes of mixtures have received disproportionately intense attention because of their interest to correlators and theoreticians, and not because they are particularly "representative" of Nature.

- **Fourth**: We note that many of the $g_E$ and/or $h_E$ values for 298 K are determined by extrapolation or derivation via the Gibbs-Helmholtz equation. Such estimates are of course better than no estimates at all, but they are, in the end, only estimates.

With these caveats in mind, we can briefly review the statistical makeup of our data collection. For the $g_E/h_E$ and extended $g_E/h_E/c_p$ data bases, mixture types are represented approximately as follows (see Tables 2 and 3 for details):

<table>
<thead>
<tr>
<th>Mixture Type</th>
<th>% of $g_E/h_E$</th>
<th>% of Extended $g_E/h_E/c_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NP/NP</td>
<td>23</td>
<td>27</td>
</tr>
<tr>
<td>NA/NP</td>
<td>25</td>
<td>18</td>
</tr>
<tr>
<td>A/NP</td>
<td>20</td>
<td>17</td>
</tr>
<tr>
<td>NA/NA</td>
<td>12</td>
<td>23</td>
</tr>
<tr>
<td>A/NA</td>
<td>14</td>
<td>11</td>
</tr>
<tr>
<td>A/A</td>
<td>6</td>
<td>4</td>
</tr>
</tbody>
</table>

Hence, about 65% of our mixtures contain a nonpolar...
species, 50% a nonassociating polar species, and 35% an associating polar species. Of the binary mixture types, A/A mixtures are the most poorly represented, accounting for only about 5% of the whole.

**PATTERNS AND TRENDS**

Figure 3 is a \( \hat{g} \) vs. \( \hat{h} \) plot for the complete \( g^\circ/h^\circ \) data base. Although this picture appears at first glance to be a scene from an experimentalist's nightmare, it (and its companion Table 2) delivers some important messages:

1. Regions I and II are very heavily represented, accounting for 48% and 24% of the data base: positive \( g^\circ \) and \( h^\circ \) are "the norm."

2. Region V is very sparsely represented. Nature appears to abhor the most inherently stable of liquid mixtures—the systems with negative \( h^\circ \) and positive \( s^\circ \).

3. Only 59% of our mixtures have positive \( s^\circ \), whereas 80% have positive \( h^\circ \). Thus, in a very gross statistical sense, the regular solution (\( s^\circ = 0 \)) is a better approximant to reality than is the athermal solution (\( h^\circ = 0 \)).

4. Negative \( h^\circ \) implies negative \( s^\circ \), and positive \( s^\circ \) implies positive \( h^\circ \) about 90% of the time. The converses are true only about half of the time:

\[
\begin{align*}
\text{Positive } h^\circ &\quad \Rightarrow \quad \text{Positive } s^\circ \quad (85\% \text{ valid}) \\
\text{Positive } s^\circ &\quad \Rightarrow \quad \text{Positive } h^\circ \quad (95\% \text{ valid}) \\
\text{Negative } h^\circ &\quad \Rightarrow \quad \text{Positive } s^\circ \quad (70\% \text{ valid}) \\
\text{Negative } s^\circ &\quad \Rightarrow \quad \text{Negative } h^\circ \quad (41\% \text{ valid})
\end{align*}
\]

5. Nature seems to provide some of our missing bounds for "largeness" of \( \hat{g} \) and \( \hat{s} \). Very approximately, according to Figure 3, we may consider \( \hat{g} < -0.4 \) and \( \hat{s} > 0.4 \) as additional criteria of "largeness." When combined with the criteria presented earlier, these bounds define the rectilinear region denoted by the dashed line in Figure 3. Systems falling outside this region may be considered "unusual."

Figure 4, the modeling plot of \( \hat{h} \) vs. \( \hat{s} \) for the complete \( g^\circ/h^\circ \) data base, without most of the "unusual" cases, conveys the same messages as Figure 3.

Ploets of \( \hat{g} \) vs. \( \hat{h} \)

It is instructive to examine \( \hat{g} \) vs. \( \hat{h} \) relations for each of the six binary mixture types. We do them in order of increasing molecular complexity

**NP/NP Mixtures**

These are shown by the open circles of Figure 3 (and separately in Figure 6 of the Appendix, available from the authors). The systems fall mainly in Regions I and VI; \( \hat{g} \) is small to modest in size, rarely exceeding 0.2 in absolute value. The Region VI mixtures mostly contain alkanes or other "inerts" of greatly different molar volume; here, the negative \( \hat{g} \) results from a relatively large positive \( \hat{s} \) ("entropy dominates"). The Region I mixtures mostly contain two alkanes or two aromatics of modest molar-volume ratio, or mixtures of an alkane with an aromatic hydrocarbon. Heat effects can be quite large for the alkane/aromatic systems, but these tend to be compensated by a large positive value of \( \hat{s} \), leading to small or modest \( \hat{g} \).

**NA/NP Mixtures**

These are shown by the triangles in Figure 3 (and separately in Figure 7 of the Appendix. Region I behavior is the norm ("enthalpy dominates"), but one finds occasional excursions into Regions II through V. Most of the latter cases are systems in which one of the substances is an aromatic hydrocarbon, a tertiary amine, \( \text{CCL}_4 \), or acetonitrile. Mixtures containing acetonitrile tend to fall in Region II; their location makes them appear to be "weak" relatives of A/NP mixtures (see below). Notice that for NA/NP mixtures, both \( \hat{g} \) and \( \hat{h} \) can be quite large.

Chemical Engineering Education
Figure 5. The complete $c^E/s^E$ data base for binaries at 298 K and equimolar composition.

A/NP Mixtures

Data for these systems are the crosses in Figures 3 (and are plotted separately in Figure 8 of the Appendix). All data fall in Regions I or II. The stronger associators (alcohols and carboxylic acids) tend to show Region II behavior when mixed with alkanes. Here, $s$ is negative and $\hat{g}$ is large and positive: so large as to lead to phase splitting in extreme cases. Mixtures of strong associators with aromatics exhibit smaller values of $\hat{g}$, owing to smaller negative, or even large positive, values of $s$. Mixtures of secondary amines with hydrocarbons behave similarly to NA/NP systems: $h$ and $s$ are positive and sufficiently comparable in magnitude so as to produce small to modest values for $\hat{g}$.

NA/NA Mixtures

As the diamond symbols of Figure 3 (and Figure 9 of the Appendix) show, these systems exhibit one of two general kinds of behavior, depending on whether the unlike species can solvate by hydrogen bonding. If solvation occurs (acetone/chloroform is the classical example), then $s^E$, $h^E$, and $s^E$ are all negative, and Region IV behavior obtains (open diamonds). If both species are proton donors or both are proton acceptors, then Region I or Region II behavior is common (solid diamonds). Quasi-ideal mixtures (very small $\hat{g}$, $h$, and $s$) are possible when the two species both have high effective polarity.

A/NA and A/A Mixtures

Data for the A/NA systems are the box symbols in Figure 3 (plotted separately in Figure 10 of the Appendix). A diversity of behavior is seen, but $\hat{g}$ is usually positive and is often large. Generalization is difficult because of the complex molecular effects in operation; association or electrostatic interactions between like molecules may be partially compensated by solvation between unlike species. Region III behavior is not uncommon, especially at low temperatures. Aqueous systems are the open boxes in Figure 3, principally in Region III.

The x symbols in Figure 3 (plotted separately in Figure 11 of the Appendix) show the very small data base for A/A mixtures. Association or solvation can occur between all pairs, sometimes leading to a near cancellation of polarity or association effects (as in many alcohol/alcohol mixtures), and sometimes not. No easy generalization can be made.

Relationships with $c^E$

Finally, we consider the excess heat capacity. The statistics in Table 4 suggest a strong correlation between the signs of $s^E$ and $c^E$. Thus a negative $s^E$ (or $c^E$) gives a positive $c^E$ (or $s^E$) about 90% of the time, while a positive $s^E$ (or $c^E$) implies a negative $c^E$ (or $s^E$) about 70% of the time:

- $s^E \rightarrow c^E$ (93% valid)
- $c^E \rightarrow s^E$ (91% valid)
- $s^E \rightarrow c^E$ (68% valid)
- $c^E \rightarrow s^E$ (73% valid)

Hence, we have the approximate equivalence

$$\text{Sign} (c^E) = -\text{Sign} (s^E)$$

Searching for correlations between the signs of $h^E$ and $c^E$, we find

- $h^E \rightarrow c^E$ (84% valid)
- $c^E \rightarrow h^E$ (91% valid)
- $h^E \rightarrow c^E$ (46% valid)
- $c^E \rightarrow h^E$ (31% valid)

Negative signs on $h^E$ (or $c^E$) imply positive signs on $c^E$ (or $h^E$) about 85% or more of the time, whereas positive signs on $h^E$ (or $c^E$) imply negative $c^E$ (or $h^E$) only about 40% of the time. Thus, we have the relatively strong implications that a negative $h^E$ (or $c^E$) gives a positive $c^E$ (or $h^E$). The converse statements are not generally true, however.

These arguments lead us to consider a plot of $\hat{c}$ vs. $\hat{s}$ (Figure 5). Quantitative judgments are aided if one adds to Figure 5 the dashed parity lines $\hat{c} = \hat{s}$ and $\hat{c} = -\hat{s}$. These lines, with the axes $\hat{c} = 0$ and $\hat{s} = 0$, divide the $\hat{c}/\hat{s}$ plane into Continued on page 77.
A BIOREACTOR EXPERIMENT FOR THE
SENIOR LABORATORY

MICHAEL L. SHULER, NAHEED MUFTI,
MICHAEL DONALDSON, RONALD TATICEK
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Many chemical engineering students are not exposed to biology through the standard curriculum. But the use of concepts related to biological reactors may be required of students since they apply not only to the bioprocess industries but also to problems in waste treatment and remediation of sites that are environmental hazards. One approach for introducing these concepts is to incorporate new examples within the existing curriculum, and the senior laboratory course offers an excellent opportunity to do just that. A biologically based experiment also provides a forum for introducing material that reinforces traditional chemical engineering principles.

The goals of our senior laboratory are given in Table 1 (based on a handout prepared by George Scheele). We will show that these goals can be met through experiments that test the oxygen transfer capabilities of two New Brunswick Scientific Bioflow III fermenters during one class period; we then examine the kinetics of yeast growth and the effects of ethanol inhibition for a batch reactor during a second class period.

STRATEGICAL APPROACH

In Cornell's senior laboratory course there are lectures, briefings before a new laboratory, and a report session. Experiments span two separate three-hour periods. Student groups consist of three students each, and a group comes to the laboratory the same days of the week for two consecutive weeks.

Because of the relatively slow response time of biological systems, designing experiments that will fit within two separate three-hour blocks is difficult. Bioprocess laboratory experiments at most universities require an extended one-day experience or make use of continuous culture devices requiring sampling over a period of many days. Our approach requires considerable prelaboratory preparation by the instructor and teaching assistant to circumvent this difficulty. By using two fermenters in batch mode, with cells already in exponential growth, and concentrating on transient responses to specific stimuli, students can acquire sufficient data to explore several important concepts.

Although we require that students practice good aseptic technique when taking samples from the reactor, we wanted a system that was sufficiently robust to minimize the consequences of any mistakes. Consequently, we chose a common yeast, Saccharomyces cerevisiae for the experiments. It grows well at low pH (4.0), and if inoculated at high cell density, it will dominate when another organism accidentally enters the reactor.

The goal in the first laboratory period is to determine volumetric mass transfer coefficients ($k_{L}$) for oxygen as a function of air-sparge rates and agitator speed. Two methods are used: unsteady-state with no cells and dynamic method with cells. During this first period, students also determine aerobic growth kinetic parameters and develop calibration curves for measuring glucose and ethanol.

In the second lab period, the effects of ethanol inhibition
on aerobic (oxygen present) growth kinetic parameters are tested. Four levels of ethanol are added to the fermenters: 15 g/L, 30 g/L, 45 g/L, and 60 g/L. Aerobic conditions are used since confounding effects from endogenously generated ethanol can be avoided. If this system were being used for ethanol production, it would be conducted under anaerobic conditions (no oxygen present). The three-hour period makes the use of anaerobic conditions impractical.

To rationalize the use of aerobic conditions, the students are given a scenario in which a two-stage process is envisioned. The first stage of the proposed process is to build up cell mass as quickly as possible using aerobic growth conditions, followed by a second-stage anaerobic fermentation to ethanol. One common method of scale-up is to hold \( k_{\text{la}} \) constant. This aspect justifies the first laboratory period; the second period is justified by requiring the students to suggest a kinetic expression that would account for the inhibitory effects of ethanol. The presumption is that such a kinetic expression could be applied to both aerobic and anaerobic growth situations.

A general introduction to biochemical engineering is given in two lecture periods focusing on oxygen mass transfer in fermenters and summarizing kinetic models for growth and inhibition. Students are given copies of a general review article on biochemical engineering written for physical scientists, an article on inhibition kinetics, and a part of a textbook describing oxygen transfer in fermenters. The topics covered in these two lectures are given in Table 2.

**APPARATUS AND PROCEDURE**

**Bioreactor System**

A diagram for the primary apparatus is shown in Figure 1. We use two New Brunswick Scientific Bioflow III fermenters with 3.3 L culture vessels, Phoenix Polarographic (Houston, Texas) dissolved oxygen electrodes, and Ingold (Wilmington, Massachusetts) pH probes. An IBM PS/2 Model 30 286 computer controls the two fermenters, and an Epson FX-850 (Torrance, California) printer prints out data at the end of the experiment. To simultaneously control the two fermenters and for data logging, we use the New Brunswick Scientific Advanced Fermentation Software Package. Standard set points are pH at 4.0, temperature at 30°C, and agitation at 250 or 350 rpm. Antifoam C (Sigma Chemical Company, St. Louis, Missouri) was added automatically. The working volume for each fermentor is 2.3 L.

We added a check valve in the gas-supply lines to allow

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**TABLE 1**

Objectives for a Senior Chemical Engineering Course

A. *In operating equipment, how to*
   - Judge response time: *i.e.*, bigger is slower to respond
   - Understand special properties or conditions: *i.e.*, flooding of a packed column
   - Develop an intuitive feeling for the behavior of chemical engineering equipment and the magnitude of process streams
   - Develop a feel for data that are reliable and data that aren't

B. *In interpreting the behavior of equipment, how to*
   - Apply the theoretical and empirical equations discussed in the lecture courses to real systems
     - Develop a sense of appropriateness
     - Recognize the limitations of theories
     - Unify material from previous courses
   - Treat data
     - Recognize the difference between independent and dependent variables; between theoretical and empirical equations
   - Develop the ability to arrange equations to analyze data
   - Develop the ability to interpret results

C. *In telling others what you have done, how to*
   - Use generally accepted conventions of written reports
     - Know the format for a good technical report, magazine article, or journal paper
     - Know the conventions of writing, such as consistent tense and person, proper paragraphing, pronoun-antecedent agreement, and correct spelling
     - Search for vague, overwritten, or unnecessary words and phrases, and to rectify problems
   - Use graphs and tables
     - To analyze data—to fulfill your needs
     - To convey ideas—to fulfill others' needs
   - Learn to synthesize the sometimes conflicting data and ideas at your disposal into a clear, logical report

**TABLE 2**

Lecture SubTopics

<table>
<thead>
<tr>
<th>The cell as a chemical reactor</th>
<th>Genetic engineering</th>
</tr>
</thead>
<tbody>
<tr>
<td>What are proteins and enzymes?</td>
<td>Batch growth kinetics</td>
</tr>
<tr>
<td>Simple enzyme kinetics</td>
<td>Kinetics of inhibition</td>
</tr>
<tr>
<td>Major intracellular components</td>
<td>Experimental methods to determine cell mass and number</td>
</tr>
<tr>
<td>The genetic code and the Central Dogma</td>
<td>Scale-up problems in bioreactors</td>
</tr>
<tr>
<td></td>
<td>How to determine ( k_{\text{la}} )</td>
</tr>
</tbody>
</table>

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for a rapid switch from air to nitrogen gas. Also, a "Y" after the flow meter and the use of clamps allowed the gas stream to be directed to either the sparger ring submerged in the liquid medium or to the headspace. For measuring \( k_a \) (with no cells present), nitrogen gas was sparged through the medium to remove oxygen; after oxygen is depleted the check valve can be used to switch to air only. Measurement of the dissolved oxygen upon re-aeration allows \( k_a \) to be calculated.\(^{[3]}\) A plot of \( \ln(C^* - C_L) \) versus time \( t \) yields a slope equal to \(-k_a\). \( C^* \) is the saturated level of dissolved oxygen, and \( C_L \) is the value of dissolved oxygen in the medium.

Cells are present for the dynamic method. In this method, air flow is stopped for a short period of time (the length of time depends on cell concentration and initial level of dissolved oxygen) and is then restarted before the dissolved oxygen drops low enough to alter cellular metabolism (e.g., below 10% saturation). The rate of oxygen uptake (or specific respiration rate) can be calculated from an oxygen balance during the period when no air is being supplied, and the \( k_a \) can be calculated from the re-aeration part of the response by including a correction for oxygen consumption by the cells.\(^{[3]}\)

A plot of \( C_L \) versus \( q_O_2 X + dC_L/dt \) has a slope of \(-1/k_a\) and is plotted from the data from the re-aeration part of the experiment. Here \( q_O_2 \) is the specific rate of oxygen uptake, \( X \) is the total biomass concentration. The product, \( q_O_2 X \), is determined from the rate of oxygen depletion when the air is off. Since oxygen transfer by surface aeration would invalidate these calculations, it is important to displace air in the headspace with nitrogen as quickly as possible. The check valve and "Y" in the gas line make it easy to switch from air sparging through the medium to nitrogen flow to the headspace to displace headspace air and to provide a nitrogen "blanket." Clearly, nitrogen sparging in the medium could not be used since oxygen removal from the medium would then be due to both cellular respiration and gas stripping.

Other pieces of equipment used in this laboratory include a spectrophotometer (Milton Ray, Spectronic 301; UV-visible wavelengths) and a bench-top shaker (New Brunswick Scientific Company, Edison, New Jersey; G24 Environmental Incubator Shaker).

**Organism and Medium**

The organism used was *Saccharomyces cerevisiae* Cuy8, obtained from Dr. Tim Huffaker's lab at Cornell. Most strains of *S. cerevisiae* (a yeast) would be acceptable. The composition of the growth medium was

- 10 g/L glucose
- 1.5 g/L yeast extract
- 4.8 g/L \( (NH_4)_2SO_4 \)
- 0.75 g/L \( KH_2PO_4 \)
- 0.24 g/L \( MgSO_4\cdot7H_2O \)
- 0.036 g/L \( CaCl_2\cdot2H_2O \) pH to 4.0

Medium was autoclaved at 121°C for 50 minutes in four 2L batches.

**Start-Up Procedures**

For the experiment to be completed in the allocated time, the fermentation must already be under way when the class begins. The inoculum is prepared by inoculating 100 mL of sterile medium in a 250 mL Erlenmeyer flask with silicon closure (for good gas transfer) using a loop of yeast from a colony on a Petri plate. Three flasks are used; they are incubated on the Model G24 shaker for 16 hours at 30°C and 350 rpm. The bioreactors were inoculated 4 hours prior to student arrival with 300 mL of inocula and 2 L fresh medium. This procedure circumvents the lag phase and ensures that the culture is in the early exponential growth phase. This procedure is critical if students are to complete the experiment within three hours.

Although the reactor itself should, in principle, be sterilized by autoclaving each day, we autoclaved the vessel for Monday's laboratory but did not autoclave for subsequent laboratory sessions. Rather, we emptied the vessel after the laboratory and cleaned and disinfected it with 70% (by volume) ethanol acidified to pH 2 with HCl. The low pH of the medium provides protection against significant contamination, and using a disinfection solution reduces the time and labor involved in laboratory preparation.

Another aspect of laboratory preparation is calibration of the dissolved-oxygen and pH probes using manufacturer protocols. The dissolved-oxygen probes are particularly sensitive to electrical interference and fouling by proteins and medium components.

**Assays:** We used two enzyme-based assay kits (glucose and ethanol) and directions for both were supplied by the manufacturer (Sigma Chemicals, St. Louis, Missouri). The assay requires a spectrophotometer capable of working at a wavelength of 340 nm. We immediately filtered samples from the reactor through a 0.22 μm filter (Millipore) at the end of a 10 mL syringe, and removed cells to prevent glucose consumption before the assay was complete.

We made optical density measurements at 660 nm, using unfiltered samples. Because of non-linearities in the relationship of optical density to dry weight, samples with O.D. > 0.300 were diluted with sterile medium. Sterile medium was used as the blank.

**LAB PERIOD OBJECTIVES**

The objectives of the first period are to measure \( k_a \) and base-line (e.g., zero ethanol) growth parameters. One fermenter is used exclusively for unsteady-state \( k_a \) measurements. Suggested conditions are two agitator speeds (250 and 350 rpm) and three air-flow rates (1.0, 2.0, 2.0, Chemical Engineering Education
and 4.0 L/min) at each agitator speed. Of course, this fermenter is not inoculated with cells.

We inoculate the second fermenter and use it to determine the maximum specific growth rate, substrate utilization rate, and specific respiration rate under aerobic conditions with no ethanol added. Additionally, we determine dynamic $k_{L,a}$ values for selected values of agitator speed and gas-flow rate corresponding to two of the conditions used in the unsteady-state experiments.

We inoculate both reactors in the second lab period, and we determine growth substrate utilization and respiration rates upon the addition of known amounts of ethanol. One reactor is challenged at 15 g/L ethanol, then 45 g/L, and the second reactor is challenged at 30 g/L and then 60 g/L.

**BRIEFINGS AND REPORTS**

For the briefing, we give the students a general statement of the problem along with the goals for laboratory periods one and two. We also provide selected instructions from the manuals for the New Brunswick Scientific Bioflow III fermenters, the enzyme assay kits for glucose and ethanol, and the Spectronic Model 301 spectrophotometer. A standard curve relating optical density at 660 nm to dry weight of the culture (developed by the teaching assistant) is also provided. We then introduce the students to the equipment and demonstrate the use of the software for fermenter control and data logging. We also demonstrate the use of Eppendorf pipetters since many of the students have not previously used them.

Based on this information, we then ask the student group leader to formulate an experimental plan and to assign duties to the other group members. Without this kind of good preparation it is impossible for the group to complete the laboratory on time.

We discuss problems in the experiments and the format of the report (written in some cases and oral in others) during the report session. We ask the students to calculate or to provide the following:

1. Calibration curves for ethanol and glucose
2. Sample calculation for $k_{L,a}$ from the unsteady-state method
3. Sample calculations for $k_{L,a}$ from the dynamic method
4. Calculation of $\mu$, the specific growth rate ($h^{-1}$), which is defined as
   \[ \mu = \frac{dX}{dt} / X \]  
   during the exponential phase of culture growth, where $X$ is the dry-weight concentration of cells (g/L)
5. Calculation of $q_{O_2}$ specific respiration rate ($mgO_2/g$ cells-h) for oxygen consumption. A value for $q_{O_2}$ $X$ is found using the procedure for dynamic $k_{L,a}$ and dividing this value by $X$ yields $q_{O_2}$.
6. Calculation of the specific glucose uptake rate, $q_{glu}$ (g-glucose consumed per g cells per hour). Note that
   \[ q_{glu} = \frac{dS}{dt} / X = \frac{dS}{dt} / X \mu = \frac{\mu}{Y_{X/S}} \]  
   where $S$ = glucose concentration in the growth medium (g/L), $t$ = time (h) and $Y_{X/S}$ is the yield coefficient or mass of cells formed per mass of substrate (glucose in this case) consumed.
7. Calculation of $Y_{X/S}$.

   Items 4 through 7 above are calculated from all experiments (0 to 60 g/L of added ethanol).

   Based on these calculations, each member of the group is expected to develop a correlation of $k_{L,a}$ with agitator speed and air-flow rate, and this correlation is compared to expected dependency of $k_{L,a}$ on agitator speed and air-flow rates. The expected dependency can be found from the combining expressions such as
   \[ k_{L,a} \propto P_{g}^{0.4} Q^{0.5} N^{0.5} \]  
   where $N$ = agitator speed (rpm), $Q$ is volumetric gas-flow rate (L/min), and $P_{g}$ is the power requirement in the aerated fermenter, with constant impeller diameter
   \[ P_{g} \approx \left( \frac{P^2 \cdot N}{Q} \right)^{0.45} \]  
   where $P$ is the power required in the unaerated fermenter, and with
   \[ P \propto N^3 \]  
   where Eq. (5) applies in the turbulent region.

   For the analysis of kinetics, the students test by fitting several possible kinetic expressions to the five available data points for $m$, $q_{O_2}$, and $q_{glu}$. We also asked them to comment on the possible effects, if any, on the yield coefficient.

   Many equations have been suggested to describe product inhibition. Three examples are
   \[ \mu = \mu_{max} \left[ 1 - \left( \frac{P}{P_{max}} \right)^n \right] \]  
   \[ \mu = \mu_{max} \left( e^{-k_{p}P} \right) \]  
   \[ \mu = \mu_{max} \left( \frac{K_{ix}}{K_{ix} + P} \right) \]  

   In the above equations, $\mu_{max}$ is the maximum specific growth rate ($h^{-1}$) and can be determined from exponential growth at zero ethanol concentration; $P$ is the extracellular ethanol concentration. Students evaluate $\mu_{max}$ from growth data during the first period (for the yeast used in these experiments, $\mu_{max}$ is about 0.4 $h^{-1}$). For these equations, we assume that the Winter 1994
dimensional space domain. The case of constant speed of for a finite time, but eventually they decay to spatially homo­

We obtained generally good results for determining k,a, particularly with the unsteady-state method. The kinetic data are more problematic since few data points are available due to the laboratory's time constraints. Further, the requirement for a high level of precision in biomass and glucose measurements is not met by every student group. Although the actual techniques are straightforward, careful attention to detail and sample handlings are required. Groups with fewer

CONCLUDING REMARKS

Equipment malfunctions, particularly with the dissolved oxygen electrodes, should be anticipated, and the techniques for preparing inocula should be followed consistently. Under some stress conditions, this strain of yeast can develop a pinkish pigment that can invalidate the optical density versus dry weight relationship.

We obtained generally good results for determining k,a, particularly with the unsteady-state method. The kinetic data are more problematic since few data points are available due to the laboratory's time constraints. Further, the requirement for a high level of precision in biomass and glucose measurements is not met by every student group. Although the actual techniques are straightforward, careful attention to detail and sample handlings are required. Groups with fewer than three students are unworkable as the students are too rushed for time to complete the assays carefully.

ACKNOWLEDGMENTS

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REFERENCES


REVIEW: Oscillations and Instabilities

Continued from page 17.

stationary states are calculated and analyzed, showing that steady-state multiplicity can occur also in this case. The effects of different kinetic mechanisms and boundary conditions on the multiplicity pattern and the stability of the steady-states are discussed.

In Chapter 10, the formation of stationary spatial patterns, the so-called Turing structures, is considered for the thermokinetic model, e.g., non-isothermal first-order kinetics. First, the homogeneous steady-state is evaluated and its stability character is determined. In the case where it is stable to spatially homogeneous perturbations and the ratio of mass and thermal diffusivities is sufficiently large, it is demonstrated that stable spatial patterns can form due to spatially inhomogeneous disturbances. On the contrary, when the uniform steady-state is unstable to spatially homogeneous perturbations (e.g., the corresponding well-stirred system exhibits limit cycle behavior), diffusion processes have no stabilizing effect. Spatial patterns can form and survive for a finite time, but eventually they decay to spatially homogeneous oscillations.

Chapter 11 deals with chemical traveling waves in a one-dimensional space domain. The case of constant speed of propagation is considered and its limitations are discussed. It is shown how quadratic and cubic autocatalysis produce traveling waves.

In Chapter 12, the broad issue of heterogeneous reactions is addressed. The aim of this chapter is only to show that also in this case, steady-state multiplicity and instability can occur due to non-linearities in the model equations. How these non-linearities can arise is discussed in some detail. In particular, the cases of activated adsorption, multi-site reaction mechanism and competitive chemisorption are considered. The chapter includes some examples of steady-state multiplicity and oscillations.

The last chapter of the first part of the book, Chapter 13, introduces the reader to the world of chemical chaos. After clarifying that more than two state variables are required for a continuous system to exhibit deterministic chaos, the authors turn to simple discrete mappings to illustrate the striking phenomenon of the Feigenbaum cascade. Then the periodic forcing of oscillatory systems is considered by illustrating some techniques for their analysis and some examples of their behavior. Subsequently, complex oscillations and chaos in autonomous systems are dealt with and the determination of the stability of limit cycles through the computation of Floquet multipliers is described. Examples are provided by a modified version of the autocatalator in an isothermal batch reactor and by two consecutive exothermic
reactions in a CSTR.

In the first chapter of the second part of the book, Chapter 14, the widely studied Belousov-Zhabotinskii (BZ) system, as an example of a solution-phase reaction, is considered. First, background information on the BZ oscillations, its chemical mechanism and its simplified three-variable model (e.g., the Oregonator) is given. Then the relaxation oscillations of the Oregonator are analyzed in some detail using the techniques developed in Chapter 5. The BZ oscillations in flow reactors are considered next, introducing the issue of bistability. The chapter is completed by the analysis of the minimal bromate oscillator, where the organic substrate is omitted.

Chapter 15 presents results for several gas-phase combustion reactions. In particular, hydrogen, carbon monoxide and acetaldehyde oxidations are considered.

Indeed, the book reaches the dual aim stated by the authors in the Preface. On one hand, it encourages more chemists "to be less afraid of mathematics" by guiding the reader through the colorful zoo of non-linear dynamics, using simple examples while avoiding the presentation and discussion of theorems in rigorous mathematical terms. On the other hand, those more familiar with the mathematical tools will find a new opportunity to appreciate the richness of "the chemical world" in terms of non-linearities.

The approach adopted throughout the book is rather pragmatic. A clear indication of this attitude is in an introduction to each chapter. It does not contain the usual list of material treated in the chapter, but rather a list of items which the reader should be able to accomplish "after a careful study of the chapter."

In presenting each new dynamic phenomenon, first a numerical example is presented in order to illustrate the physical picture, and then the mathematical tools for developing an exhaustive analysis are described. The reader is never involved in rigorous, high-level mathematical discussions, while the mathematical developments are reported in full detail. This permits smooth reading.

In the more complex area of spatially distributed reaction-diffusion systems, the emphasis is placed on the representation of the various possible dynamic behavior. The description of the mathematical tools needed for the their determination becomes inevitably more vague.

The effort expended in relating the mathematical behavior to the physico-chemical basis of the system is indeed remarkable. For this, the authors analyze in parallel two different models whose non-linearities arise from two different sources. In the autocatalator, which has been introduced and widely studied in the literature by the authors, the non-linearity is in the cubic autocatalytic step. This model has the merit, over the classical Brusselator and Oregonator, of providing probably the best compromise between simplicity and richness of dynamic behavior in an isothermal closed system. In the non-isothermal model, where two irreversible first-order reactions are considered, the exotic dynamic behavior arises from the interaction of the reaction thermal effects with the non-linear Arrhenius dependence of the kinetic constant.

On the whole, this book provides an easy and convenient entry into the difficult area of non-linear dynamics. While there are not many independent courses existing which could use this book as a text, it could certainly be used as a supplementary text for graduate-level applied mathematics and reaction engineering courses. It is most certainly a valuable reference for all who are interested in the dynamics of reaction processes.

**ChE book review**

**TEACHING ENGINEERING**

*by Phillip C. Wankat and Frank S. Oreovicz*  
*Published by McGraw-Hill, Inc., New York, NY; 370 pages, softcover $32.95 (1993)*

**Reviewed by**  
C. Stewart Slater  
Manhattan College

*Teaching Engineering,* by Wankat and Oreovicz, covers all aspects of teaching engineering and does it in a clear and concise manner. The text evolved out of an engineering graduate course on educational methods taught at Purdue University and a project funded by the National Science Foundation. Materials from the text have been successfully used in faculty-training courses given through the American Society for Engineering Education as well as through other organizations.

Although it is oriented toward helping a new faculty member to become an excellent and efficient teacher, the text can also be quite useful for any engineering educator, and can be used as the textbook for a graduate course for students who are considering teaching as a career. The text can be used by any engineering discipline and would certainly be suitable as a resource for faculty outside of engineering.

The book is written in a pragmatic "how-to" style. This method of concept-presentation allows an instructor to easily follow the points made on any of the various subjects. Educational philosophy is incorporated when appropriate, and extensive references are given for those who want more information on a particular topic. Each chapter is effectively divided into subsections and concludes with chapter comments, summary and objectives, homework problems, and references.

The first chapter, "Introduction: Teaching Engineering," Continued on page 43.
EXOTHERMIC CSTRs
Just How Stable Are The Multiple Steady States?

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This paper was prompted by a discussion with a colleague who has been teaching chemical reaction engineering for many years. During the discussion, mention was made of the fact that when there are three steady states in an exothermic continuous stirred tank reactor (CSTR), the upper one can be unstable. The colleague said that this is impossible, and he based his disbelief on the classic plot of the multiple steady states, shown in Figure 1. This particular plot was taken from Stephanopolous [1] but it appears in practically all the reaction engineering textbooks, probably starting with the book by Levenspiel [2].

This plot shows the curve of heat generated (A) and the line of heat removed (B) versus the temperature in an exothermic CSTR. The three steady states are the points of intersection (P₁, P₂, and P₃, Figure 1) of curve A and line B. Let's assume that the reactor is started at temperature T₁. At this point the heat generated by the reaction (Q₁) is greater than the heat removed (Q₂). This will cause the temperature in the reactor to rise, and the rise will continue until the upper steady state, P₃, is reached. It is easy to show, using similar arguments, that P₁ and P₂ are stable steady states and that P₃ is an unstable one. There is really no indication from this plot that P₃ could also be unstable.

We can conclude that the use of a plot such as the one in Figure 1 may lead to the misconception that the upper steady state in an exothermic CSTR is always stable, but the roots of this misconception are actually much deeper. They stem from the mistaken belief that one can rely solely on results of a steady state model to predict dynamic behavior. The steady state model can certainly provide some guidelines, but a dynamic model is needed to predict dynamic behavior.

It should be mentioned that there are textbooks (i.e., Westerterp, et al., [3] pg. 339) where dynamic analysis is discussed in detail, based mainly on the pioneering work of Aris and Amundson [4]. But in most reaction engineering courses, only plots such as the one in Figure 1 are mentioned.
We can conclude that the use of a plot such as the one in Figure 1 may lead to the misconception that the upper steady state in an exothermic CSTR is always stable, but the roots of this misconception are actually much deeper. They stem from the mistaken belief that one can rely solely on results of a steady state model to predict dynamic behavior.

as a practical means for analyzing CSTRs behavior. This should not be the case any longer. The introduction of user-friendly, interactive simulation packages which can solve nonlinear algebraic or ordinary differential equations (ODEs) has not only made the solution of dynamic nonlinear models possible but has even made it easy.

In this paper we will demonstrate the use of one such simulation package (POLYMATH) for analysis of the behavior of an exothermic CSTR. The POLYMATH package is a numerical simulation package to be used with IBM and compatible computers, and the current version (2.1.1 PC) is distributed by the CACHE (Computer Aids for Chemical Engineering Education) Corporation, a non-profit organization for disseminating educational computer programs among chemical engineering departments.*

POLYMATH has been used for almost a decade, and its structure and possible applications have been described in several publications.[5-7] From among the programs included in the package, the algebraic and ODE solver programs are the most useful for exothermic CSTR analysis. (The algebraic equation solver was described in detail in reference 5.)

The main advantage of the POLYMATH ODE solver over similar programs is that equations are typed in their mathematical form, and the user has to provide only information regarding the mathematical model (equations, initial, and final values). No technical information, such as integration method and step size, graph scaling, etc., has to be provided. After the equations have been entered, the computer time for solving even the most complicated problems is only a few seconds.

For non-stiff equations, POLYMATH uses either an explicit Euler's method or the fourth-order Runge-Kutta method for integration. Euler's method is implemented when the estimated integration error is less than 0.1 times the error tolerance. For stiff equations the implicit Euler method is used.

The structure of the rest of this paper is as follows:

• In the next section we introduce an example problem. It is essentially the same problem as Luyben presented.[8] The problem definition is reproduced for the reader's convenience.

• In the third section, different combinations of multiple steady states are demonstrated using a steady state model, while the fourth section deals with the analysis of the stability at different steady states, using the dynamic model.

• The model equations used for the reactor analysis are given in the Appendices, in a form suitable for use with the POLYMATH package.

EXAMPLE PROBLEM

The typical CSTR problems, in which a first order, exothermic reaction is being carried out is presented in many textbooks. We used a slightly modified form of an example presented by Luyben.[8]

An irreversible exothermic reaction \( \text{A} \rightarrow \text{B} \) is carried out in a perfectly mixed CSTR as shown in Figure 2. The reaction is first order in reactant A and has a heat of reaction \( \lambda (\text{BTU/mole A reacted}) \). Negligible heat losses and constant densities can be assumed. A cooling jacket surrounds the reactor to remove the heat of reaction. Cooling water is added to the jacket at a rate of \( F_j(\text{ft}^3/\text{sec}) \) and an inlet temperature \( T_{j0}^{\circ}\text{R} \). The volume of the reactor, \( V \), and the volume of water in the jacket, \( V_j(\text{ft}^3) \) are constant.

The reaction rate coefficient changes as function of the temperature according to the equation

\[
 k = \alpha \exp(-E/RT) \tag{1}
\]

The feed flow rate (\( F \)) and the cooling water flow rate (\( F_j \)) are constant. The jacket water is assumed to be perfectly

Winter 1994
mixed. Heat transferred from the reactor to the jacket can be calculated from

\[ Q = UA(T - T_j) \]  

(2)

where

- \( Q \) is the heat transfer rate in BTU/hr
- \( U \) is the overall heat transfer coefficient in BTU/(sec)(ft\(^2\))(°R)
- \( A \) is the heat transfer area

The parameter values for the process\(^8\) are shown in Table 1.

Taking into account that the inlet flow rate \( F_0 \) is equal to the outlet flow rate \( F \), we see that \( dV/dt = 0 \), and the mole and energy balances on the reactor and cooling jacket yield:

\[ \rho C_p V \frac{dT}{dt} = \rho C_p F_0 (T_0 - T) - \lambda V k C_A - U A(T - T_j) \]  

(3)

\[ \rho j C_j V_j \frac{dT_j}{dt} = \rho j C_j F_j (T_{j0} - T_j) + U A(T - T_j) \]  

(4)

At steady state these equations become

\[ F_0 (C_{AO} - C_A) - V k C_A = 0 \]  

(6)

\[ \rho C_p F_0 (T_0 - T) - \lambda V k C_A - U A(T - T_j) = 0 \]  

(7)

\[ \rho j C_j F_j (T_{j0} - T_j) + U A(T - T_j) = 0 \]  

(8)

In the third and fourth sections we will discuss the number of steady state solutions of these equation sets for the parameter values of Table 1.

**SOLVING THE CSTR STEADY STATE MODEL**

There are several ways to solve the steady state equations of the CSTR (Eqs. 6-8). The most obvious way is to solve the three equations simultaneously, but this option has the disadvantage that most solution algorithms will find only one of the solutions. If there are several steady states, some trial and error involving the initial estimates will be required in order to find all the solutions.

Another option, one which will indicate all the steady states, involves the preparation of plots similar to the one in Figure 1. To accomplish this, we first must solve Eq. (6) for \( C_A \) and Eq. (8) for \( T_j \). This gives us

\[ C_A = \frac{F_0 C_{AO}}{F_0 + V k} \]  

(9)

\[ T_j = \frac{T_{j0} + \beta T}{1 + \beta} \]  

(10)

where \( \beta = UA/(\rho j C_j F_j) \).

Next, we define heat generated \((Q_G)\) and the negative of heat removed \((-Q_R)\) as

\[ Q_G = -\lambda V k C_A \]  

(11)

\[ -Q_R = -[\rho C_p F_0 (T - T_0) - U A(T - T_j)] \]  

(12)

In order to change the temperature in the reactor continuously, a dummy differential equation

\[ \frac{dT}{dt} = 1 \]  

(13)

can be specified.

The set of equations consisting of Eq. (1) and Eqs. (9) to (13) can be typed into the POLYMATH ODE simulator. The form in which these equations are entered into POLYMATH is shown in Appendix A. (Note that in the appendix the notation "tr" is used for the temperature inside the reactor and "tin" for the feed inlet temperature.) The numerical values of the constants from Table 1 have already been introduced into these equations.

The plot obtained by using the numerical values from Table 1 is shown in Figure 3, above, which is very similar to Figure 1. The three steady states can be clearly identified as the points of intersections of the \( Q_R \) and \( Q_G \) curves, and the approximate temperatures at these points can be determined.

---

**Table 1: CSTR Parameter Values**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_0 )</td>
<td>40 ft(^3)/hr</td>
</tr>
<tr>
<td>( F )</td>
<td>40 ft(^3)/hr</td>
</tr>
<tr>
<td>( C_{AO} )</td>
<td>0.50 mol/ft(^3)</td>
</tr>
<tr>
<td>( V )</td>
<td>48 ft(^3)</td>
</tr>
<tr>
<td>( F_j )</td>
<td>49.9 ft(^3)/hr</td>
</tr>
<tr>
<td>( V_j )</td>
<td>3.85 ft(^3)</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>7.08 ( \times ) ( 10^{-10} ) hr(^{-1})</td>
</tr>
<tr>
<td>( E )</td>
<td>30,000 BTU/mol</td>
</tr>
<tr>
<td>( R )</td>
<td>1.99 BTU/mol °R</td>
</tr>
</tbody>
</table>

---

*Figure 3. Heat removed (1) and heat generated (2) as functions of temperatures when \( T_0 = 530 \) °R.*
The conditions can now be easily changed so as to get different combinations of steady states. By changing the reactor inlet temperature $T_0$, the heat removal line moves parallel to itself and one or two steady state conditions can be generated, as shown in Figure 4.

This is not the best way, however, to find the exact values of the variables at the various steady states. To do that we can rewrite Eq. (7) as a single nonlinear algebraic equation

$$f(T) = Q_0 - Q_\theta$$

This equation, together with Eq. (1) and Eqs. (9) to (12) can be entered into the POLYMATH nonlinear algebraic equations' solver program (as described in Appendix A). The results for all three steady states for $T_0 = 530 \degree R$ are summarized in Table 2.

### STABILITY ANALYSIS AND DYNAMIC SIMULATION OF THE CSTR

Once the steady states have been found, the most important factor is how stable they are. We usually prefer to operate the reactor at some particular steady state (most often at the one with the highest conversion), but instability at this steady state may cause many undesirable effects, such as highly oscillatory response to small disturbances, or drift to a different, less desirable steady state.

Stability at the different steady states can be determined by calculating the eigenvalues of the state matrix of the linearized model of the reactor. This method is widely taught in process dynamics and control courses, but is not mentioned in any of the reaction engineering textbooks. Using this method, the system of Equations (Eqs. 3,4,5) is linearized at the vicinity of a steady state. Once the state matrix which contains the multipliers of the state variables is constructed and its eigenvalues are calculated, the stability of a steady state solution is determined by the sign of the real part of the eigenvalues of the state matrix. If the real part is positive, the steady state is unstable; a negative real part indicates a stable steady state.

We have carried out such an analysis for the CSTR example which was discussed earlier. We used two different formulations of the problem. In the first formulation, we assumed pseudo steady state with regard to the cooling water temperature. That means that the differential equation, Eq. (5), was replaced by the algebraic equation, Eq. (10). The jacket's time constant is relatively small because of its small volume, with the result that steady state assumption reduces the stiffness of the problem and changes the result very little. We will henceforth refer to this formulation as the modified model.

In the second formulation, we used the basic set of equations, Eqs. (3), (4), and (5), and from this point on we will refer to it as the basic model. The calculated eigenvalues are shown in Tables 3 and 4.

For both formulations there is a positive real eigenvalue for the intermediate steady state, indicating that this steady

<table>
<thead>
<tr>
<th>Steady State</th>
<th>$T_0 (\degree R)$</th>
<th>$T_1 (\degree R)$</th>
<th>$C_\theta$ (mole/ft$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Lower</td>
<td>537.16</td>
<td>536.62</td>
<td>0.4739</td>
</tr>
<tr>
<td>2. Intermediate</td>
<td>599.99</td>
<td>594.63</td>
<td>0.2451</td>
</tr>
<tr>
<td>3. Upper</td>
<td>651.06</td>
<td>641.79</td>
<td>0.0591</td>
</tr>
</tbody>
</table>

**Figure 4.** Heat generated (1) and heat removed (2) as functions of temperature for various $T_0$ values.
state is unstable. There is also a positive eigenvalue for the upper steady state. In this case the absolute value of the positive eigenvalue is much larger in the modified model than in the basic model. That indicates that the upper steady state will be unstable when using both formulations, but the oscillations in the basic model will grow much slower than in the modified model.

These results can be verified by simulation. The equations that have to be typed into the POLYMATH ODE simulation program are shown in Appendix B for both the modified and the basic model.

Figure 5 shows the change of temperature inside the reactor when it is started up at the three different steady states. These plots were obtained using the modified model and show that the reactor operation is as expected from the theoretical analysis. The lower steady state is stable and the intermediate state is very unstable, meaning that the temperature starts to go down after about one hour and stabilizes at the lower steady state after about five hours. In the upper steady state the temperature first starts oscillating and finally goes down toward the lower steady state.

The upper steady state can be further analyzed by looking at the plot of heat generated versus temperature, shown in Figure 6. It can be seen that for both the basic and the modified formulation the heat generated creates a spiral form where the growth rate of the spiral is much smaller in the basic model. This is what is expected from the state matrix eigenvalue analysis, but this plot is completely different from the one in Figure 3 which was generated using the steady state model.

It is interesting to note that when it is integrated for a long enough time, the basic model will produce a limit cycle. This requires programs, however, that are "tuned" for integration of stiff equations for long time intervals with high accuracy, and POLYMATH is not adequate.

The conclusion from these results is clear: using a steady state model for predicting CSTR behavior at the upper steady state can lead to wrong conclusions.

Several additional questions can be asked. First, is the state matrix eigenvalue analysis really needed in order to investigate the stability at different steady states? The an-

### TABLE 3

<table>
<thead>
<tr>
<th>Steady State</th>
<th>1st</th>
<th>2nd</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Lower</td>
<td>-1.446, 0</td>
<td>-0.953, 0</td>
</tr>
<tr>
<td>2. Intermediate</td>
<td>-0.515, 0</td>
<td>3.504, 0</td>
</tr>
<tr>
<td>3. Upper</td>
<td>0.486, -2.86</td>
<td>0.486, 2.86</td>
</tr>
</tbody>
</table>

### TABLE 4

<table>
<thead>
<tr>
<th>Steady State</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Lower</td>
<td>-188.7, 0</td>
<td>-1.267, 0</td>
<td>-0.976, 0</td>
</tr>
<tr>
<td>2. Intermediate</td>
<td>-188.1, 0</td>
<td>-0.532, 0</td>
<td>3.049, 0</td>
</tr>
<tr>
<td>3. Upper</td>
<td>-187.7, 0</td>
<td>0.00746, -2.754</td>
<td>0.00746, 2.754</td>
</tr>
</tbody>
</table>

---

Figure 5. Temperature changes inside the reactor when started at different steady states, using the modified model.

Figure 6. Plot of heat generated versus $T$ in the upper steady state.
swers in most cases will be no. Dynamic simulation can be much easier and faster, and the real physical behavior of the system can be observed, as opposed to observing indirect indicators such as the eigenvalues.

Can the conditions in the CSTR be changed so that the upper steady state is stable in the three steady state regions? The reader can verify that such conditions exist by multiplying the feed flow rate ($F_0$) by three and repeating the simulation using the equations in Appendices A and B.

Is the instability of the upper steady state a result of the varying cooling water temperature, and could it be prevented if there were only two variables ($T$ and $C_A$)? The reader can verify that this assumption is not true by fixing the cooling water temperature at $T_j = 530\degree R$ and using the parameter values

$$F_0 = 40 \times 10 \text{ ft/hr} \quad \text{and} \quad \alpha = 2 \times 7.08 \times 10^{11} \text{ hr}^{-1}$$

instead of the values shown in Table 1. This set of parameters gives three steady states, with the upper one being unstable.

**CONCLUSIONS**

In this paper, we have demonstrated the applications of an interactive numerical simulation package for location and analysis of the steady states in an exothermic CSTR. We showed that the use of a plot of heat generated and removed versus temperature as the only means for analyzing the stability at the steady states may lead to wrong conclusions. Also, that using this type of analysis sends the wrong message to students, implying that they can rely solely on the results of steady state models to predict dynamic behavior.

We have also shown that dynamic simulation is preferred over other methods (such as state matrix eigenvalue analysis) for testing stability at the steady states because it is easy, it is fast, and the test is based on the real physical behavior and not on indirect numerical indicators.

**REFERENCES**


**APPENDIX A**

**Steady State Model**

Plotting Heat Generated and Heat Released versus Temperature and Finding the Steady State Solutions.

(1) $d(tr)/dt=1$
(2) $k=7.08 \times 10^{**10} \exp(-30000/1.99/tr)$
(3) $beta=150 \times 250/(62.3 \times 1.0 \times 49.9)$
(4) $tj=(530+beta * tr)/(1+betta)$
(5) $ca=0.5/(1+48 * k/40)$
(6) $qg=30000 * k * ca * 48$
(7) $tin=530$
(8) $rhocp=50 * 0.75$
(9) $qr=-(rhocp*40*(tin-tr)-150 * 250*(tr-tj))$

- To change feed temperature change tin value in equation (7)
- To find the steady state solutions change $Eqn (1)$ to:
  (1) $f(tr) = qg - qr$
  and use the algebraic equation solver program
- To change feed flow rate change the number 40 in equations (5) and (9) to the desired value
- To fix the cooling water temperature at $T_j=530$

**APPENDIX B**

Dynamic Simulation of the CSTR—Modified and Basic Models

(1) $d(ca)/dt=40 \times (0.5 - ca)/48 - k*ca$
(2) $d(tr)/dt=(qg - qr)/(rhocp*48)$
(3) $beta=150 \times 250/(62.3 \times 1.0 \times 49.9)$
(4) $tj=(530+beta * tr)/(1+betta)$
(5) $k=7.08 \times 10^{**10} \exp(-30000/1.99/tr)$
(6) $rhocp=50 * 0.75$
(7) $qg=30000 * k * ca * 48$
(8) $qr=-(rhocp*40*(530-tr)-150 * 250*(tr-tj))$

- To change feed temperature change $tin$ value in equation (7)
- To find the steady state solutions change $Eqn (1)$ to:
  (1) $f(tr) = qg - qr$
  and use the algebraic equation solver program
- To change feed flow rate change the number 40 in equations (5) and (9) to the desired value.
- To fix the cooling water temperature at $T_j=530$
- To check additional steady states use the values shown in Table 2 as initial values.
- To change the feed flow rate change the number 40 in equations (1) and (8) to the desired value.
- To fix the cooling water temperature at $T_j=530$
- To change from modified to basic model replace $Eqn (4)$ by the following equation:
  (4) $d(tr)/dt=49.9*((530-tr)+beta*(tr-tj))/3.85$
Random Thoughts . . .

MEET YOUR STUDENTS

5. Edward and Irving

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Raleigh, NC 27695-7905

The scene is a dormitory room, shared by two senior engineering students. Irving is hunched over his computer, looking at an open manual next to the keyboard, as Edward breezes in.

Ed: "Yo, Irv—shut it down and move it out...it's party time."
Irv: (Silence)
Ed: "Come on, ace—the brew is losing its head...up and away!"
Irv: "Chill out, Eddie—I'm trying to figure out how to install this upgrade on my operating system. Why don't you go on ahead and I'll get there later?"
Ed: "Right—just like last week, when you were going to get there in fifteen minutes and you never showed at all."
Irv: "I told you I got involved with the control homework and lost track of time...anyway, you know I don't enjoy these parties—you guys are lunatics."
Ed: "We can't be lunatics, we're engineers—we're all nerds, we solve differential equations for kicks, most of us wear glasses...besides, I knew the campus security guard wouldn't really call the police last Friday—he just likes to blow smoke. Here, I'll bet I can figure that out...a few line commands here, a couple of mouse clicks there, and we're off for the bright lights and the beautiful...
Irv: "Eddie, get your grubby hands off that machine and let me read the manual and do it right. Remember how you were going to help me program my VCR to record Star Trek last week, and you didn't need the instructions, and we ended up with a two-hour PBS special on pancreas transplants?"
Ed: "That was only because I..."
Irv: "And how about that physics lab where you shorted out the whole building? 'Let's just do it—lab manuals are for weenies,' he says, just before the explosion."
Ed: "Yeah, but don't forget whose crazy idea got a patent application on his summer job...your problem is you spend so much time studying about what you're planning to do and worrying about why it might not work that you never get around to doing it...but it's ok, read all night if you can stand it, I'm out of here...oh, and don't forget, I asked Jake and Marty and Amy and a couple of the others to get together here tomorrow to study with us for the design test."
Irv: "Dammit, Eddie, why do you keep doing this to me? You know I study better alone—besides, you have an attention span of about twenty seconds, and if those jokers are over here you can forget studying or anything else but..."
Ed: "No way—I'm really serious this time. I just like to have people around—keeps things from getting too dull."
Irv: "Too dull? You..."
Ed: "Later, my man. I'll save some foam for you..."
Irv: (Low growling noise)

Ed and Irv have been best friends since elementary school, and no one was surprised when they enrolled in the same engineering school and became roommates. What was surprising was that they became friends in the first place, since their personalities are polar opposites. Ed loves big parties, and even if he doesn't know a soul when he walks in, everyone knows his life story by the time he leaves. Irv, on the other hand, doesn't like parties at all except for small quiet gatherings of people he knows well. Privacy is a sacred concept to Irv and a relatively alien one to Ed. They react much differently when faced with unfamiliar tasks or situations. "Let's try this out and see what happens," says Ed, as he dives in. "Hold on—let's think it through," responds Irv, as he dips his toe in the water.

The two of them have dramatically different approaches to schoolwork. Irv puts on some soft music, arranges his books on his desk, and immerses himself. Even when Ed is there, puttering around the room, fixing himself a snack, watching TV, or even talking directly to Irv, Irv goes right on working, occasionally mumbling responses to questions he really didn't hear. Ed sometimes tries to work like that but can't do it; he's constantly up and down, making comments about what he's reading or asking Irv questions about it, and if he hears a conversation down the hall or suspects that one might be about to start, he's off like a shot to make sure he doesn't...
miss anything. He likes to see how others approach problems and to try out his solution ideas on them, and he drives Irv crazy by assembling crowds to study or work on homework assignments when Irv wants to work in solitude.

Edward is an extravert and Irving is an introvert. Although the popular ideas of these terms (the extravert is the one at the party wearing the lamp shade and the introvert is the one hiding under the couch) are exaggerations, they have some basis in reality. Extraverts tend to be gregarious and active; introverts tend to be reserved and contemplative. Extraverts are energized by being with people—the more the better—while introverts find it draining to spend much time with people they don't know well, and they may need to go off somewhere by themselves afterwards to recharge their batteries. Extraverts need to experience things to understand them; introverts want to understand them first.

Science and engineering require the strengths of both types—the thoughtfulness, capacity for sustained concentration, and desire for understanding of the introvert and the quick thinking, verbal fluency, and willingness to take risks of the extravert. Introverts may spend so much time thinking about potential difficulties that they never quite get around to trying out new ideas, while extraverts are comfortable with trial-and-error learning and will not wait too long to take action. Lacking the introverts' characteristic cautiousness, however, extraverts may get into trouble by jumping into things before thinking them through, and being less able to focus on one task for a long time, they are more likely to accept superficial problem solutions. Extraverts are well suited to jobs like technical sales and management that require strong interpersonal and communication skills and jobs like consulting and emergency troubleshooting that require quick thinking and responding, while introverts work better in areas like research and design that allow them to take information in, process it introspectively, and then respond.

While both extraverts and introverts can become excellent scientists and engineers, the usual way these subjects are taught—straight lectures, homework done individually, minimal hands-on experience—stacks the deck in favor of the introverts. Extraverts tend to have shorter attention spans and find it hard to maintain their focus in long lectures. They also do much of their best learning interactively—discussing, arguing, working out their ideas by bouncing them off others; if they are forced to work individually all the time, they lose their most effective learning tool.

Several instructional techniques make classes more effective and enjoyable for both extraverts and introverts. Give students several minutes of small-group exercises during each class period—answering or generating questions, solving problems, or brainstorming. These exercises give extraverts occasions for activity and introverts opportunities to reflect on the course material. Bring experimental demonstrations—preferably hands-on—into lectures (for the extraverts) and give minilectures on interpretation of experimental results in laboratory courses (for the introverts). Use interactive computer tutorials and simulations: extraverts will enjoy the active learning they provide and introverts will get practice in trial-and-error analysis in a relatively risk-free environment. Assign some homework to teams of three or four rather than to individuals. Some introverts may complain about having to work in groups, but the extraverts will appreciate getting to function in their preferred learning mode for a change, and both types will learn the course material better while improving their interpersonal, leadership, and communication skills.3

Epilogue: Ten Years Later. Following graduation, Ed went to work as a product development engineer in the polymer division of a chemical corporation and received several patents for new membrane formulations. After two years he decided that he enjoyed working with customers more than synthesis reactors and extruders, moved into marketing, and is currently associate marketing director in charge of international sales. Irv went to work for an environmental consulting firm, spent two years designing stack gas scrubbers, went back to graduate school for a PhD, and is now an associate professor at a large university not far from where Ed lives. They get together at least once a year. Ed always proposes making the rounds of his favorite bars with some drinking buddies he's sure Irv will like. Irv always looks pained, makes some reference to lunatics, and counters with a proposal to take in a chamber music concert or a poetry reading. Ed rolls his eyes in mock disgust, says something about "engineering nerds," and they compromise on dinner with their wives at a good restaurant and drinks afterwards at a quiet jazz lounge. They both thoroughly enjoy this routine and wouldn't think for a moment of changing it.

REFERENCES

1. Lawrence, G., People Types and Tiger Stripes, 2nd ed, Center for Applications of Psychological Type, Gainesville, FL (1982)
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 interns and coop assignments typify such experiences; however, reports of more unusual cases are also welcome. Description of 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, Texas 78712.

THE M.I.T.PRACTICE SCHOOL

Intensive Practical Education in Chemical Engineering

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One of the most satisfying engineering activities is to apply an appropriate blend of theory, intuition, and experience to the solution of a practical problem. In general, engineers learn their theory and principles in the academic classrooms and laboratories; they cultivate practical intuition and experience on the job. Naturally enough, it may be asked if the academic training should also include some practical development as well. The new engineer could then approach a first job with some knowledge of how it "really works." To this end, there exists a variety of cooperative education and industrial internship programs.

In this article, we will describe a unique program of practical education at the graduate level. The David H. Koch School of Chemical Engineering Practice (the "Practice School") is administered by the Department of Chemical Engineering at M.I.T. Students who are admitted to the Practice School spend a semester working at off-campus industrial stations. The semester at the stations replaces the conventional Master's research thesis. Upon successful completion of the Practice School, plus two semesters of graduate lectures in Cambridge, students are awarded the degree of Master of Science in Chemical Engineering Practice.

The Practice School stations are maintained at host companies, which provide office facilities and student tuition and stipend support. Each station is staffed by a Director and an Assistant Director (both faculty of the Department residing year-round at the station) and a secretary from the host company.

Practice School students work within the company, on the company's problems, using the company's resources and equipment, but they are not company employees—they work for academic credit under the guidance of the station faculty. They are given a good deal of responsibility for planning and execution of the work, rather than perfunctorily performing a predefined set of steps. For the host company, the Practice School is like a small consulting firm, working for company clients within a format designed to accomplish a great deal in a short time.

A BRIEF HISTORY

The Practice School is seventy-seven years old, and its continuous operation has been interrupted only by the two World Wars. It came about through the initiative of M.I.T. alumnus A.D. Little and the support of Chemical Engineer-

Barry S. Johnston has been Assistant Professor and Director of the Midland Station since 1992. He holds a PhD in chemical engineering from Northwestern University. Prior to coming to M.I.T., he worked in the chemical and nuclear industries.

Thomas A. Meadowcroft has been Assistant Professor and Director of the West Point Station since 1993. A Practice School graduate, he holds a PhD in chemical engineering from M.I.T., where his thesis was on distributed control systems.

Aleksander J. Franz was recently the Assistant Director of the Midland Station. A Practice School graduate, he is now a PhD student at the University of Michigan.

T. Alan Hatton is Chevron Professor and Director of the Practice School. He holds a PhD in chemical engineering from the University of Wisconsin. He conducts research in novel separation processes and interfacial phenomena.
ing Director W. H. Walker. Little, remembering his formative years in industry, sought to have industrial experience made available to students on a regular basis. With funding from George Eastman of Kodak, five stations were set up at companies in the northeastern United States.

In the early years, each host company provided a laboratory and workshop for its station, but presently the Practice School maintains no laboratories, and the students' time is devoted entirely to company projects. What has not changed is the residence of M.I.T. faculty at the stations and the practical nature of the work.

There have been some thirty host companies for the stations over the years. There are currently two stations: the Midland Station at the Dow Chemical Company in Midland, Michigan, and the West Point Station at Merck Pharmaceutical Manufacturing Division in West Point, Pennsylvania. A comprehensive history of the Practice School and its contributions to chemical engineering is available in a monograph by Mattill.11

HOW IT WORKS

Either between or after two semesters of graduate lectures on campus, a class of five to eleven students spends one semester in Practice School. These students all have Bachelor's degrees (about half from M.I.T. and half from other schools), predominantly in chemical engineering. They stay eight weeks at one station, have one week off, and then go to the other station for another eight weeks. At the end of this schedule, each student will have worked on four technical projects, contributed to eight written reports, delivered at least four talks, and led at least one technical team.

In the months before the students arrive at a station, the resident faculty solicit project topics from the host company, and together they prepare projects, each designed to occupy a team of students for four weeks. They also identify the company resources that will be needed to support the project. For each project, the faculty write a Problem Statement expressing the client's objectives and providing background information and a suggested strategy for the students. The students are divided into groups of two or three, and in each group a group leader is appointed.

A typical work calendar is shown in Figure 1. After an orientation to the company and the Practice School, each group receives a Problem Statement and is introduced to its client. By the end of the first week, each group submits a written Investigative Memorandum in which the students demonstrate their understanding of the problem, present relevant background information, and propose the method by which they intend to accomplish their objectives. The students must also exhibit a satisfactory understanding of the safety requirements of their project. In the associated Proposal Conference, one student from each group makes a formal oral presentation to the clients, faculty, and students. The Proposal Conference is a useful forum for review and modification of project plans.

One week later, another student from each group presents an oral Progress Report. By this time, significant progress is expected, and members of the audience often respond with valuable suggestions. With one week remaining, each group leader chairs an informal meeting of the group, the client, and the faculty in which the form and substance of the remaining work are negotiated and agreed upon. The project culminates in the writing of a Final Report (occasionally the size of a small Master's thesis) and the oral Final Presentation by the group leader. The faculty critique two preliminary versions of the report before accepting the final draft. A typical Final Report outline is shown in Figure 2.

The schedule is repeated for a second project, with new group assignments and leaders. At the conclusion of the two projects, the faculty give letter grades and evaluate each student with respect to technical ability, creativity, motivation and initiative, leadership, and communication skills.

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Figure 1. First-month Practice School calendar.
The students perform a similar evaluation of each other. For many it is the most thorough discussion of their strengths and weaknesses they have ever received. After a week's break, the students go to the next station for two more projects, following a similar schedule. Grading and evaluation at the second station are independent of that at the first.

The objectives of a Practice School project are deliberately ambitious. Students normally find they must work sixty to eighty hours a week. Careful planning of the work and effective organization of the group thus become crucial skills. Working in groups is often a new experience for the students. The group leader, in particular, can gain valuable experience in planning, allocating resources, encouraging the team, and making decisions. Each student has at least one turn as group leader.

The faculty attempt to keep abreast of the students' progress, challenge their thinking, supply information and suggestions, and direct them to resources. The students work as needed with a variety of host company personnel such as librarians, laboratory technicians, research scientists, technology specialists, computer experts, plant operators, and process engineers. Both faculty and students are bound by confidentiality agreements in their handling of the host company's information.

The students live in apartments that cost about as much as they would have to pay in Cambridge. To provide some diversion, the faculty arrange weekend activities that vary with the preferences of the individual class and can be as simple as dinner and a movie or as challenging as bicycling, cross-country skiing, or canoeing. During the weekend between projects there is time for an overnight trip to an area resort for skiing or sightseeing.

CASE HISTORIES

Consistent with the wide range of technologies and activities that fall within the province of chemical engineering, students in the Practice School may expect a diversity of work topics. The majority of projects involve an operating process, but the work may also include research, design, or simulation. Three case histories are described below, with the descriptions written to give a clear idea of the students' work while challenging the group thus become crucial skills. Working in groups is often a new experience for the students. The group leader, in particular, can gain valuable experience in planning, allocating resources, encouraging the team, and making decisions. Each student has at least one turn as group leader.

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CASE 1: Refrigerated Separation

Figure 3 shows a continuous separation process. The column feed and overhead streams are cooled by a cascade refrigeration unit that provides coolant at two temperatures, the higher for the feed cooler and the lower for the condenser. The clients wanted to increase production at an upstream reactor and felt that the column and refrigeration unit were limiting.

The students began by determining the material and energy balances. They obtained flows, temperatures, and pressures from plant instrumentation and requested chemical analyses of several streams, using this information to develop and validate an ASPEN PLUS model of the process. A check of the column temperature profile suggested that little separation was being achieved in the upper portion of the column. After performing staging calculations, the students concluded that the reflux ratio could be reduced without affecting the overhead purity, as shown in Figure 4. This would reduce the load on the refrigeration system as well as increase column capacity.

The students then analyzed the operation of the refrigeration unit. They quantified the split of refrigeration capacity between the two sides of the cascade, showing that the overall capacity is increased as the cooling is diverted from the lower to the higher temperature side. The column staging calculations indicated that more feed cooling and less overhead condensing would not adversely affect the separation. Hence, they recommended operating conditions that increased both column and refrigeration capacity.

Beyond the immediate production increase from changes in operating conditions, the students also estimated the capacities of several heat exchangers, both within the refrigeration unit and associated with the column. From this they provided the clients with a list of equipment upgrades to allow further production increases. Furthermore, the students traced the service piping and recommended valve settings that would improve coolant distribution without requiring hardware modifications.

With the client's permission, the students supervised a plant trial to test their recommendations. Following the students' instructions, the plant achieved a record production rate while maintaining product specifications.

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**Figure 2. Table of Contents from a typical Final Report**

*Chemical Engineering Education*
Case 2: Reactive Batch Distillation

A product is made by sequential substitution at active sites

\[ A - B_3 + 3C \rightarrow A - C_3 + 3B \]

The batch process is run in a steam-heated kettle, and volatile compounds are separated in an overhead still. After an initial distillation to remove by-product B, the kettle is run under vacuum to remove excess reactant C, which is then recycled to the kettle to begin the next batch. Sharply increased demand for the product necessitated a production increase. In addition, there were unacceptable variations in product consistency from batch to batch.

The students approached the problem in three ways. One student began laboratory experiments to generate a consistent set of kinetic data; another attempted to model the batch distillation using BATCHFRAC software; and a third began reviewing the process operating data. It sometimes happens that an initial approach must be abandoned. In this project, the batch modeling was dropped and the students concentrated on process experimentation to effect improvements.

Chemical analyses allowed the unsteady material balance to be determined. The students discovered that by rearranging process steps, several non-productive steps could be omitted entirely. In particular, they could reduce the contamination of recovered reactant C with by-product B. They reached their conclusions from the scrutiny of process data coupled with basic stoichiometric calculations.

The students ran several trial batches in the process equipment to test their recommendations, which required some adjustment of sleep schedules to accommodate round-the-clock production. The simplified batch scheme increased the purity of recovered reactant C, which in turn improved product consistency from batch to batch. In addition, product yield increased. Hydraulic calculations indicated that the column pressure drop was significantly higher than expected. Subsequent examination of the column proved that the packing was crushed. The clients have realized significant production gains from the students' work. In addition, the students' kinetic data have proved useful to company engineers designing a new continuous process for the product.

Case 3: Quantitative Risk Assessment of a Storage Facility

A volatile and flammable chemical is stored in a refrigerated tank. The tank is protected from overpressure by rupture disks, but the clients were concerned that the protection might be inadequate, especially in case of fire.

The students examined the equipment and the safety procedures. They constructed fault trees leading to a BLEVE (boiling liquid/expanding vapor explosion) or a UVCE (unconfined vapor cloud explosion). They made heavy use of the literature, as well as interviewing plant safety organizations. From these sources they assigned probability values to the steps in the fault trees and thus derived the overall probability of each incident.

The students found and applied correlations for damage from projectiles, blast waves, and thermal radiation. They deployed the PHAST code to calculate the dispersion of the chemical in an atmospheric release and thus estimated the consequential damage to the plant and to the surrounding community.

Having specified the paths by which incidents could occur, the students identified several improvements to operating procedures and safety equipment. They designed a new pressure-relief system, using an in-house code. Heat transfer calculations led to recommendations for the number and placement of water deluge nozzles. From their risk assessment, they could express quantitatively the benefit to be gained from implementing each recommendation. The estimated probability of incident was reduced by two orders of magnitude. The final report was abstracted for inclusion in the host company's process safety guidelines.
THE BENEFITS

The Practice School is an educational program operated for the benefit of the students, but it can only continue if the host company feels that its money is being well spent. For the company, the Practice School provides teams of talented engineers who can mount energetic attacks on important tasks. During their relatively short stay in Practice School, students are undistracted by the multiple duties and concerns of regular employees and are able to direct undivided attention to the problem at hand. The focus and intensity of the students' efforts is often inspiring to company employees.

What the students lack in practical engineering experience, they sometimes make up for by a fresh approach to problems. Often the solution to a problem is found in the creative assembly of company resources. The students do make original contributions, and occasionally they demonstrate new techniques of analysis which are then picked up by the company. Company personnel who devote a few hours a day in supporting the student group can see their investment produce a significant amount of accomplished work.

Clients are generally pleased with the quantity and quality of the work. Responses to surveys in recent years indicate that 90% of the clients would like to have another Practice School project. Many prospective clients, however, fear that the students will require too much of their time, and this possibility is especially troublesome for oversubscribed production supervisors whose plants are running lean on personnel. While the short duration of a project is appealing to some clients, others have requested that projects be longer, or that less time be spent in writing and presentations.

Students attending Practice School may experience an unprecedented level of professional involvement. The host companies offer them important tasks; decisions will be made and money spent, based on their work. Students are excited to find that their efforts have resulted in significant cost savings or production increases; they acquire the confidence which follows the accomplishment of a demanding task. From observing other groups, they appreciate the variety of activities and applications of engineering.

While knowledge from academic classrooms is offered as separate subjects, a Practice School project is likely to require that this separately acquired knowledge be integrated. Thus the reactor performance may be limited by the heat exchanger area, and the distillation column fails because of reboiler piping. Furthermore, what the homework problems normally gave as background information now has to be obtained or estimated. The students must quickly assimilate and deploy procedures and software that may be new to them. Since different companies may use different tools for similar purposes, the students must adapt to what is available at each station.

The students benefit from working with experienced engineers and scientists at the host companies. This can give them a deeper understanding of particular technical concepts, practical details of equipment operation, shortcut design and estimation techniques, or a sense of what constitutes reasonable and realistic industrial practice. Experienced engineers can illustrate how problems are best approached and what to watch out for. The students may also observe the sorts of jobs available in industry, which may influence their own career decisions. In addition, the students have more access to faculty guidance than in the typical campus lecture course.

Finally, the students are able to improve their communication skills. Reports are not only written, but they also must be revised. The faculty are concerned with content and presentation, questioning the choice of verb as well as the accuracy of the energy balance. Each student's oral presentation is evaluated for delivery as well as for composition. Before each talk there is a faculty review of the visual aids, to assess both the organization and the clarity of the material. The Informal Progress Report offers a chance to improve meeting skills. Working in groups, the students gain practical knowledge of interpersonal relationships, sometimes under stressful circumstances. The experience of being a group leader is particularly motivating to previously shy or reserved students.

CONCLUSION

The intensity of the Practice School would be impractical to maintain for more than a short time—students can find the experience exhausting. Each group has written and revised two documents and prepared three oral presentations each month; they have often had to adjust sleep schedules to follow production runs; they have met and listened and read and discussed and debated and calculated and defended until they want no more.

Appreciation of the benefits seems to grow with time. Practice School graduates have been particularly strong in their subsequent support of the program and the Department. Students later tell us that through the Practice School they gained a sense of how much can be accomplished, how decisions can be made from incomplete and contradictory information, how scarce resources can best be allocated, and how new information can quickly be assimilated.

The Practice School does not pretend to be the only way to learn; however we are confident that its contribution to chemical engineering education is unique and valuable.

REFERENCES


set the tone for the book by describing the importance of teaching. An overview of the components of good teaching is presented along with a list of learning principles.

Chapter 2 focuses on efficiency, which is important for faculty in both teaching and research. Since most faculty have a myriad of responsibilities, this chapter helps by dealing with topics such as setting goals, establishing priorities, and maintaining "to-do" lists, so that efficiency can be increased.

Chapter 3, "Designing Your First Class," is an excellent step-by-step guide for any new assistant professor and leads the reader into the following chapters for more detailed information. Course objectives and textbooks are the subject of Chapter 4; the topics include taxonomies of educational objectives, teaching approaches, textbook selection, and addressing ABET course requirements.

Chapter 5 covers problem solving and creativity, both of which have been the focus of many engineering studies over the years. Development of effective problem solving strategies is very important to an engineering student's success and the subject is concisely presented here. Teaching students to be creative is also addressed. This chapter has a particularly thorough reference listing.

Chapter 6 describes lecture format and style. Since lecturing is by far the most popular style of teaching engineering, this chapter is quite important—improving one's lecture style significantly benefits any course. The chapter treats topics such as the advantages/disadvantages of lecturing, improving lecture content, organization, performance aspects, and interaction with students. The problem of how to effectively teach large class sizes is also addressed.

Chapter 7, "Nontechnological Alternatives to Lecture," presents some options to the lecture format, such as discussion, cooperative group learning, panels, debates, and "quiz shows,"—all of which are used in other educational fields. Independent study, mastery learning, and self-paced instruction are also covered.

"Teaching with Technology," Chapter 8, describes some of the delivery techniques useful to teaching. The delivery media profiled include television and video, and computers. The audiotorial method is also mentioned.

"Design and Laboratories" are featured in Chapter 9. Both topics are quite important to engineering education and are crucial to the accreditation process. Although they are not extensively covered in this chapter, they are effectively summarized. General aspects of incorporating design throughout the curriculum, as well as teaching design projects, are presented. Laboratory structure for different student levels is also reviewed.

Chapter 10, "One-to-One Teaching and Advising," covers listening skills, tutoring and helping students, and advising and counseling strategies. Proper advising of research students from undergraduates through doctoral candidates is presented.

Chapter 11 reviews the various aspects of "Testing, Homework, and Grading," while Chapter 12 explores "Student Cheating, Discipline, and Ethics." It is designed to assist faculty in preventing cheating and also addresses how to incorporate the subject of ethics into the curriculum.

"Psychological Type and Learning," Chapter 13, focuses on the natural differences among students which need to be considered when teaching plans are made and in the teacher's interactions with students. Both Piaget's and Perry's theories of cognitive development and their application to engineering education are presented in Chapter 14. Learning theories are explained in more detail in Chapter 15, which includes further discussion of learning and teaching styles, Kolb's learning cycle, and student motivation.

"Evaluation of Teaching" is covered in Chapter 16, and topics ranging from promotion and tenure to professional development are mentioned in Chapter 17. Information for graduate students interested in finding an academic position is presented in Appendix A, and a sample outline for a course on teaching is presented in Appendix B.

Overall, this is an excellent book. It brings together all the topics necessary for developing as a superb teacher. The authors incorporate a significant amount of material into the 370 pages and do so in a way that is easy to follow and to use for improving one's performance as an engineering educator. I am sure that students would want to see this book on the professor's required reading list for next semester!

UNIT OPERATIONS HANDBOOK
Vol. 1: Mass Transfer
Edited by John J. McKetta
Marcel Dekker, 270 Madison Ave., New York, NY 10016
$350 for set of Vols. 1 & 2 (1993)

Reviewed by
Scott Lynn
University of California, Berkeley

In the Preface, the editor of this handbook describes it as "up-to-date" and "presented by world authorities in their specialties." That statement is, perhaps, only half-accurate. Many of the contributors are certainly the grand old men in their respective areas—but the overside of the title page notes that the contents of this volume were previously pub-
The object of this column is to enhance our readers' collection of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested, as well as those that are more traditional in nature and which elucidate difficult concepts. Please submit them to Professors James O. Wilkes and Mark A. Burns, Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

DESIGNS TO DEMONSTRATE THE CRITICAL STATE

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Emphasis on design considerations has led to a critical state apparatus that is easier to fabricate and use than what has been offered in the literature. There, focus has been on CO$_2$ as the working fluid in capillary tubes.$^{[1,3]}$ When Halpern and Lin$^{[1]}$ followed the technique of Banna and Mathews,$^{[2]}$ their tubes "failed to demonstrate critical behavior." Halpern and Lin present an extensive experimental portion that convincingly conveys that their tubes work, but it is not clear whether this is due to usage technique or fabrication technique. The previous two papers, as well as one by Smith and Boyington,$^{[16]}$ all basically use a capillary-fill technique that involves introducing CO$_2$ gas and then condensing it with external liquid nitrogen cooling. Smith and Boyington also do a solid CO$_2$ load, but this is generally regarded as unsatisfactory due to difficulties of quantifying granular solid CO$_2$ volumes.

DESIGN ISSUES

The essence of design, compared to, say, analysis or synthesis, is the open-endedness of the question. It is recognized at the outset that multiple solutions to a design problem could work, and at least several should be initially considered. Contrast that philosophy to the uniformity in the scope of the three cited papers—their exclusive consideration of CO$_2$, for example, may be due to the oldest paper in the series$^{[3]}$ or to a physical chemistry laboratory text.$^{[4]}$ Perhaps the roots of influence go back even further. Moore$^{[5]}$ begins his discussion of the critical region by pointing out that the first gas to be studied in the critical region was carbon dioxide—work done by Thomas Andrews in 1869. Dodge$^{[6]}$ implies the industrial importance of CO$_2$ in the introduction to his chapter on refrigeration and reinforces that impression with an extensive section on solid carbon dioxide processes.

Design, on the other hand, should respect history and in this case might begin with the priority criterion to make critical phenomena visible, perhaps even to highlight the vanishing meniscus or "critical opalescence"$^{[7]}$ that occurs in transition through the critical state. Realizing that these effects could be expected in any critical state situation, one might find the question shifting: "What working fluids might have critical conditions most readily obtainable in the laboratory, and can they be made visible?"

Some working fluids with mild critical conditions are gaseous at ambient laboratory conditions and have a particular disadvantage in that special efforts are needed to handle them compared to solids or liquids. Thus, true to the genuine

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SAFETY

Critical pressures are above atmospheric and so safety from explosion must be considered in addition to toxicological safety. Pressures that will be generated can be calculated from a thick wall formula involving an inside and outside radius as well as a simpler thin wall capillary tube formula [8]

\[ S = \frac{R_0^2 + R_1^2}{R_0^2 - R_1^2} p_1; \quad S = \frac{p_1 D^2}{2 t} \]

(1)

where

- \( S \) = maximum stress that may be experienced in the tube material
- \( R_o \) = outside tube radius, 3.5mm
- \( R_i \) = inside tube radius, 0.75mm
- \( p_1 \) = pressure inside the tube
- \( D \) = tube diameter, equal to 2 \( R_o \), 7.0mm
- \( t \) = tube thickness, equal to \( R_o - R_i \)

For the 7-mm capillary tubes used and with the 33.7 bar critical pressure of n-pentane as an example, the two formulas in Eq. (1) yield (with 1.0133 bar/atm and 14.7 psi/atm) comparable results of 536 and 622 psi, respectively, for the experienced stress. Perry's Chemical Engineering Handbook, pages 23-60, gives the maximum stress (a yield stress or close relative, modulus of rupture) of 6,000 to 10,000 psi for borosilicate (Pyrex) glass. This represents a safety factor of about ten and is intended to secure occasional mild excursions above the critical pressure.

FABRICATION

The "Safety" section above explicitly mentions the capillary, and the earlier sections hinted that a capillary glass tube was used. Thermal transport questions include: Can the capillary volume be heated uniformly and can molecules exchange, on the microscopic scale, between liquid and gas states, sufficiently to ensure quasi-equilibrium? On both points a spherical cavity might be best. Thus, if a capillary is used, shortness would be desirable. However, sufficient length should be provided so that definition of a meniscus is promoted and meniscus activity is easily followed.

The cited papers [1-3] produced capillary tubes of approximate respective lengths 20, 35, and 20 cm. It is not clear why the long lengths were used (since shortness is desirable) unless the manifolding arrangements in some way required it.

Our end product was a 10-cm capillary, and fabrication began by sealing one end of the capillary with a gas/oxygen torch used for glass blowing. The small portion of the other end was drawn out in a tapered neck. This made the sealing step easier and may have helped in the purging process. Presence of the slight restriction due to the tapered neck may have promoted arrest of backflow. The length of the tube was measured and the required (quantitative information follows) height of the liquid meniscus noted. At that height (with pure saturated vapor above it) the contents in the constant volume capillary will have the critical specific volume when heated to the critical temperature.

The detailed technique is to inject more than the required amount of liquid with a syringe through the capillary neck. Low toxicity fluids like n-pentane or diethyl ether will, at ambient, partially vaporize and purge the capillaries of all gases except the pure vapor. This purge continues until the correct liquid amount is obtained. The tube is then quenched in a cold bath, and the tube neck is sealed with a blob of molten glass and annealed with a second or two of reducing flame. With some practice, the slightly drawn neck is easily reheated, quickly and specifically, without disturbing the rest of the container. The molten glass blob at the end of a glass rod is applied with a tamping acting that again thickens out the previously slightly drawn neck. Previous wall thicknesses (or greater) upon which the safety calculations were based, can be achieved. Again briefly, Figure 1 illustrates the situation within a second of sealing. The shape of the drawn neck is indicated. Filling with the syringe has been straightforwardly accomplished. The tube is in its cold bath with flame and partially melted glass rod ready. The shape after the closure, tamp, and anneal steps is also shown. With

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**TABLE 1**

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<td><strong>Critical Parameters</strong></td>
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<td><strong>Fluid</strong></td>
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<tr>
<td>Carbon Dioxide</td>
</tr>
<tr>
<td>Isobutane</td>
</tr>
<tr>
<td>n-Pentane</td>
</tr>
<tr>
<td>Diethyl ether</td>
</tr>
<tr>
<td>111-Trichlorotrifluoroethane</td>
</tr>
<tr>
<td>Perfluoroethane</td>
</tr>
</tbody>
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* From Refs. 10 and 11; other from Ref. 7.
practice, one person of normal talent can perform the purge and seal step, but it is easier with two people.

**USAGE**

Since the working fluids have critical temperatures of about 200°C, tubes can be placed in a glycerol or silicone oil bath. (As an aside, another advantage of these working fluids over CO₂ is that special cooling, as with a fire extinguisher, is not required to rapidly cool from supercritical down to temperatures at the upper edge of the critical state. The ambient air and higher critical temperature here provide sufficient gradient for cooling, the point being to save time in the set up, demonstration, cool off, and take down.) Slow heating with stirring of the bath causes the tubes to move slowly through the critical state. These shorter tubes evidently have none of the mass transport resistance to equilibrium (and the attendant need to be rotated) noted by Halpern and Lin. This in itself is a significant simplification of procedure.

In cases where the critical composition is not obtained during fabrication, the meniscus slowly rises or falls until it disappears, which indicates a saturated liquid or saturated vapor condition, respectively, the temperature of which can be noted. Thus the saturation boundary ("steam dome") can be constructed directly on a temperature versus specific volume plot. Figure 2 shows this with our data. We have estimated the uncertainty involved in reading, simultaneously, the slowly rising temperature and the slowly moving meniscus. Specific volume, $v$, is found from room temperature liquid and vapor specific volumes $v_l$ and $v_g$, along with meniscus height, $h$, and the tube length, $L$, from the relation

$$v = xv_g + (1 - x)v_l; \quad x = \frac{h}{L - h} \frac{v_g}{v_l}$$

(Dividing the right side by the numerator yields Eq. 2.

The letter $v$, for specific volume, is just the reciprocal of the density; the gas and liquid densities are indicated, again, by the $g$ and $l$ subscripts, respectively.) Note that $M_g$ and $M$ are the gas and total mass, respectively, and that $h$ and $L$ refer to liquid height and total height in the closed capillary. Capillary cross-section is $A$. Some rearrangement of Eq. (2) yields the $L$ over $h$ ratio

$$\frac{L}{h} = 1 + \left( \frac{x}{1 - x} \right) \frac{\rho_l}{\rho_g}$$

The densities and quality must still be found. Quality can

![Figure 1. Illustration of the drawn neck, flame, and molten glass rod at the moment of quench and seal.](image-url)
be obtained from Eq. (2)
\[ v_c = x v_g + (1 - x) v_i \] (4)
The quantity 304 \( \times 10^{-6} \text{m}^3/\text{mol} \) can be combined with the 72 molecular weight to yield the critical specific volume, \( v_c \).
The Handbook of Physics and Chemistry (HPC) value for the liquid density, about 0.63 g/cc, agrees well with the Rackett equation:
\[ v_1 = v_c Z_c^{-(1-\gamma)0.2857} \]
of 0.66 g/cc; where
\[ T_r = \frac{298}{466.7} \]
\[ Z_c = 0.262 \]
\[ v_c = 304/72 \text{ cc/g} \]

Iterative approaches such as the Redlich/Kwong approach could have also been used.

In addition to having a remarkably complete tabulation of quantitative thermodynamic property data, Smith and Van Ness also has a wealth of such information in the problems. On page 319, for example, Antoine's equation is given for n-pentane. It predicts to many places the saturation pressure, temperature pairs given on page 2378 of HPC. (That data would make a wonderful basis for constructing an Antoine-type equation. That is not our purpose here, but it could be included—students need to go through such an effort at least once in their career to appreciate correlations and other sources for such information.) The saturation pressure at, say, 25°C, could be used with the ideal gas law to find \( v_g = 503 \text{ cc/g} \), but we cannot expect this to be very accurate. It could be used as a starting value for an iterative scheme for a more accurate value. It is on the order of the 3-to-4 g/l that one might expect from Section 3-72 of Perry's Chemical Engineering Handbook, where ethane and butane are 1.4 and 2.6 g/l, respectively. n-Pentane is not listed there, but let us assume the 4 g/l value, or \( v_g = 250 \text{ cc/g} \). This could also be used in an iterative scheme (3 cycles with Redlich/Kwong yields 318 cc/g). With \( v_i = 1/0.63 \text{ cc/g} \) and \( v_c \) having the only value before calculated, Eq. (4) will yield \( x = 1.1\% \) with \( v_g = 250 \text{ cc/g} \) or \( x = 0.83\% \) with \( v_g = 318 \text{ cc/g} \). In either case, Eq. (3) then will lead to \( h = 0.37 \text{ L} \) when rounded to two significant digits.

Other issues could be pursued. We could start with Eq. (3) and form
\[ \frac{L}{h} = 1 + \frac{x}{1-x} \left( \frac{p_l}{p_i} - 1 + 1 \right) = 1 + \frac{x}{1-x} \left( \frac{1}{1-y} \right) \] (5)

We might like to ignore the gas-to-liquid density ratio here by considering the parameter \( y \) as unity minus the density ratio. Dropping the density ratio is introducing error into \( y \). Propagation of error (\( y \) approaching 1) in standard fashion
\[ \delta \left( \frac{L}{h} \right) = \delta \left( \frac{L}{h-1} \right) \]
produces a singular form, as would direct comparisons of exact and approximate expressions. The singularity can be cast in terms of densities, and l'Hopital's rule will close. Probing density uncertainties, however, might be more meaningful, with the characteristic form
\[ \frac{\delta (L/h)}{\delta y} = \frac{\delta p_l + \delta p_g}{p_l + p_g} \]

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**REFERENCES**
MATHEMATICAL MODELING OF AN EXPERIMENTAL REACTION SYSTEM

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Usually, one objective of a laboratory experiment is measuring the values of a dependent variable as it changes with an independent variable, or determining the values of some characteristic constants or parameters of a system. It is also useful to teach the students how to build up a mathematical model of the system under investigation and to think of possible analytical or numerical solutions to the model.

Models which describe the transient period of the system (e.g., start-up or shut-down) contain differential equations which can be solved either analytically or numerically (if the model is relatively complex). Steady-state models (with uniform dependent variables) usually contain algebraic equations.

The objective of this paper is to simulate the dynamics of a CSTR during different stages of its continuous operation. Mathematical models will be developed, along with analytical and numerical solutions, and together, these will be compared with experimental results.

A CLASSICAL EXPERIMENT

The reaction between ethyl acetate and sodium hydroxide in aqueous solutions is demonstrated in many chemical engineering labs. It is characterized by its constant density, and it is safe and easy to operate and analyze. The reaction rate is well established, and the mechanisms have been discussed in detail. The overall reaction rate is regarded as a second-order reaction, particularly at low temperatures.\[1-3]\]

In this study, the experiment is operated batchwise to determine the order of the reaction and the reaction-rate constant. These kinetic data are used to simulate the dynamics of the continuous mode operation.

SET-UP AND PROCEDURE

The saponification of ethyl acetate occurs quickly, so it is more convenient to measure the concentration by following the change in conductivity than to titrate aliquots since the latter need sampling, quenching (to stop the reaction in the sample), and back-titration.

In a batchwise mode and at zero time, one liter of sodium hydroxide (0.1 N) and one liter of ethyl acetate (0.1 N) are thoroughly mixed at room temperature (23°C). The conductivity is recorded at suitable intervals of time, and the concentration can be read from a suitable calibration curve. The order of the reaction and the rate constant can be deduced from these batchwise data by a suitable differential and/or integral analysis. Both methods give a second-order and a reaction-rate constant, \( k = 6.1 \text{ mol/min} \).

Continuous operation, which is the objective of this study, is illustrated in Figure 1. Solutions of sodium hydroxide and ethyl acetate (at equal concentrations) are pumped first to the head tanks (to eliminate fluctuations in flow rate caused by direct pumping to the reactor) and then to the reactor at suitable, but equal, flow rates. The speed of the stirrer is adjusted by the stirrer speed control, while temperature control is achieved through the heater temperature control and the cooling coil. The conductivity is recorded at suitable intervals of time. Notice that at zero time the reactor is empty. During the startup and filling of the reactor, both concentration and volume change with time until the reactor overflows; then the concentration will change with time until steady state is reached.

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MATHEMATICAL MODELS AND ANALYTICAL SOLUTIONS

Once students determine the order of reaction and the rate constant from the batch data and become familiar with the system, they are in a position to mathematically model and develop a transient analysis of the continuous mode operation of the stirred reactor. Three stages can be modeled:

1. From beginning to overflow
2. From overflow to steady state
3. Steady state operation

Obviously, the first and second stages are transient, while stage three is represented by a steady-state model. In this study, analysis is restricted to identical concentrations and flow rates of reactants. We let

\[ C = \text{molar reactant concentration in the reactors; mols/liter} \]
\[ C_0 = \text{molar reactant concentration in feed; mols/liter (M)} \]
\[ F = \text{flow rate; liter/min} \]
\[ k = \text{reaction rate constant; liter/mols-min} \]
\[ r = kC^2, \text{the rate of reaction; mols/min-liter} \]
\[ t = \text{time; min} \]
\[ V = \text{volume of the reacting system; liter} \]

**Stage One**

This stage is semibatch. There is no output because the reactor contents do not yet reach the overflow level. A material balance on either NaOH or ethyl acetate (both reactants are at the same concentration and flow rate) gives:

\[ \text{rate of accumulation} = \text{rate of input} - \text{rate of consumption} \]

Therefore

\[ \frac{d}{dt} (VC) = FC_0 - VkC^2 \]  

or

\[ V \frac{dC}{dt} + C \frac{dV}{dt} = FC_0 - VkC^2 \]

But \( V \) is a function of time, and since the system is of constant density and flow rate, a total mass balance gives

\[ \frac{dV}{dt} = F \quad \text{or} \quad V = Ft \]

since at \( t = 0 \), \( V = 0 \). Equation (2) then becomes

\[ Ft \frac{dC}{dt} + CF = FC_0 - Ft kC^2 \]

or

\[ \frac{dC}{dt} = \frac{C_0}{t} - \frac{C}{t} - kC^2 \]  

Equation (3) is subject to \( C = C_0 \) at \( t = 0 \). This equation can be solved using the substitution

\[ u = \exp(k \int C \ dt) \]

Equation (3) becomes, after some manipulation,

\[ t^2 \frac{d^2u}{dt^2} + t \frac{du}{dt} - kC_0 tu = 0 \]

which can be solved via Bessel functions by using the substitution \( z = t^{1/2} \). Equation (4) becomes

\[ z^2 \frac{d^2u}{dz^2} + z \frac{du}{dz} - 4kC_0z^2u = 0 \]

which is a modified Bessel equation, the general solution of which (in terms of \( t \)) is \[ u = A_1 I_0 \left( \sqrt{4kC_0t} \right) + B_0 K_0 \left( \sqrt{4kC_0t} \right) \]

where \( I_0 \) and \( K_0 \) are the modified Bessel functions of the first and second kind of order zero, respectively, and \( A \) and \( B \) are constants to be determined by the boundary conditions and the nature of the problem.

At this point, students can be asked to carry out several interesting exercises:

1. Perform the steps required to get Eqs. (4) and (5).
2. At \( t = 0 \), \( u = 1 \), greatly simplifying Eq. (6). Show that \( B \) must vanish.
3. We are looking for a relation between \( C \) and \( t \); thus Eq. (6) should be written in terms of \( C \).
4. If task 3 above is performed, it can be shown that

\[ C = \sqrt{\frac{C_0}{kt}} \left( \frac{I_1(2\sqrt{kC_0t})}{I_0(2\sqrt{kC_0t})} \right) \]

where \( I_1 \) is the modified Bessel function of the second kind of order one. This equation shows that \( C \) is not defined at \( t = 0 \), although at this initial time \( C = C_0 \). It is a good exercise for the students to show that this condition is implicitly
satisfied by expanding the modified Bessel functions, considering only the first few terms.

**Stage Two**

The second stage is continuous, but not yet steady. The concentration is changing with time but the volume of the reactants is constant. A material balance takes the form:

\[ \text{rate of accumulation} = \text{rate of input} - \text{rate of output} - \text{rate of consumption} \]

or

\[ \frac{dC}{dT} = FC_0 - FC - kVC^2 \]  

and therefore

\[ \frac{dC}{dT} = \frac{C_0 - C}{\tau} - kC^2 \]  

where

\[ T = t - \tau = \text{time in minutes} \]

\[ \tau = V/F = \text{time constant} \]

At steady state, \( C = C_s \), which is a particular solution to Eq. (9). Substituting

\[ C = C_s + \frac{1}{z} \]  

changes Eq. (9) to a linear first-order differential equation which can be solved by the integrating factor method. The final solution is

\[ C - C_s = \frac{1}{B \exp(AT) - \frac{k}{A}} \]

where

\[ A = \frac{1}{\tau} + 2 kC_s \]

\[ B = \frac{1}{C_i - C_s} + \frac{k}{A} \]

and \( C_i \) is the concentration at the beginning of stage two (e.g., at \( t = \tau \)).

Students can be asked to derive Eq. (11) by starting from Eqs. (9) and (10). It is interesting to check Eq. (11) at \( T = 0 \) and at steady state (e.g., as \( T \to \infty \)) and to think of a special form of the equation suitable for short times.

**Stage Three**

This is the easiest stage to model. A material balance requires that

\[ \text{rate of input} = \text{rate of output} + \text{rate of consumption} \]

or

\[ FC_0 = FC + Vr \]  

Therefore

\[ FC_0 = FC_s + kVC_i^2 \]

and

\[ k\tau C_i^2 + C_s - C_0 = 0 \]  

where \( C_s \) is the steady state concentration. If \( k \) is known, \( C_s \) can be predicted, or if \( C_i \) is measured, \( k \) can be calculated.

Notice that Eq. (13) can be derived directly from Eq. (9) where at steady state \( dC/dT = 0 \) and \( C = C_s \).

**NUMERICAL SOLUTIONS**

Numerical solutions are required whenever analytical solutions are not possible or are difficult to obtain. A suitable Runge-Kutta subroutine (e.g., IVPRK or DIVPRK from IMSL) can be used to solve the initial value problems, Eqs. (3) and (9). Concentrations from Eq. (7) can be calculated using IMSL special functions (DBSIO and DBSII). Equation (3) is not defined at \( t = 0 \), but it can be shown (by Taylor series expansion) that

\[ \left( \frac{dC}{dt} \right)_{t=0} = -\frac{1}{2} kC^2 \]

This condition should be considered in the numerical solution. Notice that the initial condition for stage two is that \( C = C_1 \) and \( T = 0 \) (or \( t = \tau \)), where \( C_1 \) is the concentration at the end of stage one.

![Figure 2](image1.png)  
**Figure 2.** Analytical and numerical profiles (perfectly matched) of reactant concentration for different initial concentrations.

![Figure 3](image2.png)  
**Figure 3.** Analytical and numerical profiles (perfectly matched) of reactant concentration for different initial concentrations.
Equations (3) and (9) were solved numerically and the solutions were compared to the analytical solution from Eqs. (7) and (11). Figures 2, 3, and 4 show these theoretical profiles for different cases of initial concentrations and for different values of rate constant \( F = 0.23 \text{ l/min}, V = 2.8 \text{ l} \). Notice that both numerical and analytical profiles coincide, i.e., they match perfectly. Both the analytical and the numerical solutions are compared to experimental results (shown in Figure 5) for the case of 0.1 N initial concentration, a volume of reactants of 2.5 l and a total flow rate of 0.24 l/min.

**DISCUSSION**

Continuous operation of the CSTR setup as shown in Figure 1 can serve several useful functions:

1. It can foster a realization of some practical problems, such as fluctuations in flow. A possible remedy is the use of head

\[ \text{Figure 4. Analytical and numerical profiles (perfectly matched) of reactant concentration for different rate constant values.} \]

\[ \text{Figure 5 Theoretical profile of reactant concentration as compared to experimental results.} \quad (C_0 = 0.1 \text{ M}, V = 2.5 \text{ l}, F = 0.24 \text{ l/min}). \]

Theoretical performance of the continuous mode operation is shown in Figures 2, 3, and 4. There is almost no difference between numerical and analytical solutions, as can be clearly seen from the figures. They match perfectly. This confirms the correctness of the analytical solutions.

Both solutions are compared with experimental results, as shown in Figure 5. A discrepancy between theoretical and experimental results is noticed in the initial period of the start-up operation. It is not difficult to predict, theoretically, the concentration at any time, but limitation of solutions in the reactor at the beginning of the start-up makes it difficult to accurately measure the concentration. Stirring during this initial period causes air bubbles, and this will affect the performance of the conductivity meter. A possible solution to this problem is to increase the flow rate (in new runs) or to measure the concentration using other means. Students should think of possible limitations to these solutions.

Students will find it interesting to consider the possible reasons for this discrepancy. They should first think of experimental errors and then check the assumptions of the model in order to think of new models, if they are required. They will quickly come to a realization of the difference between models and reality.

Another interesting point is the approach to steady state concentration. As can be seen from the figures, a steady state condition is approached asymptotically. Thus, depending on the significant figures required by the experiment, different values of experimental steady-state concentrations can be recorded, and they will represent a percentage of the theoretical steady-state value which can be achieved from stage three by using Eq. (13).

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**REFERENCES**

AN INTEGRATED DESIGN SEQUENCE
Sophomore and Junior Years

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The recent information explosion in science and engineering requires careful selection of what topics to present to the undergraduate. In the limit, as the amount of material covered in class approaches infinity, student comprehension approaches zero; the inverse is also true. Both limiting conditions are intolerable. It is important to back away from saturation coverage and to focus on the material that future engineers will need.

The future engineer will need to understand (analyze, optimize, synthesize, evaluate) the interaction of a series of steps that work together to achieve some desired result. The engineer (today and in the future) must be able to

- Work in teams to solve a problem
- Identify the need to know information
- Locate material to satisfy these needs
- Learn the content material
- Solve the problem with appropriate methodology
- Communicate effectively

The design sequence presented in this paper requires students to practice and develop all of these skills. They learn to recognize the interrelationship between courses; they learn that the courses are not isolated, only to be forgotten as soon as a grade is received.

Our faculty members agree that a common goal of producing graduates with the above skills is the most important aspect of our undergraduate program. Under the leadership of two or three faculty, all other faculty teaching the affected courses participate in the design projects. We discuss the undergraduate curriculum and adjust course emphasis if necessary; if an instructor feels that students do not have adequate mastery of a prerequisite subject, similar adjustments are made. We believe that any design project which requires students to learn for themselves, which demonstrates that engineering is more than a series of well-defined problems at the end of some chapter, which demonstrates that engineering knows no traditional course-work boundaries, and which forces students to synthesize material as it is learned, will benefit the student and, ultimately, produce a better engineer.

We recently introduced an integrated design project that spans the sophomore and junior years. A single chemical process design is analyzed, synthesized, and evaluated over the course of these two years. The first-semester sophomore project focuses on material balances and applies simple economic criteria based on the costs of raw materials, products, and by-products. Each subsequent semester requires additional knowledge, and by the end of the junior year the design yields an economic optimization of an improved process which the students synthesized and which required selection of operating conditions and sizing of chemical reactors, heat exchangers, pumps, compressors, separators, and recycle rates. The economics include both capital costs and operating costs such as pay-back period (time value of money is not introduced until the senior year).

These are group design projects that are integrated into
The rationale for this approach is uncomplicated. We want to prepare our students for a group senior-year design project, for a sequence of individual comprehensive problems required in the senior year, and ultimately, for a forty-year career in chemical engineering. These senior-year design activities are described elsewhere.\textsuperscript{2,3}

As a result of the design projects, students develop a number of personalized strategies for life-long learning—they learn self-evaluation and experience team work, they recognize the role of economics in decision making, they appreciate the need to understand basic principles, and they understand the various sources of engineering information. Since (group) oral and written reports are required most semesters, they also learn the importance of developing communication skills.

In addition to the direct impact on students, faculty are provided with the necessary input to assess student performance in their application of engineering principles. The feedback provided by the senior-year design projects affect the content of the sophomore/junior design projects. This is one mechanism we use to ensure that graduates meet minimum standards of knowledge and skills. The feedback directly measures learning and aids in curriculum development and improvement.

ABET is in the process of changing the design and engineering science requirements to eliminate the "bean counting" in favor of an "integrated design experience" throughout the curriculum, ending in a capstone course. The program described in this paper is one type of integrated experience which appears to satisfy these new criteria.

This paper will briefly summarize the design sequence, review some of the experiences the students had during the sequence, describe changes in student development, report on the "student culture" that has evolved, and attempt to explain why these changes took place. The paper will focus on the first-semester junior design for the 1992-93 year to illustrate how the process operates.

**REVIEW OF DESIGN SEQUENCE**

A single chemical process is the basis for the design sequence during the sophomore and junior years. Each subsequent semester's design requires additional knowledge and more detail, including mastery of the previous design. All chemical process designs used for this sequence are symbolized by a generic process block diagram (see Figure 1). These include four essential elements: a pre-reactor system, a chemical reactor system, a recycle stream, and a post-reactor system (i.e., one or more separation units).

![Figure 1. Generic chemical process](image)

We introduce first-semester sophomore students to a simple process flow sheet that includes a reactor, a separator, and a recycle stream. We give them cost data for feed and product streams; we provide several feed stocks and recycle rates and require the students to select operating conditions.

In the second semester we give the students a more complicated flow sheet that includes heat and work units. Utility costs are provided and are included in the evaluation. Students learn that heating, cooling, and power cost money. The advantage of high conversion at elevated pressures is offset by the high cost of running the gas compressors. This affects the selection of operating conditions. As the students' understanding of the process is enhanced, the quality of their decisions improves.

In the first semester of the junior year, we cover thermodynamics, heat transfer, and fluid flow. For the first time, students learn how to calculate the area of heat exchangers, to evaluate the work/heat requirements for systems of staged compressors with intercoolers, to determine the number of adiabatic (equilibrium) reactors in series, to handle the non-ideal behavior of gas mixtures, and to determine the size of process piping. All of these studies are needed for the new design. For the first time, capital costs are considered in the analysis. The optimum operating temperature and pressure changes because of this change in the objective function.

The final design in the second semester of the junior year differs in one major aspect. We do not give the students a flow diagram as a starting point. We provide kinetic information that yields different reactor performances and require the students to examine the separations units of the post-reactor system. Combining their experience from the previous designs with the new information on separations and kinetics, they synthesize a new, improved, process.

**Details of the First-Semester Junior-Year Design Project**

A few details, taken from the first-semester junior year, are presented here, and they illustrate the types of activities that result from the design sequence. Recent first-semester juniors involved in their third design continued their investigation of a process for the production of ammonia from synthesis gas. Figure 2 shows the process flow sheet provided...
to the students with the problem statement. It is a "caricature" chemical-process diagram and includes certain attributes that have been distorted. They are not tricks, nor are they necessarily realistic. They are often naive design choices meant to focus students' attention on a specific concept. Two examples are absence of any heat integration and compressing a vapor when pumping a liquid is possible. From this flow sheet, we expect students to discover a need to know more about separations and reaction kinetics to develop a credible design. This established groundwork for the following semester's content. The "caricatures" included in Figure 2 and the problem statement are:

1. High concentration of CO₂ in the feed
2. Questionable solubility data for CO₂ in liquid NH₃
3. Fixed reactor cost independent of temperature, pressure, concentration, and flow rate
4. Single-stage compressor for feed

Students started this design with valuable experience gained from previous projects with a somewhat simpler ammonia process flow sheet. They had discovered the high cost of gas compression and the effect of conversion on process profitability (that the higher conversions were obtained at lower temperatures and higher pressures). The problem statement had provided cost information on feed material, equipment, and a wide range of utilities along with introductory relationships for estimating the capital costs for major equipment units.

The students soon realized they were not able to evaluate chemical conversion for this new feed material and did not understand how to reduce the cost of compression. Also, the relationship for heat-exchanger costs required knowledge of the area, and they could not calculate the area. They could not deal with non-ideal gases. They had unmasked several "needs-to-know." These needs were satisfied by the concurrent class work.

Figure 3 is a composite design that represents the students' response to the project. The major characteristics are

- The reactor operated at low pressure (in spite of lower conversion)
- A three-stage compressor replaced the single-stage compressor
- A 3-7 stage adiabatic reactor with intercooling was used to obtain high conversion
- A single-stage condenser replaced the two-stage system
- High recycle rates were required.

While group solutions differed in detail, all the groups presented a modified flow sheet that was an improvement over the one they were given. They had all correctly identified the need for class content, had learned that content, and had applied it to the design. They had gained the confidence to challenge and to make changes to the original flow sheet.

Students are traditionally trained to mimic what they have seen and heard, but this seldom translates into an ability to make meaningful changes. Individually, they fear looking foolish—but as a group they are braver, more willing to express their ideas and opinions. Previously, they had probably had little practice in challenging things that were presented to them—the "caricature" problem helped them recognize that they can contribute better ideas.

Students wanted to use a chemical process simulator to perform the many required calculations, but prior to their junior year, our students are not allowed to use a simulator for class problems or projects. Having observed seniors working with the software, the juniors wanted to exploit this tool. Faculty encouraged them to use it whenever appropriate; however, no class time was spent in instructing students on its use. The juniors solved this problem by finding knowledgable colleagues (in this case, seniors) and asking them how to use it. In response, the seniors set up individual tutoring sessions and were available to help as needed. Given this self-discovered need-to-know, the juniors picked up the fundamentals quickly, gaining proficiency with practice. They took the initiative and learned what was necessary on their own. This is how our sophomores and juniors learn about plotting, spread-sheeting, and graphics software; no formal class time is devoted to these activities.

**ILLUSTRATIVE STUDENT EXPERIENCES**

In navigating a passage from the starting point represented by Figure 2, and the destination represented by Figures 3, students encountered many obstacles that had to be overcome. How the students hurdled these barriers is revealing. Some of their solutions follow:

![Figure 2. Ammonia (caricature) process flowsheet](image)
**Event 1.** Most design groups established a computer simulation as a first step. They studied the effects of changing recycle ratio, pressure, and temperature on the conversion. It was only after many hours (days) of toil that they considered economics and found that the system was an economic disaster. Unlike those groups, one group chose to consider economics first. They contrived what they labeled a "magic black box" containing a chemical process to produce ammonia. This box cost nothing to build and operate, it converted 100% of the limiting reactant to product, and all the energy released in the reaction was converted to steam that was sold at the highest value provided in the problem statement. This was the best conceivable case that satisfied a material balance; the simple analysis took little time and required no simulation. This group came directly to the conclusion that the system was an economic disaster.

The other groups did not focus on the goal and developed information on the performance of a system that could not possibly achieve the goal. They eventually came to the same conclusion, but they wasted significant time in the meantime. The professor had advised them to focus continuously on the goal (economics) and not to set it aside for later consideration, but the advice had little impact. When the one group presented their "little black box" concept to the class, the other groups realized (without being told or criticized) how they had wasted time by not focusing on the goal.

**Event 2.** The design problem, as originally stated, had no payback. The students were shocked! (This was probably their first experience with a totally unexpected result.) At this point the design objective was modified, with the new objective of minimizing losses. Students were also encouraged to suggest the maximum price that could be paid for feed material in order to get a positive payback and to consider any recommendation that would make the process profitable. The groups considered several alternatives to reduce the feed costs:

- Paying only for the reactants and not for the inert CO₂ portion of the feed
- Removing the CO₂ from the feed and selling it as a by-product
- A combination of the above

The "magic black box" analysis showed that there was a possibility of a five-year payback period if high yields and low capital costs could be achieved. Among the alternatives considered for making the process profitable were:

- Separating the CO₂, H₂, and N₂ from the purge stream and selling them all in pure state
- Reacting the NH₃ and CO₂ in the product gas to produce urea

The students found references showing that the composition of the product gas, the temperature, and the pressure are all appropriate for feeding directly to the reactor unit of a urea plant. Applying the "little black box" showed that there was an opportunity to obtain a reasonable payback period. It was now time to consider details on how to reduce the capital costs and increase the yield.

**Event 3.** Many groups recommended the removal of CO₂ from the feed, and the most common reason given for doing this was to reduce the amount of CO₂ in the product ammonia. Several groups concluded that the reduction in equipment and operating costs would be significant. One group found their way into the library and came up with flow sheets for ammonia plants showing a water scrubber that removed the CO₂ (they also found design information on the scrubber, but did not understand how to use it). Another group found out that CO₂ could not be tolerated in the reactor because it poisoned the catalyst—this uncovered the fact that no design would work unless the CO₂ was completely removed before the reactor or unless a new catalyst was found. The critical importance of catalyst behavior was identified.

It became evident to the students that their design was at risk until they understood more about reactor design and separations. The direction the students took at this point depended on their assumptions, but whatever direction they took, the merit of their design depended upon the validity of the assumptions they made. Until the assumptions were justified, their solution offered a higher-than-necessary risk of failure. To reduce the risk, students saw the need for future course content covering reactor design, separations, and the properties of the catalyst.

**Event 4.** The ammonia is removed in a partial condenser. This presented a major problem for the students. It required a condensable material to be removed from a non-condensing gas—a situation for which calculation of the heat transfer rate involves simultaneous heat and mass transfer considerations. Initially, the students thought they could not deal with this complex system because it was not included any-

**Figure 3.** Improved (student composite) ammonia flow sheet

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where in the curriculum. Once they recognized the problem and brought it to the attention of the faculty, however, it was added to the concurrent course material. The coverage of radiation and numerical solutions to unsteady state heat transfer had to be reduced, but this was not judged to be a serious problem.

This last event demonstrates that when a major problem arises, it can be taken care of by the faculty and the necessary principles can be added to the curriculum. For lesser problems which are brought to the faculty's attention, the students are referred to other sources of information (such as the seniors). Many smaller problems, however, are never even brought to the faculty's attention and are simply solved by the students on their own—obviously, a very satisfying development.

**DISCUSSION**

The design sequence represents a framework for the curriculum. Students need to know where their education is taking them and how the materials they study fit in—seldom do they simply accept the professorial assertion that, "Trust me, it is critical for you to know this material." After discovering the importance of course material on their own, students usually pursue an understanding of all course materials more aggressively. In other words, students who know where they are going are more likely to get there!

The goal of this comprehensive sequence is made clear to the students. They will be expected to learn how to analyze, design, and handle comprehensive chemical processes on their own; they are told that problems in their senior year and beyond, throughout their careers, will require this ability. They observe the effort the seniors put into these problems and understand that they, too, will at some point be presenting and defending their solutions before a panel of professors or supervisors.

Each semester begins with all the ideas from all the groups on the table. Then each individual group has to analyze this new information, rejecting the poor ideas and selecting those ideas that are worthy of follow-up. The teams listen to all of the other presentations, acquiring a good understanding of a variety of feasible solutions to their problem.

In our department, the program's effectiveness is enhanced by the department "culture." Graduates and seniors, excited about what they are doing, pass their enthusiasm on to the other students. Also, we find that motivation is not a problem if students can observe their progress toward a final goal. In a sense, our department may be viewed as a one-room schoolhouse; faculty offices, the classrooms, and the undergraduate computer room/work area/lounge are all on the same floor. In this close-knit setting, students can see that they are doing things that they could not do the previous semester, and that seniors are more capable than juniors and juniors are more capable than sophomores. The culture provides beneficial peer pressure as well as a student network where upper-level students support lower-level students.

Although the culture described above has existed in our department for many years, it is not a prerequisite to successful use of such coordinated design projects. If the projects are viewed by faculty and students as a coordinated framework for the curriculum, features of the culture will spontaneously emerge. A few faculty may become champions, but all will actively participate. Sophomores will seek assistance from juniors, who in turn learn from seniors.

It is not necessary to develop design projects from scratch. We seek new project ideas from colleagues in other departments as well as from those in industry and government. We recently got an idea from a departmental seminar speaker, and we have also obtained ideas from former students. Over the years we have developed several successful projects for the sophomore-junior sequence, and we would be happy to share them with others.

Questions often arise regarding the opportunity for students to free load and be carried along by the group. This has not been a problem—probably because of peer pressure and knowing that the time will come when each of them must appear alone to answer questions from a faculty or employer panel.

Introduction of the design sequence has not reduced the amount of course content provided. While our students still have ample opportunity to solve differential equations and integrate the Navier-Stokes equations, some changes in subject material were made. The major impact on course content was made previously when we decided to incorporate modest design activity in each course. The subsequent integration of the design into a single problem for each semester and to retain a single theme for the problems over four semesters was expected to reduce the time taken away from formal course work. The amount of time the students elected to devote to the design has increased and exceeded our expectations. There is some concern about the excessive time many students spend on these problems.

**CONCLUSIONS**

The integrated design process involves features that are largely overlooked (or dismissed), but which can significantly impact a students' overall development. Some of these features are

**Focus** • Students must focus on a goal. Once they understand what they are expected to accomplish, they can appreciate the process used to achieve the goal, the relevance of the course work, and the progress they have made toward that goal each semester.

**Group Projects** • Students benefit from group participation in the design sequence in several ways. Groups are more willing than individuals to express new ideas and to make
judgments. They find comfort in numbers and are less fearful of looking foolish. While individual students are unlikely to have sufficient experience to manage a design problem, the situation is different for several students working together. The sum is truly greater than the parts.

**Culture (One-Room Schoolhouse)** • Students benefit a great deal from observing the performance of other students at the same level as well as in the levels above and below theirs. It is obvious to them that the higher-level students can do what they cannot do, and that they can now do what they could not do earlier. Upper-class students can be a great help to other students in their courses, telling them what to expect in future courses and why they need to know the subjects they are studying.

**Need-to-Know** • Students are more motivated to understand and to retain knowledge and principles when their studies are the result of a sequence of events that begins with a need-to-know. The steps following the need-to-know are to gather information, learn the necessary principles, and apply principles to an original problem.

**Depth and Breadth** • It is essential that students be exposed to a wide range of knowledge. It is also essential for students to pursue some knowledge in depth and to understand how it is applied to the development of chemical processes.

All the items listed above have a common element: they require the student to take an active, rather than a passive, role in learning. Their design skills (not the subject of this paper) are significantly advanced by this process. Students' success in this program provides them with additional attributes resulting from focused participation in activities invariant with time—attributes that will serve them well throughout their professional careers.

**REFERENCES**


**REVIEW: Unit Operations Handbook**

Continued from page 43.

lished in *Encyclopedia of Chemical Processing and Design*, edited by McKetta and Cunningham, first printed in 1976 and reprinted at one- to two-year intervals through 1990. Many of the sections do not appear to have been updated since their first appearance. The most recent reference found by this reviewer in any section was from 1986; most of the sections cite nothing more recent than the 1970s. The section on batch distillation cites only a single reference that was published in 1958, while the section on packed towers short-cuts cites only material from two chapters in the 4th edition of *Perry’s Handbook*, which appeared in 1963.

As a result, many of the sections are seriously out of date. For instance, the section on absorption presents an overly long, highly empirical example for calculating steam stripping that makes no use of computer techniques. The section on packed column internals (as well as the introductory section on distillation) contains nothing about packings that have been introduced in the past decade. The section on the costs associated with gas adsorption cites the price of activated carbon that prevailed in 1977, which may or may not correspond with current costs when the M & S cost index is employed.

As is to be expected in a multi-authored handbook, the sections are uneven in quality. Many (but by no means all) of the sections are highly tilted toward petroleum processing. The section on estimating naphtha cuts in distillation, for instance, uses so much oil-company jargon that it is almost unintelligible to someone who wasn’t working in that area in the 1960s. A diagram of the VLE data for methanol/water shows a non-existent tangent pinch, and absorption is described as a purely physical phenomenon (despite the use of the alkanol amines to remove acid gases). To illustrate the separation of azeotrope-forming compounds by distillation, using benzene to break the ethanol/water azeotrope, a four-column sequence is presented even though the use of three columns is more common and two columns can do the job.

Some of the examples used to illustrate principles are curious: The case of an absorber with a pinch at the bottom tray is illustrated with a column in which an insufficient stream of pure water is used so that only a specified fraction of the SO2 is removed from a flue gas. No mention is made of the improbability of a) using water, with its low capacity for SO2, as the absorbent, or b) not using a stream of absorbent that is sufficiently large to shift the pinch point to the top tray when designing a scrubber to remove SO2.

In a similar exercise, natural gas is used to strip H2S from crude oil in a process deemed advantageous because it would be once-through for both the gas and liquid streams. No mention is made of the fact that the H2S will subsequently have to be recovered before the natural gas can be used for any other purpose, and that this requirement may make its use as the stripping medium somewhat less attractive.

Of course, much of the basic material on the key unit operations (adsorption, distillation, liquid-liquid extraction, crystallization, etc.) is timeless and can bear retelling by a master in the field. Nevertheless, one may question the value of a handbook of this type in which many of the sections are one to two decades out of date in the first year of its publication.
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In the first place, all men agree with the familiar maxim,
"If you don't have a thing, simulate it."

Desiderius Erasmus[1]

This early reference to simulation points up a certain ambiguity in our current use of the word. On one hand, a simulation (especially a computer simulation) tends to be regarded as a representation or prediction of the behavior of a real thing to a considerable degree of accuracy. On the other hand, the word can also mean making a pretense of — so a simulation could be a counterfeit or sham object. Error bars are usually lacking in the results of a simulation for process design, and this may fool us into believing that our simulation is of the first kind when it is actually of the second kind.

To illustrate this, consider a simple separation process based on an example in Douglas' Conceptual Design of Chemical Processes.[2] In this process, acetone is to be removed from an air stream (containing ~1.5 mol % acetone) by absorption at atmospheric pressure in water at 25°C. The aqueous solution is subsequently distilled to recover the acetone. Design specifications call for 99.5% of the incoming acetone to be removed in the absorber, and 99.5% of the acetone in the resulting feed to the distillation column to be recovered in the top product at a composition of 99% acetone. The entering air stream flows are 687 lb mol/hr air (G) and 10.3 mol/hr acetone.

A pencil-and-paper calculation, using the absorption factor (L/mG) as a parameter, shows that when

\[ \frac{L}{mG} = 1.4 \]

the required water flow (L) is 1943 lb mol/hr and, from the Kremser equation, 12.1 ideal stages are required in the absorber.[3] But a computer calculation by the Chemos modeling program (developed at the University of British Columbia) shows that the desired acetone removal cannot be obtained at the hand-calculation design point and that much higher water flows are needed. The difference is due to greatly differing values for the predicted equilibrium ratio, m, in the absorption factor, where

\[ m = \frac{y^*}{x} = \frac{\gamma_1 P^0}{P} \]

where

- P total pressure
- \( P^0 \) vapor pressure of pure acetone at system temperature
- \( \gamma_1 \) activity coefficient of acetone in solution

While \( P \) is specified and \( P^0 \) can be predicted to good accuracy, the value of \( \gamma_1 \) may be in some doubt.

The value used by Douglas (\( \gamma_1 = 6.7 \), giving \( m = 2.02 \)) is referenced to page 14-15 of Perry's Handbook[4] where it occurs in a table used in an example calculation (Example 2), but no source is given for the table. The value used by the Chemos program came from a binary data bank containing parameters for the Wilson equation obtained from Hirata.[5] But the only entry then present in the Chemos data bank for the acetone-water system was set 504 from Hirata, which refers to equilibrium at 150°C. The default method used by the Chemos program for extrapolating to other temperatures assumes that the values of

\[ (\lambda_{12} - \lambda_{11}) \quad \text{and} \quad (\lambda_{21} - \lambda_{22}) \]

in Eqs. (9) and (10) are independent of temperature and gives a value for the activity coefficient of acetone at infinite dilution in water at 25°C to be

\[ \gamma_1^\infty = 19.61 \]

Alternatively, the "athermal model" could be chosen, which
The minimum solvent rate from the absorber is an important parameter for design since it sets a lower bound for the energy requirements if this stream is to be subsequently distilled... this may enable a go/no-go decision to be made for this route early in the design process.

assumes that $\Delta G^{0}/RT$ is independent of $T$ and gives (see Eq. 7)

$$\gamma_i^{0} (25^\circ C) = \gamma_i^{0} (150^\circ C) = 12.64$$

Obviously, either of these predicted values would require proportionately larger liquid flows to keep the absorption factor at a reasonable design value. Since all of this extra water has to be distilled, the size and energy requirements of the recovery column would also be greatly increased.

Extrapolation of activity coefficient values from one temperature to another always introduces extra uncertainty. It can be avoided in this case since the Hirata data collection contains results at 25°C. Using the values of the Wilson parameters calculated by Hirata for that data gives

$$\gamma_1^{0} = 4.69$$

which would reduce the water flow to 70% of the amount originally calculated. Gmehling's data collection[6] has this same data[7,8, set 232] and one other at 25°C. Gmehling's fit of the Wilson equation to the Beare[7] data gives

$$\gamma_1^{0} = 7.00$$

and to the Taylor[8] data gives

$$\gamma_1^{0} = 6.44$$

Since data set 503 in Hirata is the same as data set 232 in Gmehling, the difference between the calculated $\gamma_1^{0}$ values (4.69 versus 7.00) must either be due to different assumptions made in data reduction or be caused by different criteria for goodness of fit.

DATA REDUCTION

Each of the referenced authors assumes that all non-idealities may be described by the liquid-phase activity coefficient ($\gamma_i$) so that the phase equilibria may be represented by

$$y_i = \frac{x_i y_i^{0} P^{0}}{P}$$

(1)

where the mole fractions in the vapor and liquid phases ($y_i$ and $x_i$) and the total pressure ($P$) are from the experimental data, and the pure component vapor pressure ($P_i^{0}$) is given by the Antoine equation

$$\log_{10} (P_i^{0}) = A - \frac{B}{(1 + C T)}$$

(2)

The coefficients (A,B,C) used by the two authors differ slightly: Hirata, et al., calculate the values of

$$P_{acetone}^{0} = 230.05 \text{ mm Hg}$$

and

$$P_{water}^{0} = 23.76 \text{ mm Hg}$$

while Gmehling, et al., use

$$P_{acetone}^{0} = 230.91 \text{ mm Hg}$$

and

$$P_{water}^{0} = 23.69 \text{ mm Hg}$$

at 25°C. The effect of these differences is very slight, as can be seen in Table 1.

EXPERIMENTAL DATA FITTING

The Wilson equation for the activity coefficient of each component in a binary mixture can be written

$$\ln \gamma_1 = -\ln(x_1 + \Lambda_{12} x_2) + x_2 \left( \frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{x_1 x_2} \right)$$

(3)

$$\ln \gamma_2 = -\ln(x_2 + \Lambda_{21} x_1) - x_1 \left( \frac{\Lambda_{12}}{x_1 + \Lambda_{12} x_2} - \frac{\Lambda_{21}}{x_1 x_2} \right)$$

(4)

A nonlinear regression method must be used to find the values of Wilson's parameters ($\Lambda_{12}, \Lambda_{21}$) that best fit a set of experimental data. The choice of the measure of goodness of fit (objective function to be minimized) and of the regression method may affect the final values of the parameters.

Hirata, et al., use a nonlinear least-squares method to minimize the function

$$F = \sum_{i=1}^{n} (Q_{exp} - Q_{calc})^2$$

(5)

where $n$ is the number of experimental points and

$$Q = x_1 \ln \gamma_1 + x_2 \ln \gamma_2$$

(6)

The independent variables are the values of $L_{12}$ and $L_{21}$. Since the excess free energy of mixing is given by

<table>
<thead>
<tr>
<th>TABLE 1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Experimental and Calculated Activity Coefficients for Acetone(1) in Acetone-Water system at 25°C</strong></td>
</tr>
<tr>
<td>$x_1$</td>
</tr>
<tr>
<td>(0)</td>
</tr>
<tr>
<td>0.0194</td>
</tr>
<tr>
<td>0.0287</td>
</tr>
<tr>
<td>0.0449</td>
</tr>
<tr>
<td>0.0556</td>
</tr>
<tr>
<td>0.0939</td>
</tr>
<tr>
<td>0.0951</td>
</tr>
<tr>
<td>0.1310</td>
</tr>
<tr>
<td>0.1470</td>
</tr>
<tr>
<td>0.1791</td>
</tr>
<tr>
<td>0.2654</td>
</tr>
<tr>
<td>0.3538</td>
</tr>
<tr>
<td>0.5088</td>
</tr>
<tr>
<td>0.7852</td>
</tr>
</tbody>
</table>

* Obtained by linear extrapolation for the first four data points.

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\[ \Delta G^F = RT(x_1 \ln \gamma_1 + x_2 \ln \gamma_2) \]  

Hirata's solution best fits the excess free energy for an isothermal data set.

Gmehling, et al., use the non-linear simplex method to minimize the function

\[ F = \sum_{i=1}^{n} \left( \frac{Y_{\text{exp}} - Y_{\text{calc}}}{Y_{\text{exp}}} \right)^2 + \left( \frac{Y_{\text{exp}} - Y_{\text{calc}}}{Y_{\text{exp}}} \right)_2^2 \]  

and they relate the values of \( A_{12} \) and \( A_{21} \) to the interaction energy between components \( i \) and \( j \) (\( \lambda_{ij} \)) by the relations

\[ A_{12} = \frac{V_i^L}{V_i^L} \exp \left[ \frac{-\lambda_{12} - \lambda_{11}}{RT} \right] = \frac{V_i^L}{V_i^L} \exp \left[ \frac{-A_{12}}{RT} \right] \]  

\[ A_{21} = \frac{V_i^L}{V_i^L} \exp \left[ \frac{-\lambda_{21} - \lambda_{22}}{RT} \right] = \frac{V_i^L}{V_i^L} \exp \left[ \frac{-A_{21}}{RT} \right] \]  

where \( A_{ij} \) and \( A_{ji} \) serve as the independent variables for minimization of \( F \). The molar volume of pure liquid \( i \) is \( V_i^L \).

Gmehling, et al., use the volume at 25°C for all data sets, and Chemos calculates the saturated liquid volume at system temperature and uses this to extrapolate to other temperatures, assuming that \( \lambda_{ij} = \lambda_{ji} \) remains constant.

The minimization function used by Hirata, et al., (Eq. 5) is recommended on thermodynamic grounds by Reid, et al.,(59,203) but it weights the error in the logarithm of the activity coefficient of a component by the mole fraction of that component. Consequently, the final values of the parameters that result from minimizing this function are less influenced by errors in the activity coefficients of components at high dilution than are the corresponding values for the minimization of the function used by Gmehling (Eq. 8).

The predicted value of the activity coefficient of acetone is less than the value obtained from the Beare data set over almost all of the composition range when Hirata's values of Wilson's parameters are used (see Table 1), whereas Gmehling's values exceed the experimental ones at the lowest concentrations.

If Wilson's equation fit the data perfectly, then the two minimization functions would give the same value of \( \gamma_i^* \). The observed difference could be because the equation is inappropriate, or the data is erroneous, or both are wrong. Leaving aside the choice of equation for the moment, two tests on thermodynamic consistency of the data are reported in Gmehling. The "area" test\(^{20}\) evaluates

\[ \int_0^1 \ln \left( \frac{Y_1}{Y_2} \right) dx_1 \]

which should equal zero for isothermal data. The "point" test\(^{10}\) calculates \( \gamma_i \) from experimental T, P, and \( x_i \) for each point, and evaluates

\[ \sum_{i=1}^{n} \frac{Y_i(\text{calc}) - Y_i(\text{exp})}{n} \]

This test requires values of \( \partial \rho / \partial x_i \) which are obtained by fitting a smooth spline curve to the P-x_i data. The Beare data set meets the criteria set by Gmehling for the area test but fails the point test, while the Taylor data fails both tests. The experimental acetone activity coefficient has an s-shaped curve with mole fraction instead of increasing with increasing negative slope as \( x_i \to 0 \), and the experimental water activity coefficient has a minimum of 0.916 at a mole fraction of acetone of 0.147 instead of increasing monotonically from 1.0 at \( x_i = 0 \). These differences may be the result of systematic experimental errors. In any event, they make prediction of the activity coefficient very uncertain at low concentrations of acetone (\( x_i < 0.15 \)).

**PREDICTED VALUES**

Prediction methods based on ASOG or UNIFAC can be used for this system. The ASOG method described by Pierotti\(^{111}\) is summarized in Table 8-17 of Reid, et al.,(14) and predicts \( \gamma_i^* = 7.78 \) at 25°C. While prediction methods cannot be better than the data they are based on, Pierotti had access to Shell Oil Company data books values that may not be generally available. Using UNIFAC by running Aspen Plus\(^{81,12}\) predicts values of the Wilson equation parameters that give \( \gamma_i^* = 11.49 \).

**SIMULATION EXPERIMENTS**

Table 2 lists values of \( \gamma_i^* \) from various sources. Any one of these values (except perhaps the two highest) might be chosen as a basis for design in the absence of other information, but the most likely values to be selected are either of the two values from data compilations 4.69\(^{14}\) and 7.00\(^{16}\), or the Aspen/Unifac value of 11.49.

**TABLE 2**

<table>
<thead>
<tr>
<th>Value of ( \gamma_i^* ) for the Acetone (1)-Water System at 25°C (Various Sources)</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.69</td>
<td>Hirata, et al., 1975(^{14}) (Beare data)</td>
</tr>
<tr>
<td>6.44</td>
<td>Gmehling, et al., 1977(^{16}) (Taylor data)</td>
</tr>
<tr>
<td>6.70</td>
<td>Perry, et al., 1973(^{13}) (Example 14-15)</td>
</tr>
<tr>
<td>6.93</td>
<td>Perry, et al., 1984(^{13}) (Example 14-21)</td>
</tr>
<tr>
<td>7.00</td>
<td>Gmehling, et al., 1977(^{16}) (Beare data)</td>
</tr>
<tr>
<td>7.78</td>
<td>Reid, et al., 1987(^{10}) (Table 8-17)</td>
</tr>
<tr>
<td>8.96</td>
<td>Perry, et al., 1963(^{14}) (Examples 14-31,14-32)*</td>
</tr>
<tr>
<td>11.49</td>
<td>Aspen/Unifac, 1991</td>
</tr>
<tr>
<td>12.64</td>
<td>Chemos - athermal extrapolated from 150°C</td>
</tr>
<tr>
<td>19.61</td>
<td>Chemos - default extrapolated from 150°C</td>
</tr>
</tbody>
</table>

* \( \gamma \)-value back-calculated from value of \( m \) used in examples
Table 3 lists the results of some Aspen simulations taking the same feed-gas flows and product specifications as were used in the hand-calculation example. The absorber was represented by the ABSBR block (the RADFRAC block gave almost identical results), the equation-of-state option set was SYSOP8A (Wilson/Redlich-Kwong/Henry's Law), and N₂ (used instead of air as the non-absorbed gas component) was declared an unsymmetrical (Henry's Law) component. A specification statement was used to adjust the liquid flow rate to satisfy the design requirement on the acetone leaving in the gas stream. Since the entering gas contained no water vapor, the simulation showed some evaporation of the water (~23 lb mol/hr). This evaporation required more heat than was provided by the absorption of acetone so that in all cases the water leaving the bottom of the tower was cooler than the entering liquid—by 13°F at the lowest flow rates and by 3°F at the highest.

It was not possible to obtain convergence of the simulation with less than 12 stages at absorption factors as low as 1.4. We used all three data sources to model a six-stage absorber which gave a liquid flow rate ranging from 1460 lb mol/hr for the lowest activity coefficient (Beare/Hirata) to 5030 lb mol/hr for the highest (Unifac/Aspen) (see Table 3). In a second series of tests, we increased the number of stages to the maximum that could be solved (minimum liquid rate that would converge). The solutions varied from six stages at 1460 lb mol/hr liquid (Beare/Hirata data) to ten stages at 3538 lb mol/hr (Unifac/Aspen). Even this considerable range may underestimate the extent of our ignorance since other equations (Van Laar, Margules, NRTL, Uniquac) could have been fitted to the equilibrium data. Also, we made no attempt to convert ideal stages to real packing—this step is commonly regarded as being much less accurate than the prediction of equilibrium relationships.

**IMPLICATIONS FOR DESIGN**

The minimum solvent rate from the absorber is an important parameter for design since it sets a lower bound for the energy requirements if this stream is to be subsequently distilled. Depending on energy costs, this may enable a go/no-go decision to be made for this route early in the design process. (Douglas[23] considers a number of other process alternatives.) If the go/no-go decision turns out to be dependent on \( \gamma^- \), then clearly it becomes essential to get better data.

If the range of \( \gamma^- \) values all lead to feasible absorber-stripper designs, and the designs are optimized, there is still no escaping the necessity to circulate more water when higher values of \( \gamma^- \) are assumed. If the process were designed and constructed based on the Hirata databook value, and the real value turned out to be that predicted by Unifac, then the process would fail to meet the required air-pollution discharge standards. The chemical engineer who replaced the original designer might spend some time trying to improve the packing or tray efficiency, to no avail. If the apparently conservative Unifac value was used and the Hirata value was correct, the process would work—but it would be more costly than it should be. A contractor proposing this design might find his bid rejected as being non-competitive.

**VARIATIONS IN HISTORICAL VAPOR-LIQUID EQUILIBRIUM DATA AT 760 mmHg**

If the absorbed acetone is to be recovered by distillation, equilibrium data at constant pressure (760 mmHg) are required; it is much easier to make equilibrium measurements under these conditions, and many more data sets are available. Whereas Gmehling, et al., only list two data sets for acetone-water at 25°C, they report ten sets for the same system at atmospheric pressure. Table 4 lists the \( \gamma^- \) values (predicted from the Wilson equation parameters at 100°C) for these data sets, arranged by year of publication. For four of these sets, the \( \gamma^- \) values are also available from data compilations of Hirata, et al.,[14] and of Ohe,[15] who used the same measure of fit as Hirata. In some cases the different fitting methods have resulted in greatly different values of \( \gamma^- \) (34.83 compared to 11.81 for the 1952 data set, for example), even though that data satisfies both measures of thermodynamic consistency.

The more extensive data allow different activity coefficient equations to be compared. Hirata only fits the Wilson equation, but Gmehling fits each data set with five equations (Margules, Van Laar, Wilson, NRTL, and Uniquac) and compares their goodness of fit by evaluating

\[
\sum \frac{|y_{1exp} - y_{1calc}|}{n}
\]

Table 4 lists the equations that are reported to best fit the data and the corresponding \( \gamma^- \) predicted by that equation. No clear picture emerges, since NRTL is best for five sets, Continued on page 67.

**TABLE 3**

<table>
<thead>
<tr>
<th>Data Source</th>
<th>Stages</th>
<th>Water Flow ( L/KG ) (geometric mean)</th>
<th>A=L/KG</th>
<th>K(acetone)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beare/Hirata</td>
<td>6</td>
<td>1460</td>
<td>2.16</td>
<td>1.041 - 0.782</td>
</tr>
<tr>
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Beware The Use of an Ideal Gas

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Only a foolish person ignores a warning. Julius Caesar heard the words of this warning in one of Shakespeare's great tragedies:

Beware the ides of March

but upon hearing them, he simply inquired as to who uttered them. Brutus (who was one of the assassins) replied that they were said by a soothsayer. History tells us that Caesar did not heed the warning and reveals the consequences of his inattention.

In contemporary life, we find the following warning on cigarette packs:

SURGEON GENERAL'S WARNING
Smoking causes lung cancer, heart disease, emphysema, and may complicate pregnancy

As I still see people smoking, it is apparent that they, like Caesar, choose to ignore warnings.

The purpose of this paper is to direct your attention to another warning: when too much attention is placed on the teaching of ideal gases, troubles can result. I hope to convince you that neglecting this warning can also be dangerous.

I fully expect that you will introduce the equation of state of an ideal gas to your students during their chemical engineering education. But I encourage you to limit the discussion to a much greater extent than you may have practiced in the past. My reasons for this cautionary note are several.

I will begin my discussion by considering just what influence I may have on my students after they graduate and leave the university setting. Since I will not always be at their elbow, I hope I will have taught them how to cope without faculty assistance. I want them to be able to view subjects from a general perspective and to decide just what skills they have that may be applicable to the problem at hand.

One of the educational experiences the students will have had is an introduction to the equations of state and their use, both in the prediction of the pressure, volume, and temperature (PVT) properties of fluids and in the determination of the values of other thermodynamic properties. While I (and others who are conversant with the subject matter) know just when the predictions of the ideal gas equation of state can be used to estimate the properties of fluids, my experience has been that students have not had sufficient exposure to the subject to make such a judgment.

Because of the difficulties I have encountered in trying to dissuade students from their near devotion to the use of an ideal gas, in this paper I will limit my comments to ideal gases. It has been my experience that once students have been exposed to ideal gases, finding some way to unlearn this equation of state is more difficult than was teaching them a more realistic equation of state in the first place. I will begin by first introducing the compressibility factor and then using it to define an equation of state for a real fluid.

The Compressibility Factor and Its Relationship to Real Gases

I will first consider systems whose variables of state, pressure, volume, and temperature are sufficient to set the equilibrium state. Since these variables occur frequently, I will use the symbols PVT when referring to them throughout this paper. This limits our considerations to gaseous systems.
whose only work mode is P-V work.

The defining equation of the compressibility factor of any real gas can be written as

\[ z = \frac{PV}{nRT} = \frac{PV}{RT} \]  (1)

where
- \( R \) universal constant known as the gas constant
- \( V \) molar volume
- \( z \) the compressibility factor

\( R \) is not dimensionless but has units which depend upon the choices of units for the variables \( P, V, n, \) and \( T \). This can be seen most clearly by inspection of Eq. (2):

\[ R = \frac{PV}{nT} \]  (2)

While Eq. (1) serves as the defining equation for the compressibility factor, it also represents the equation of state for any real gas. I feel that students should be introduced to the general subject of equations of state for gases by means of the compressibility factor and Eq. (1).

The compressibility factor is important for at least two reasons:

1. **It is dimensionless.** Although that point may seem simplistic and not worthy of note, I believe it is a mistake to overlook its importance since dimensionless quantities are used a great deal in chemical engineering, both in empirical representations of experimental data and in theoretical considerations. This fact should be pointed out to the students—the compressibility factor may be the first dimensionless variable they encounter in their education.

2. **The variable, \( z \), is subject to direct experimental measurement.** I stress this point since I believe that measurement is a topic essential for all engineering. I point out that a series of experimental measurements of the PVT behavior of a known quantity of gas can be made, and that we can thus determine a numerical value for \( z \) directly from its definition given by Eq. (1). Once the \( z \) values have been determined, they can be presented as tables or plots.

The factor \( z \) is a variable when we obtain values of it for real gases by direct experimental measurement. This means that \( z \) is not something which has a constant value.

When we consider gases which follow the ideal gas equation of state, we see that the compressibility factor is a constant identically equal to unity. Unfortunately, no known gas follows the ideal gas equation of state over all of its equilibrium states. Its very name should make it completely clear that it is an idealization, and thus an ideal gas serves as a limit for the behavior of real gases under certain specialized conditions. It is imperative that students make note of the above italicized words. Real gases follow ideal gas behavior only as limiting cases.

An ideal gas is any substance whose pressure, volume, and temperature behavior can be represented by

\[ PV = nRT \]  (3)

where \( R \) is the gas constant (the other variables were defined in Eq. 2).

The ideal gas "law" is given considerable attention in many texts and by many of my colleagues in teaching chemistry, physics, and chemical engineering, but I do not join their ranks. The time I spend in teaching an ideal gas is very limited. While I can understand the importance of an ideal gas in the historical development of an equation of state, I feel that too much attention is given to it in most instances.

What is particularly troubling to me is that I have seen far too much evidence that all this attention does not lead to student understanding of equations of state or their application. Rather, it has been my experience that students use an ideal gas under all circumstances—whether or not it is applicable.

My thoughts concerning an ideal gas are summarized in the following paragraphs.

**MY CASE AGAINST THE IDEAL GAS EQUATION OF STATE**

Please note that I do not refer to it as a "law." A law is something which should have near-universal validity, and the equation of state for an ideal gas does not meet that criteria.

**EXHIBIT I**

*It is a qualitative equation of state, at best, and its quantitative predictions can be very far from reality.*

If we divide both sides of Eq. (3) by \( nRT \), we find

\[ \frac{PV}{nRT} = 1 \]  (4)

Comparison of Eq. (4) to Eq. (1), which is the defining equation for the compressibility factor, indicates that the ideal gas equation of state predicts that \( z \) is a constant identically equal to 1. But inspection of Figures 1 and 2 (next page) reveals that this is not true.

While the value of the compressibility factor depends on the magnitude of the reduced temperature and the reduced pressure, it has a value of unity only in the following exceptional cases:

- All isotherms in the limit as \( P \to 0 \)
- Isotherms with \( T \) values which are \( \sim<2.5 \). The compressibility factor is unity twice for these isotherms: once at the zero pressure limit and once at the point where it crosses the line \( z=1 \).
I do not believe that these cases are sufficient to allow us to use the ideal gas equation of state to predict the phase behavior of most gaseous materials.

I can almost see a glow in the eyes of some of you upon reading the words above, and I can hear your rebuttal:

"What you say is true, but there are an infinity of points on a straight line, and thus the ideal gas must predict the correct value of \( z \) for an infinity of equilibrium states. Aren't you satisfied with something which works correctly infinitely often?"

This is music to my ears, and I respond:

"I was hoping you would ask that,"

... and I explain why...

There are an infinite number of points on a line, and if we use a notation introduced by Georg Cantor, we can say that this infinity is represented by a Hebrew character, aleph 1. Infinities do not stop with aleph 1, however, and the infinity of possible geometric curves known as aleph 2 (which represents the isotherms for real gases) is of a greater infinity than aleph 1. Aleph 2 is infinitely larger than aleph 1. Thus, I can say that ideal gas behavior is followed in only a miniscule number of cases. It is too simplistic to represent the PVT behavior of real gases. More information concerning Cantor's classification of infinities can be found in references 2-4.

The following example serves to illustrate just how much error can be introduced into predictions made by assuming that gases are ideal rather than real.

**EXAMPLE**

Propane is stored at 1000 psia and 300°F in an insulated vessel. Use the generalized compressibility chart to determine \( V \) under these conditions.

**SOLUTION**

Calculating values for the reduced pressure and the reduced temperature, I read a value of \( z = 0.55 \) from Figure 1, the generalized compressibility chart. This allows me to calculate \( V \).

**Figure 1.** Generalized compressibility factor for the low pressure range.

**Figure 2.** Generalized compressibility factor for the high pressure range.
\[ V = \frac{(0.55)(10.73)(760)}{1000} = 4.52 \text{ ft}^3/\text{lb}\cdot\text{mole} \]

This result can be compared with the value of 8.22 ft³/lb-mole which is the value predicted using an ideal gas. Thus, the ideal gas equation of state predicts that a volume approximately twice the actual size would be necessary to contain the propane. I do not consider this to be a particularly accurate prediction and feel you would agree with me, especially if I asked you to pay for the difference necessary to construct and install a storage tank which was nearly 100% oversized!

This example does not represent the worst possible case. If I had attempted to make a prediction of the volume of a gas present at its critical point, the ideal gas equation of state would have failed to an even greater degree.

**EXHIBIT 2**

It fails to predict the existence of the liquid state.

The ideal gas predicts that all isotherms must have the mathematical behavior shown in the following equation:

\[ PV = \text{Constant} \quad (5) \]

This is the equation of a rectangular hyperbola and its predictions are known as Boyle's "law." The equation does have some validity, and the early investigators of the critical point noted the approach of the critical point by observing the breakdown of this equation. I wish to note an interesting characteristic which is relative to this discussion—the slopes of all isotherms which satisfy Eq. (5) are everywhere negative. This is all well and good if we want the material to satisfy a condition of stability and remain in a single phase. Real substances do not satisfy the stability criteria for all states, however, and other phase(s) appear. If you have any doubt concerning this, consider that the surface of the earth is approximately 80% water; if you have further difficulty with it, I suggest you try to go for more than one day consuming only gas and not any liquid. While you may survive the experiment, I am confident you will not reject an opportunity to partake of liquids when they are presented to you following the exercise.

**EXHIBIT 3**

It Violates the Third Law of Thermodynamics.

This is a most serious crime. The laws of thermodynamics are so universal and pure that it is unthinkable to consider ways that fail to follow their dictates. If the ideal gas is used to predict the behavior of entropy as the absolute temperature approaches zero, it predicts a value of - . This is certainly specious, for while there is some disagreement about the numerical value of this limit, the third law of thermodynamics informs us that it approaches a finite limit and this limit is not -. In one sense, it is foolish to even attempt to use the ideal gas equation to predict any behavior as the absolute temperature approaches zero. The ideal gas equation is valid only for substances which are at elevated temperatures, and zero is hardly an elevated temperature.

I summarize my case thusly:

*The ideal gas is too simplistic to represent the behavior of real gases and fluids over the vast majority of cases of interest to chemical engineering. Thus, I should like to have it delivered to Walt Disney World where it can join with other fairy-tale characters and live happily ever after. It would quickly become a great tourist attraction and with the passage of time could become as celebrated as Donald Duck and Mickey Mouse.*

I am aware that there are those who will attempt to defend an ideal gas as an equation of state that provides an introduction to the general topic and serves as a starting point for any subsequent discussion of a real gas. But I do not accept this as a valid defense. It has been my experience that once a student learns the equation of an ideal gas, it is only this equation of state that is retained in his memory, and it is used under all circumstances, whether or not it is applicable.

A prime example of this is a recent experience I had when grading a problem I had included on a PhD qualifying examination. I had given a quantity of steam at a temperature greater than its critical temperature and had asked the students to determine the energy interaction necessary to bring the steam to its critical state at constant volume. Five out of the eight students used the ideal gas law in attempting to solve this problem. Since an ideal gas never has a critical temperature, it was, of course, impossible for them to locate the critical point and thus to determine the magnitude of the energy interaction. One student even went so far as to state that the gas was incompressible.

A gas is incompressible? This certainly was news to me! There are no gases which are incompressible!

I have no idea where such ideas find their origin. I expect that it was just a reflection of the fact that the student felt a great deal of pressure at the time of the examination, and he was merely grasping at straws. If so, he certainly selected a most inappropriate one.

I am very much of the opinion that it is more difficult to convince a student to "unlearn" something than it is to teach the correct approach in the first place. While it may take a little longer for the student to see the general relationship among the PVT variables when real gases are considered, the time will be well spent. It is certainly worthwhile to invest a little additional time in introducing gases by using the com-
pressibility factor. Ideal gases simply present too many problems. The following is another case in point.

**A PARADOX . . .**

The compressibility factor can be written in the virial form as a power series in reciprocal specific volume, and if we do this and perform some algebraic operations on the resulting equation, we find

\[
\frac{RT}{P} - V = -\frac{B(T)RT}{PV} - \frac{C(T)RT}{PV^2} - \cdots
\]  

(6)

where B(T) and C(T) are the second and third virial coefficients of the substance of interest.

We introduce a new symbol, \( \alpha \), to represent the expression which appears on the left-hand side of this equation. We now want to pass to the limit at \( P \to 0 \). Whenever \( P \to 0 \), \( V \to 0 \), \( V^{-1} \to 0 \), and \( PV \to RT \). Thus, we can write

\[
\lim_{P \to 0} \alpha = \lim_{P \to 0} \left( -\frac{B(T)RT}{PV} - \frac{C(T)RT}{PV^2} - \cdots \right)
\]  

(7)

The limit of the right-hand side reduces to \(-B(T)\). This is a completely general result and all equations of state must satisfy this condition.

I next ask a student to evaluate the limit of \( \alpha \) as \( P \to 0 \). The student reasons that real gases must approach ideal gas behavior as \( P \to 0 \), and he introduces the expression \( PV = RT \) into the defining equation, only to find that it becomes identically equal to zero! This result is in conflict with the result given by Eq. (7).

Q. How do you explain this apparent paradox?

A. When \( P \to 0 \), \( \alpha P \to 0 \), and \( PV \to RT \) even though \( \alpha \to 0 \). Thus, the result the student obtained resulted from his being led into a trap. An ideal gas can do many nasty things to you. It is best to avoid traps.

Dodge has commented on this paradox, and he concludes:\(^5\)

In explanation of this we may say merely that there is no ideal gas. It is an imaginary gas introduced for convenience and one must not expect an actual gas to have the behavior postulated for an ideal gas even as \( P \) approaches zero.

Those words were published nearly fifty years ago. I can’t help but wish that they had been read by textbook authors and others who present an ideal gas as an acceptable equation of state. It simply isn’t.

Could the student have avoided the trap? I don’t know. I recall being present at an oral exam a number of years ago and seeing a graduate student led into the same trap. He became unnerved when he recognized his error and was unable to resolve the paradox at that time.

The best advice is to avoid traps whenever possible. Help your students learn to build a better mouse trap rather than be caught by one.

**OTHER PROBLEMS RESULTING FROM AN IDEAL GAS**

Having considered some of the difficulties resulting from the use of an ideal gas on the macroscopic level, I would now like to examine some of the problems encountered when we consider an ideal gas at the microscopic level. I think it will become quite clear that an ideal gas can lead to some conclusions that don’t make a great deal of sense.

Both real and ideal gases exert pressure on the walls of those vessels used to contain them. This pressure certainly results from the momentum exchange between the gas molecules and the confining walls. The kinetic theory of gases assumes that the gas is composed of molecules which are in motion and which experience collisions with the surrounding walls and with one another. There is no term in the ideal gas equation of state which even attempts to account for the volume occupied by the molecules themselves. (You might note that the parameter b in the van der Waals’ equation of state does take this into account.) Thus, the molecules of an ideal gas are considered to occupy zero volume.

If the molecules have zero volume, this introduces the following difficulties:

- The molecules exert a pressure so they must have a mass.
- If their volume is zero, their density must be infinite.
- The molecules have a viscosity which is proportional to the square root of the temperature.

If the gas molecules have no volume, how is it possible for them to have a viscosity?

I suggest that you return to the words of Dodge. An ideal gas is an imaginary gas which exists only in textbooks. It can lead one astray even under those conditions where it is supposed to be valid.

Do not teach it as your introduction to equations of state!

I expect that some discussion of an ideal gas is necessary, but I suggest that you point out some of the limitations I have discussed in this paper and that you make minimal references to ideal gases.

**REFERENCES**

ERROR BARS IN PROCESS SIMULATION

Continued from page 61.

Margules for two, Wilson for two, and Uniquac for one. Restricting the comparison to the six sets of data that satisfy both of the thermodynamic consistency tests gives a score of three for NRTL, two for Wilson, and one for Unifac.

Based only on the "good" data, only on the Gmehling measure of fit, and only on the Wilson equation, this subset still yields values of $\gamma_i^*$ ranging from 7.41 to 11.81. If the Hirata measure is also included, the range is from 7.41 to 34.83. For many distillation calculations the different data sets would yield similar results, but in this example, if the bottom product from the tower has to have a very low acetone concentration to meet discharge standards, or to be recycled to the absorber, then $\gamma_1$ approaches $\gamma_i^*$ and the scatter is important.

At first sight it appears that the more recent sets of data show less variation, but note that three of these sets are smoothed data, at equal x increments. Some of these may have been obtained by interpolating smoothed bubble-point and dew-point curves, with no simultaneous measurements of x and y. Applying the point consistency test to these data may be tautologous.

CONCLUSION

The error bars in chemical engineering design may be much wider than is commonly believed. This is especially true for non-ideal systems at limiting concentration—a region of operation approached by many absorbers designed to meet discharge specifications for air pollution abatement.

There are warnings in the literature:

Finally, it must be emphasized that the biggest limitation to further developing the models is not theoretical insight or computational shortcoming, but the lack of good, relevant, experimental phase equilibrium data.

Fredenslund[10]

Most chemical engineering textbooks, however, are silent on this and treat experimental data as given, with no error bars. To avoid being fooled, or fooling others, data sources must be properly referenced. This may require finding out where the numbers in a computer data bank came from. When possible, the range of uncertainty of the input data should be reported and the consequences of that range carried through to the final design. At that point it may be necessary to put the simulation aside and go back to the laboratory.

REFERENCES

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TEACHING AS AN EXERCISE IN PROJECT MANAGEMENT

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Stepping from the industrial world into the academic world can be a daunting, but challenging, experience. After almost twenty years in industry, including some ten years in project management, I returned to academia and found myself facing the question of how I could best apply my industrial experience to at least partially compensate for my lack of teaching experience. I felt that several aspects needed to be addressed: first, I needed an overview of the position, including all of its duties and responsibilities; second, I needed to understand the role that lectures and exams play, and their interrelationship, in addition to an understanding of the grading system; and third, consideration had to be accorded the students and their abilities and aspirations. I concluded that some of the fundamental philosophies of project management that I had practiced in industry could be applied to teaching, and that a number of analogues existed between the two professions.

THE PROFESSOR'S ROLE

In constructional project management, the role of the project manager is to build something—anything from a house, say, to a nuclear power plant. Overseeing the construction involves meeting deadlines and specifications. In most cases, however, both time and specifications are subject to change, and this in turn affects costs—so the project manager often has to strike the best balance he can between time, specifications, and costs. In addition, he stands between the contractor and the client, and, whether or not he is employed by either of them, he must satisfy both of them. Contractual obligations must be met and personal differences must be overcome if they exist.

The professor is similarly positioned between the requirements of the university and the needs of the students. The university requires a certain academic standard (the specification) in upholding the reputation of the institution, while the students seek an education, within a certain time frame, that will qualify them for a professional position in society.

Cost is also a factor, just as it is in project management. Additional fees are incurred when a student, who does not meet the academic specification, fails and graduation (and earning power) is delayed. It is idealistic to hope that all students will pass, but students who fail should serve as an incentive for reviewing and improving teaching standards.

Another aspect of cost is the value of the service provided. While a project manager is well aware of the costs involved when a contractor stands idle for an hour, is the professor fully aware of the costs involved when he cancels a class? A significant number of dollars can be involved if you consider his salary, his time commitment to a particular course, the students' fees for the course, and the number of students enrolled in the class (not to mention government subsidies). Professors should feel an obligation to make the best use of the allocated time and to provide a service that is commensurate with the overall cost.

LECTURES AND EXAMS

Lectures have been defined as the transfer of knowledge from the professor's notebook to the students' notebooks without that knowledge having passed through the mind of either of them. If this is true, why not just hand out copies of the notes at the beginning of the term? If we presume that students absorb only a small amount of knowledge through the writing process, then we must assume that the bulk of their knowledge is obtained outside the classroom. Consider the opposite extreme—a highly gifted lecturer who can hold the class spellbound for an hour at a time. Can we assume that those students will automatically achieve top grades? Of course not. There is obviously still a need for acquisition of knowledge outside even the best lectures. An integral part of
the learning process is usually some form of self-study—
most people maintain that what they know best is what they
learned on their own, through their own efforts. It seems,
therefore, that the most efficient method of teaching would
be to create a self-learning environment, with the direction
and inspiration coming from the lectures.

From the point-of-view of a project manager, the end
result is what really counts—and for students the end result
(the final examination) is also what counts. The normal
progression of giving lectures and then giving a test on the
lecture material can be reversed with good results. The tech­

cical content and the required standard for the final exam­
ination can be set in advance, just as specifications for
engineering construction are pre-set. Setting such instruc­
tional objectives allows the professor to adopt a manage­
ment-by-objectives approach to teaching and gives the
students direction. Further guidance can be provided
through regular assignments that have a similar content as
the final examination, with the lectures providing guidance
on how to execute the assignments.

Students need other skills in addition to technical skills,
and some of them (particularly written communication and
mathematical computation) are demonstrated in the exami­

nations. Assignments throughout the course help to develop
these skills, and the final examination is to some extent a
measure of the development of these skills during the course.
There is an analogue with athletes or musicians who practice
avidly for the big event—students need to practice their
skills before attempting the final examination; such practice
comes through regular execution of assignments.

STUDENT'S ASPIRATIONS

The obvious end result of a student's aspirations is a de­
gree. That is the goal of all students, and each course can be
viewed as one step along the way. In general, the more
demanding the steps, the more valuable the degree. The
aspirations of the students are no different from those of the
university—to achieve a high academic standard. Human
nature, however, provides some inertia to the process and
fosters a tendency to take the line of least resistance, creating
short-term goals of merely surviving from one examination
to the next. It is therefore important that the students have an
overall vision of the program.

In construction, it is obviously foolish and expensive to
build something that cannot be used, or to have to rebuild
something that was built wrongly. It is also important for the
sequence of construction to be correct and logical. The same
principle applies to a student’s educational program and even
to the individual courses within that program. Expertise
should be developed in a logical and constructive manner.
Students accept hard work when they can see a tangible
return for the effort they put forth. They find a measure of
satisfaction if their examination grade reflects that effort,

and, if they can find some satisfaction in each of the approxi­
mately fifty courses they take in the engineering curriculum,
they will graduate with a sense of achievement.

There is a before-and-after perception of a degree, just as
there is in any project, where the completed project never
seems quite as good as its initial visualization. Figure 1
shows a mind's-eye conception of a new house before its
construction and the actual view of that same house after
completion. It is obvious from the illustration that some time
must be allocated to reap the full benefit of good landscap­
ing. The same principle applies to a degree: often, a number
of years can pass before a satisfactory job related to an
individual's expertise is secured. It should also be accepted
that the degree may have a few poor grades in its construc­
tion, just as a house may have some bad workmanship. This
is part of the student's overall experience, and ultimately, a
good engineer is an engineer who has the foundation of a
solid basic education around which to frame a career.

PLAN OF ACTION

To structure a course from a project-management perspec­
tive, definite goals and certain specified levels of acceptance
are required. The course should be monitored with respect to
time and performance so that the required standard is achieved
on the due date, precise specifications for the structure of the
final examination should be set in advance, and the steps
toward the final examination and final grade should be clearly
indicated. As an example, when the final examination em­
Continued on page 73.

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Figure 1
PRESENTATIONS ARE USED EXTENSIVELY FOR COMMUNICATION AND PERSUASION IN ALMOST ALL PROFESSIONS. IN PARTICULAR, ENGINEERS MUST BE ABLE TO PRESENT WELL SINCE OFTEN THEIR TECHNICAL EXPERTISE ALONE WILL NOT GET THE JOB DONE—THEIR IDEAS MUST BE "SOLD" THROUGH VERBAL PERSUASION IN ORDER TO BE IMPLEMENTED. "IF ENGINEERS CANNOT INFORM OTHERS OF WHAT THEY HAVE DONE, THEY MIGHT AS WELL NOT HAVE DONE IT."[1] IN THE DEPARTMENT OF CHEMICAL ENGINEERING AT LOUGHBOROUGH WE RECOGNIZE THIS FACT AND AS A RESULT HAVE INCREASED THE USE OF PRESENTATIONS IN OUR UNDERGRADUATE COURSES. WE ALSO BELIEVE THAT PRESENTATIONS CAN BE EFFICIENT LEARNING EXPERIENCES BECAUSE PRESENTERS MUST UNDERSTAND THE MATERIAL THEY ARE PRESENTING.

IN THE PAST, THE METHOD OF ASSESSING A PRESENTATION WAS LEFT TO EACH INDIVIDUAL STAFF MEMBER, AND IT USUALLY CONSISTED OF ASSIGNING A MARK BASED ON THE ASSESSOR'S IMPRESSION OF THE PRESENTATION. WE FELT THAT BETTER GUIDELINES WERE NEEDED SINCE

- THE PROPORTION OF TOTAL MARKS FOR PRESENTATIONS IN OUR COURSES IS EXPANDING.
- THE GRADER'S IMPRESSION OF THE PRESENTATION CAN BE SUBJECTIVE AND WE WANTED TO ELIMINATE ANY POTENTIAL FOR BIAS.
- WE WANTED TO BE ABLE TO SHOW OUR STUDENTS THE BASIS OF THE ASSESSMENT AND TO IDENTIFY THEIR STRENGTHS AND WEAKNESSES FOR THEM SO THEY COULD BOTH IMPROVE AND CONSOLIDATE THEIR SKILLS.

STUDENTS HAVE IN THE PAST CRITICIZED PRESENTATION ASSESSMENTS AS BEING SUBJECTIVE AND OF VARIABLE QUALITY, AND AS A POSSIBLE SOLUTION TO THE PROBLEM THEY HAVE SUGGESTED THAT ADDITIONAL STAFF MEMBERS ALSO moderate AND GRADE THE PRESENTATION. BUT OBSERVING AND ASSESSING PRESENTATIONS IS TIME-CONSUMING, AND WITH THE RECENT WORSENING OF STAFF-STUDENT RATIOS IT IS SIMPLY NOT POSSIBLE TO ASSIGN ADDITIONAL STAFF TO ASSESS AND moderate ALL STUDENT PRESENTATIONS. THEREFORE, IN ORDER TO ELIMINATE INCONSISTENCIES, WITHOUT INCREASING STAFF INVOLVEMENT, A MORE FORMAL METHOD OF ASSESSMENT HAS BEEN DEVISED AND IS BEING PRESENTED IN THIS PAPER.

ASSESSMENT IS ONLY ONE FACET OF EFFECTIVE TEACHING, HOWEVER. INSTRUCTION AND FEEDBACK ARE ALSO IMPORTANT, SO SOME SUGGESTIONS RELATING TO THESE COMPONENTS ARE ALSO INCLUDED IN THIS PAPER. BUT SINCE A BASIS FOR ASSESSMENT MUST BE IN PLACE BEFORE METHODS FOR INSTRUCTION AND FEEDBACK CAN BE ESTABLISHED, THIS PAPER WILL CONCENTRATE ON OBJECTIVE ASSESSMENT AS A FIRST STEP TOWARD IMPROVING THE TEACHING OF PRESENTATIONS. HANZEVACK AND McKean[1] DEAL IN GREATER DEPTH WITH PREPARING STUDENTS FOR THEIR PRESENTATIONS.

A CHECK-LIST APPROACH

ONE ESSENTIAL AND INESCAPABLE DIFFICULTY WITH ASSESSING A PRESENTATION IS THAT IT MUST BE DONE IN "REAL TIME" AND THE ASSESSMENT PROCESS ITSELF INTERFERES WITH OBSERVING THE PRESENTATION. IT IS POSSIBLE TO USE VIDEO TO RECORD AND REPLAY THE PRESENTATION, THEREBY SEPARATING DATA-GATHERING AND ASSESSMENT (AND IT IS ALSO A POWERFUL TOOL FOR SHOWING STUDENTS THEIR MISTAKES), BUT THAT METHOD CONFLICTS WITH THE SCARCITY OF TIME ALREADY MENTIONED. ALSO, VIDEOTAPEING REQUIRES EXPENSIVE AND COMPLICATED EQUIPMENT AND EXTRA PERSONNEL TO OPERATE IT.

REAL-TIME ASSESSMENT MUST BE SIMPLE AND SHOULD NOT DISTRACT FROM THE OBSERVATION. THIS CAN BE ACHIEVED BY USING A PRINTED FORM WITH PRE-DEFINED HEADINGS RELATING TO THE DIFFERENT ASPECTS OF A PRESENTATION. MARKS AND COMMENTS (FOR LATER STUDENT FEED-BACK) ARE RECORDED UNDER THE DIFFERENT HEADINGS DURING THE COURSE OF THE PRESENTATION. THE FORM USED BY THE AUTHOR IS SHOWN IN Figure 1.

divided into three sections, which are described in the following paragraphs.

**KEY**

The presenter must be satisfactory in each of these six categories for the presentation to be a success. The grade for each category is, therefore, a simple yes or no. For example, the presenter is either **audible** or not; the visual aids are either **readable** or not; etc.

**Personal and affiliation details** indicates the speaker’s name, department, course, etc. Most students assume that their listeners know who they are and even what they are going to talk about. The speaker must state these details, however, even when talking to friends or colleagues. We are training them for real-life presentations where the audience will, in general, not be known to them.

It is also important to **state the topic and aim** of the presentation; that is, what they intend to achieve by making the presentation. Audiences need as much help as possible in how to listen to a presentation, so clearly stating its aim is important. Is the presentation a sales pitch, or a funny story? The speaker must clarify the aim of the presentation. It is generally helpful for the assessor to record the stated topic at this point and then refer back to it at the end of the presentation.

One of the most effective ways for a presenter to alienate an audience is to miscalculate the length of the presentation and either run under or over the time allotted for it. In the first case the listeners may be irritated if they allotted too much time for the presentation and could have been doing other things. They may also perceive an unstated message that the topic is not as important as claimed. Most presentations are intended to “sell” something (such as a product, an idea, a design), and during the presentation the speaker usually has the undivided attention of the person(s) who will make the decision to “buy.” Obviously, the speaker should use the available time (but no more) in order to make the most effective case possible.

On the other hand, when a presentation runs over the allotted time, the speaker is probably keeping the listeners from other tasks which they expected to accomplish. They are most often distracted and annoyed by this usurping of their time, and the impact of the presentation is thus diluted. In the worst case, of course, the audience will walk out before the point of the presentation has been made.

The assessor should record the time taken by the presentation in order to gauge the degree of under- or overrun. Students often assume that doing more than is required will result in a higher

---

**PRESENTATION ASSESSMENT**

| Occasion: ____________________ | Start: : Finish : Date: ____________ |
| Name: ______________________ | Mark: __ out of: ____ Order: __ of: __ |

**KEY** Any presentation must be satisfactory in these key areas

<table>
<thead>
<tr>
<th>Item</th>
<th>Y/N</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Audible</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Readable visual aids</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stated personal and affiliation details</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Stated topic and aim</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Used the available time</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Made the point(s)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**INTERACTION WITH AUDIENCE**

<table>
<thead>
<tr>
<th>Item</th>
<th>Y/N</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Connected them to the topic and aim</td>
<td></td>
<td>Scale</td>
</tr>
<tr>
<td>Enjoyment</td>
<td>1 2 3</td>
<td></td>
</tr>
<tr>
<td>Understanding</td>
<td>1 2 3</td>
<td></td>
</tr>
<tr>
<td>Respect/sensitivity - presenter/audience</td>
<td>1 2 3</td>
<td></td>
</tr>
</tbody>
</table>

**TECHNIQUE**

<table>
<thead>
<tr>
<th>Item</th>
<th>Scale</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Content and relevance</td>
<td>1 2 3</td>
<td></td>
</tr>
<tr>
<td>Detail and logical structure of material</td>
<td>1 2 3</td>
<td></td>
</tr>
<tr>
<td>Use/lack of prompts, signposting</td>
<td>1 2 3</td>
<td></td>
</tr>
<tr>
<td>Quality and use of visual aids</td>
<td>1 2 3</td>
<td></td>
</tr>
<tr>
<td>Summary</td>
<td>1 2 3</td>
<td></td>
</tr>
<tr>
<td>Question handling</td>
<td>1 2 3</td>
<td></td>
</tr>
</tbody>
</table>

Delivery/posture/mannerisms/etc - comments:

**SCORING**

Give 3 marks for a "Yes" and 0 marks for a "No"; for the categories with a scale response, the point on the scale is the mark; you may also give 0 marks in these categories. There are two extra marks for general impression. The total possible is 50.

**Figure 1. Presentation Assessment Form**

Winter 1994
mark, and they should be made aware of the fact that this is not the case with presentations.

The last category, made the point(s), concerns the overall effectiveness of the presentation. The assessor should ask the questions: What was the main point? Would I buy it? Am I convinced? Referring to the topic and aim that were noted at the beginning of the presentation is helpful in determining if the presenter accomplished those aims.

— INTERACTION WITH AUDIENCE —

"Connected them to the topic and aim" means explaining the relevance of the topic to the audience. For example, "enzymes are important because . . . ." The next two categories, enjoyment and understanding are self-explanatory.

In the last category in this section the grader looks for a mutual respect and sensitivity between the presenter and the audience. For example, was the audience bored or talking among themselves while the speaker continued, blissfully unaware? Some other things to look for and include in this category are if the style of the presentation was suited to the type and size of the room it was given in, and did the presenter correctly judge the audience's previous knowledge of the subject, altering his or her presentation accordingly? For example, a sensitive speaker would not explain something that had already been explained by a colleague in a session of presentations; it would be sufficient to say, "as so-and-so has already mentioned."

— TECHNIQUE —

The categories in this section are for grading the mechanics of the presentation. Content and relevance is an assessment of whether too little, sufficient, or too much material was presented and whether or not it was pertinent to the topic and aim of the presentation. The arrangement of the material and the quality of the argument's development is scored under detail and logical structure.

Most speakers need prompts to remind them of the important points they want to present. Bad presenters read the entire presentation, putting their audience to sleep, but a good speaker appears to know the subject well and delivers the material in an interesting and engaging manner, using such elements as visual aids as prompts.

Signposting indicates whether or not the speaker has explained the structure and charted the current position of the presentation as well as where it is going. Examples of signposting are, "I shall begin by talking about..." "Then I will...," and "We have now reached the last section of...." Signposting is quite helpful for the audience members.

The quality and use of visual aids category is for grading the quality and appearance, as well as facility of use, of the visual aids. It is different from the readable visual aids category in the first section which is a simple test of readability.

The other headings in this section are self-explanatory, and the last section is for recording general impressions and any comments that do not fit into any of the above categories, such as excessive "uhms."

OTHER FACTORS

I have found that for short presentations the above headings are sufficient for grading purposes. Occasionally, however, the headings could and should be expanded. For example, if the speaker is presenting the results of experimental work, a category could be added to indicate if a diagram was used to explain the experimental rig, or whether data was correctly presented on graphs.

SCORING

Bearing in mind that presentation assessments are made in "real time," the scoring must be done at the time of the presentation or the information must be noted on the checklist so that the scoring can be done at a later date. It would be ludicrous to be too precise. My method is to give 3 points for a "yes" and 0 points for a "no" in the Y/N column, and a 3 for "good," a 2 for "average," and a 1 for "bad" in the scale category. This gives a maximum of 48 points. To make it a nice round 50 points I often add an extra 2 "discretionary" points.

Some readers may feel that a scale with only three points is too coarse, but I feel that in the majority of cases it is difficult to be any more accurate. It is still possible, for example, to give 0 points in a category if the presenter was appalling and 4 points for a performance that was exceptionally good (although this last score should be used sparingly because it changes the total marks).

As the students progress through their courses and become more proficient, they should satisfy the key requirements; therefore, the weighting given to these categories should be progressively reduced. The mark for a "yes" could be cut to 2, and then to 1, and perhaps a negative mark could be given for a "no" if they have had sufficient training and practice to know better. After all, experienced presenters should be audible and should produce readable visual aids. The number of points on the scale could also be increased to five (0,1,2,3,4). It is not possible to score to a finer precision than five points.

In scoring the use-of-time category, marks should be subtracted for serious overruns as well as underruns (unless the presenter has given a good explanation for not using all of the available time). Overrunning the allotted time can never be justified.

I normally give the first presenter in the session a few extra marks since it is the most difficult slot for both the presenter and the assessor.
PRACTICALITIES

It is easy to set up a session of presentations. All that is needed is a room, some chairs, an overhead projector, and a screen. The audience can consist of the group of presenting students, and in that case the session can also become an effective teaching situation since students tend to listen to their peers, especially when the work presented is similar to their own. The assessor should sit as far from the presenter as possible in order to check the speaker's audibility and the visibility of the visual aids. Keeping in mind that it is difficult for an audience to concentrate for more than an hour at a time, breaks should be scheduled during the series of presentations. We have found that eight ten-minute presentations during a 2 - 2.5-hour period is a workable session.

It is helpful to spend some time preparing students before they make their presentations. Hanzevack and McKean recommend a brief lecture in addition to written guidelines, and they also provide a useful summary for distribution to the students. The most important point to be stressed is that the audience wants the presenter to do well. Most students are very nervous about giving a presentation, but their fears can be somewhat allayed by convincing them that the audience is on their side.

Students should also be shown the assessment form before they give their presentation so they will be aware of the aspects that are being observed and graded.

The best presentations are always given without notes, so students should be encouraged from the very beginning to present without using them. Suggest that they use their overheads as prompts. It is also important to stress how much time they have for the presentation and that they will be penalized for running beyond that limit. Since presenters often try to include too much material, they should be made aware of the importance of tailoring their presentation to the available time. A good guideline to give them is, "If in doubt, leave it out."

The audience should be encouraged to ask questions since one of the best ways to determine if the speaker understands the material is from the way he or she handles questions. When the audience is made up of peer presenters, a scheme can be devised to provide a material reward for questioning—that is, marks can also be given for questions. For example, each student can be allowed a certain number of questions, with a mark given for each of them (provided the question is relevant and hasn't already been asked!).

Most presentations discuss work done by the student, but the mark given for the presentation should be only for its effectiveness. Marks for the technical content should be assessed separately, although the impression formed from the presentation may also have some impact on the other mark. For example, we run second-year laboratories where the total mark of 100 is split 30 for the experimental work, 40 for the written report, and 30 for the presentation. The quality of the experimental work is marked in the first two of these categories, but if the presentation indicates a lack of understanding by the student, the mark achieved in the first two categories can be affected.

The completed assessment form, with both the good and bad points highlighted, should be shown to the presenter. At the end of the session the assessor should comment on some general points, remembering to find something positive to say about each presentation, no matter how dire it was. Constructive criticism goes a long way in helping to correct a presenter's deficiencies. Good presentations are given by confident presenters, so it is beneficial to build up the student's confidence.

REFERENCES


TEACHING AS AN EXERCISE . . .

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braces problems that have a time limit for solution, the student should have had experience (practice) with similar problems on prior assignments and tests throughout the course. Feedback from those problems can be quite valuable in monitoring the student's progress through the steps leading to the final examination.

Lectures are a means of presenting basic material and guiding students to problem solutions, and they should be structured in that fashion. They should be well-directed toward an end condition, with the professor delivering the necessary information as efficiently as possible. The problems should be sufficiently varied to test all of the student's problem-solving skills.

Students who are motivated to learn through good self-study habits should be recognized for their efforts and be awarded grades that reflect their initiative as well as their skills. Grades should not be scaled to some inflexible scale dictated by policy or statistics. Those students who get an "A" should have earned it.

CONCLUSION

It is possible to meet both the requirements of a university system and the aspirations of its students by applying conventional project-management philosophies to teaching. This method of teaching also provides appropriate direction for the student, making his education meaningful and productive, and leaving him well-prepared for a career in industry where project-management philosophies are applied daily.
A FIRST-YEAR
INTRODUCTORY SEMINAR

KEVIN MYERS, LAWRANCE FLACH, AMY GROSJEAN
University of Dayton
Dayton, OH 45469-0246

Advising undergraduate students is an important task for engineering faculty. Not only must it be done well, but it must also be done efficiently. Advising first-year students is particularly challenging because at that point the students are involved in only a few engineering activities and have only a vague idea of what engineering actually is. Most of their time and effort is focused on simply surviving their mathematics, chemistry, physics, and general education courses. Typical engineering curricula do not offer the first-year student an opportunity to learn what an engineering career really involves and whether or not it is the correct course of study for them.

In an effort to address and overcome this problem, many departments have added engineering courses to their first-year curricula. Some universities have added design courses, while others have added introductory engineering courses. These courses typically use various combinations of videos, lectures, plant trips, guest speakers, and faculty and student presentations. Students are usually graded on their performance on homework assignments, written and oral reports, and examinations.

The University of Dayton previously required all first-year engineering students to complete a two-credit hour course, "Introduction to Engineering," and it was attended by students from all of the engineering majors. Faculty members from each engineering department taught sections of the course, but this led to substantial variation in the course emphasis and quality. Attempts were made to coordinate and improve the course, but in 1987 it was dropped in a move to control the rising number of credit hours required for graduation. Since then some of the engineering departments at the University of Dayton have added required, no-credit introductory seminars for their first-year students.

COURSE STRUCTURE

The seminar course "Introduction to Chemical Engineering" is offered to incoming chemical engineering students and is described in the university bulletin as an "introduction to the chemical engineering faculty, facilities, and curriculum, including a survey of career opportunities in chemical engineering." It was originally conceived through our efforts to improve the effectiveness of advising. The program outlined in Table 1 was developed to improve communication between the students and their advisors.

The seminar provides an opportunity for the faculty to share information with the students and offers the students an opportunity to ask questions which they may otherwise hesitate to ask during a one-on-one visit with their advisor. It also attempts to involve the first-year students in departmental activities and to demonstrate that there is fun, challenge, and reward in the work of the department and in the field of chemical engineering.

The primary reason for teaching the course on a no-credit basis is that most of our students would be subject to a tuition surcharge for exceeding the university's maximum
Up to this point in the program the students have only been told about chemical engineering. The fifth meeting consists of a tour of our departmental laboratories and includes demonstrations of some of the equipment. The tour is conducted by upper-level students who describe the work they are performing in our transport phenomena, unit operations, and process control laboratories.

| TABLE 1  
Schedule of Class Meetings |
<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>• Departmental welcome and faculty introduction; announcement of student AIChe kick-off meeting</td>
</tr>
<tr>
<td>• Discussion of chemical engineering, highlighting career opportunities. Video presentation</td>
</tr>
<tr>
<td>• Job-experience presentations by senior students</td>
</tr>
<tr>
<td>• Job-experience presentations by practicing engineers</td>
</tr>
<tr>
<td>• Tour of chemical engineering laboratories</td>
</tr>
<tr>
<td>• Computer/word processing tutorial</td>
</tr>
<tr>
<td>• Joint meeting with junior/senior seminar</td>
</tr>
<tr>
<td>• Registration advising</td>
</tr>
</tbody>
</table>

number of credit hours for full-time students (students are charged a flat tuition for taking from twelve to seventeen credit hours). Since it is a no-credit course and we are not really interested in increasing the students’ workload, grading is on a pass/fail basis. Attendance at all class meetings is the sole criterion for determining whether a student passes or fails the course. Any student who misses a class meeting is required to attend a faculty-approved student AIChe meeting to make up for their absence. This attendance policy is clearly explained during the first class meeting, and since the course does show up on the students’ transcripts, very few students miss class. During the four years that it has been taught, no one has failed the course.

The course meets once a week for eight weeks, and covers the topics listed in Table 1. Originally we met every two to three weeks in an attempt to distribute the course throughout the semester, but the result was poor attendance since many students forgot about scheduled class meetings.

Involving the student AIChe chapter in the seminar was designed to provide a service activity for that organization as well as to alleviate the faculty workload associated with the course. This involvement, coordinated by a student assistant, has been surprisingly effective. The upper-level students are very enthusiastic because they believe that they have important information to share with the first-year students, and the first-year students are often more at ease asking questions of upper-level students than of faculty. An added bonus is that attendance of first-year students at AIChe activities has also increased since the introduction of this course. This is probably due to improved communication between upper-level and first-year students.

A student-faculty social is held after one of the seminar meetings, and the first-year students are encouraged to attend so that they can meet faculty and upper-level students in an informal atmosphere.

COURSE SPECIFICS

At the first meeting, the departmental faculty is introduced and the structure of the course is explained. The student AIChe officers are also introduced and given the opportunity to discuss the purpose and activities of AIChe as well as to announce the first meeting of the year.

The second meeting is designed to give the first-year students a broad overview of chemical engineering as a profession, including its history, future prospects, skills required, industries involved, and job opportunities. This is accomplished through a presentation by the faculty coordinator, followed by the showing of an AIChe video, "Frontiers in Chemical Engineering."

The third and fourth meetings expose the first-year students to actual chemical engineering job experiences, first by senior students and then by practicing engineers. In both instances we attempt to cover the spectrum of chemical engineering industries and job types. To illustrate, at the most recent presentations, the senior students discussed working with environmental, consumer products, automotive, and petroleum companies, while the practicing engineers discussed their work in research, technical sales, and manufacturing. The first-year students' enthusiasm for these presentations is indicated by the large number of questions they ask. They are particularly interested in the internship and cooperative education programs.

Up to this point in the program the students have only been told about chemical engineering. The fifth meeting consists of a tour of our departmental laboratories and includes demonstrations of some of the equipment. The tour is conducted by upper-level students who describe the work they are performing in our transport phenomena, unit operations, and process control laboratories. For many of the first-year students this is their first visual exposure to chemical engineering, and they are usually quite impressed by the work of the upper-level students. Hearing an upper-level student say things like "We're studying the recycling of plastics in this injection molding device" or "I'm working on the redesign and instrumentation of this heat exchanger" is probably equivalent to an entire semester of simply discussing chemical engineering in a classroom.

The sixth meeting is used to introduce the departmental personal computer facilities that are available to the students. Since they are all required to write papers in their
courses, the first-year students are usually pleased to learn that word processing facilities are available to them. Upper-level students present a tutorial on the computers, while the department provides each first-year student with a computer disk. We have found that use of the computer facilities is a convenient way to get our first-year students involved in department activities.

At this point the first-year students attend an upper-level seminar given by a guest speaker. This joint seminar not only shows the first-year students the type of seminar they will be attending in later years but it also provides additional interaction with upper-level students.

The final meeting of the course occurs near the midpoint of the semester and is devoted to a discussion of midterm grade reports and registration for the next term. Since the first-year students have never registered on campus (their first-term registration is handled through the mail), it is important to instruct them in the logistics of registration and to ensure that they register for the correct courses. After a short introduction by the faculty, this meeting is turned over to upper-level students, thereby giving the first-year students both the faculty and student viewpoints concerning registration.

FACULTY AND STUDENT PERCEPTIONS

During the last class meeting we ask the students to complete a course evaluation that poses three questions:

1. What do you believe was the purpose of this course?
2. Do you feel that the course accomplished this purpose?
3. What would you do to improve this course?

Most of the students correctly identify that the purpose of the course is to initiate communication between the faculty and the new students and to provide them with information about chemical engineering. They also recognize that the course offers an opportunity to get to know one another. The students feel that the course accomplishes these goals. Typical comments include: "I feel more comfortable about what I am trying to become. Now I know what it is."; "I found it [the course] very helpful."; and "It didn't waste any time and accomplished its purpose nicely." On occasion, students found that chemical engineering was not what they were interested in, and we were able to effectively counsel them concerning alternate programs of study.

We were surprised when the students suggested that the course could be improved by expanding its scope (the course met only five times the first year it was taught). The students requested that we add the meeting with practicing chemical engineers, increase their interaction with upper-level students, and provide more information concerning student chapter AIChE activities.

The upper-level students have always been happy to assist us with this course. They feel that they have useful information and experiences to share with the first-year students. They do a good job, although they sometimes say things that make the faculty cringe, such as "I don't really use chemical engineering in my job."

We have been pleasantly surprised by the success of this course. We were worried that the students might see it as a waste of time since it is a no-credit course that requires only their attendance. Based on the evaluations, however, this does not appear to be the case. The current format appears to be optimal; there is a substantial amount of contact time, and the first-year students are exposed to chemical engineering in a variety of contexts. The course ends at the middle of the term, before the students lose interest, and allows them to subsequently focus all of their attention on the more rigorous courses. Also, involvement of the first-year students in departmental activities, particularly in student AIChE activities, has increased since the course was added to the curriculum.

Since we see all the students on a regular basis and have an opportunity to share information with them and answer their questions, we feel our advisory role has been improved. We have also noticed that the students know what to expect and are better prepared for their individual advising meetings. We feel that the small amount of time and effort required to conduct this course is a good investment in our first-year students.

CONCLUDING REMARKS

Both faculty and students are pleased with this introductory seminar. It is an effective and efficient means of initiating communication between the department and its first-year students, and the increased contact between faculty and students enhances our advising program. The seminar also encourages the first-year students to participate in departmental activities and is a good service project for the student AIChE chapter.

REFERENCES

1. Landis, R.B., "National Survey on 'Introduction to Engineering' Courses," California State University, Los Angeles, CA (1992)
5. Sproull, R.D., "An Introduction to Chemical Engineering: A First-Term Freshman Course at OSU," presented at the 1987 ASEE Summer School for Chemical Engineering Faculty, North Dartmouth, MA
EXCESS FUNCTIONS

Continued from page 23.

octants, denoted by numerals I through VIII. We make the following observations:

1. $c^{\theta}_{\mathbf{P}}$ is usually larger in absolute value than is $s^{\theta}$; for the systems shown in Figure 5, $|\epsilon| > 1$ about 85% of the time.

2. Octants IV, V and VI are very sparsely occupied. Thus the following behaviors are unusual:

   \[
   s^{\theta} \Theta \text{ with } c^{\mathbf{P}}_{\mathbf{P}} \Theta
   \]

   and

   \[
   s^{\Theta} \Theta \text{ with } c^{\mathbf{P}}_{\mathbf{P}} \Theta \text{ and } e^{\mathbf{P}}_{\mathbf{P}} < - s^{\theta}
   \]

   Other octants have reasonable representation.

3. $\epsilon < -1$ is an unusually large negative $\epsilon$; positive values of $\epsilon$ can, however, be considerably larger than unity.

The above observations lead to a few generalizations. Mixtures with negative $h^\mathbf{P}$ and $s^\mathbf{P}$ usually have positive $c^\mathbf{P}_{\mathbf{P}}$; mixtures with negative $c^\mathbf{P}_{\mathbf{P}}$ usually have positive $s^\mathbf{P}$ and $h^\mathbf{P}$. For NP/NP mixtures, $c^\mathbf{P}_{\mathbf{P}}$ is usually negative, though exceptions are observed (e.g., for mixtures of CCl$_4$, with an aromatic hydrocarbon). For NA/NP mixtures, $c^\mathbf{P}_{\mathbf{P}}$ is often negative, though exceptions occur (e.g., when the polar species is a ketone). For all other mixtures, positive $c^\mathbf{P}_{\mathbf{P}}$ is the norm; exceptions obtain, e.g., for quasi-ideal mixtures of components with similar effective polarity.

THE EXCESS-PROPERTY DECK OF CARDS

To stimulate interest in this method, a card game has been devised for use in class. Each card has the name of a common chemical written on one side, and the other side is blank. There are 52 cards in the deck, with representations of possible mixture types approximately as indicated above. The cards are shuffled and someone pulls out two cards without looking at the compounds. The signs on $g^\mathbf{P}$ and $h^\mathbf{P}$ for the mixture are then guessed. (The best guesses are $\Theta$.) Then, an "entropy coin" is taken out to determine the sign on $s^\mathbf{P}$. (Since the chances are about even, a coin flip is as good as any other guess.)

At this point the compounds are revealed and the mixture behavior predicted based on the probabilities and connections given in the tables. Finally, if the Appendix is available and it has the system (or a related one), it is possible to see how good the predictions are; if not, one of the group contribution methods for activity coefficients could be used to predict the sign on $g^\mathbf{P}$.

This is one of those exercises where quick students can often surpass the instructor in accuracy, though good fun is almost always had by all involved.

CLOSURE

The $g$ vs. $h$, the $h$ vs. $s$, and the $c$ vs. $s$ diagrams are effective props for displaying and categorizing the excess-property behavior of binary liquid mixtures. The six-type mixture-classification scheme, when used in conjunction with the diagrams, allows one to make some broad generalizations about liquid-mixture behavior. Thermodynamic arguments are few and classical in nature.

It would be foolish to ignore molecular concepts as aids for further organizing and explaining the results presented in this paper. In fact, the required level of molecular argument seems to be relatively modest, and precedents exist. We are preparing a "molecular exegesis" of this Field Guide which will be a second paper in this study.

The Appendix, which is available to interested readers by writing the senior authors, contains an enormous amount of information, which we use in various ways. For example, one can employ selected data in conjunction with the $g$ vs. $h$ or the $h$ vs. $s$ diagrams to illustrate and explain trends in families of binary mixtures containing a common component with a series of homologs. Educators will have no difficulty devising their own examples with this data collection and finding variations on the card game. There are a thousand stories here!

DEDICATION AND ACKNOWLEDGMENTS

This paper was dedicated to Hendrick C. Van Ness on the occasion of the celebration of this 65th birthday. Support for developing much of the material was provided to M.M.A. in the form of a Rensselaer Distinguished Teaching Fellowship, while his preparation of the manuscript was supported by the donors of the Proteus F. Trope Fund.

REFERENCES

The average professor must evaluate, or enlist the help of others in evaluating, a great number of report assignments written by students. How can that professor arrive at a grade rapidly, objectively, and reproducibly? The following offers a pragmatic and proven solution to this problem.

Evaluating technical texts is a dynamic task and no single method for doing so can be perfect. All professors challenge students in their own particular and personalized way, and through the years they find that their grading methods change and improve as new procedures appear in the literature and become known. In order to become involved in the quest for improved grading methods, some crucial questions must first be answered:

- **Is report writing considered an essential part of engineering apprenticeship?**
- **Is enough time taken in teaching students how to write a report and check the feedback, or is the teaching assistant left to struggle along on his own?**
- **How objective is the professor when evaluating a report?**
- **Can the same mark for the same report be arrived at both today and a month from now?**
- **Is flawless composition required, or are the calculations the only thing that matter?**

Arriving at a report grade can be as fascinating as a chess game. The grader tests the writer as much as the writer probes the grader. The various methods used to evaluate technical writing have been explored by Plung, but they are not suitable for the case at hand. They evaluate only continuous text and require rewriting to arrive at a score, whereas the reports we are dealing with contain text, figures, calculations, appendices, and nomenclature, and the number of assignments as well as the time pressure do not allow for rewriting.

My basic premise is that the grading system must be corrective, instructive, and simple. I have extracted ideas from all of the known methods and have added other, specific, items that apply to the learning process, with the result that over the years a pragmatic scoresheet has evolved which is effective in generating good-quality reports.

### SCORING GUIDE

A basic scoring guide is presented in Table 1. It addresses all the basic items that contribute to the quality of a report: efficiency or timeliness, overall presentation, quality of editing, technical level, and quality of calculations, tables, and figures.

It is essential that the students become familiar with the scoring guide before writing their reports. This is the instructive aspect of the method since the students can calculate their own grades and improve them at will before submitting the report. The method's corrective side comes from the fact...
that the basic items failed or violated are clearly stated, and the students are challenged to refine and improve their presentation.

The grader assigns either a "1" or a "0" to each item on the scoring guide, according to whether or not it has been satisfied. Items that are not applicable receive a "-" and are not entered on the score calculation. This is the simplicity of the method. After reading the report the professor can arrive at a precise and reproducible score in only a matter of minutes. The score is arrived at by dividing the total of numbers "1" by the total number of items judged. Table 2 shows a typical score sheet.

The system is also quite flexible and can be adapted to any number of situations. Items can be added to the list (or deleted), as necessary, to suit the type of assignment being graded.

DISCUSSION

I have used this system for several years now, with excellent results. The students are usually surprised and intrigued

TABLE 1
Scoring Guide for Written Technical Communications

<table>
<thead>
<tr>
<th>1. Work Efficiency</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>□ 1.1 Submitted on first requested date</td>
<td></td>
</tr>
<tr>
<td>□ 1.2 Submitted on second requested date</td>
<td></td>
</tr>
<tr>
<td>□ 1.3 Submitted with one granted extension of deadline</td>
<td></td>
</tr>
<tr>
<td>□ 1.4 Submitted with repeated extensions</td>
<td></td>
</tr>
<tr>
<td>□ 1.5 Submitted on an arbitrary date</td>
<td></td>
</tr>
<tr>
<td>□ 1.6 First or second version accepted</td>
<td></td>
</tr>
<tr>
<td>□ 1.7 Third or later version accepted</td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>2. Overall Quality of Presentation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>□ 2.1 Absence of scratches and visible corrections</td>
<td></td>
</tr>
<tr>
<td>□ 2.2 Required margin is observed</td>
<td></td>
</tr>
<tr>
<td>□ 2.3 Divisions of subject or text are clearly visible</td>
<td></td>
</tr>
<tr>
<td>□ 2.4 Correct linkage to prior sections or parts of work</td>
<td></td>
</tr>
<tr>
<td>□ 2.5 Figures and tables are on separate sheets</td>
<td></td>
</tr>
<tr>
<td>□ 2.6 Writing is easily readable</td>
<td></td>
</tr>
<tr>
<td>□ 2.7 Writing is readable with some effort</td>
<td></td>
</tr>
<tr>
<td>□ 2.8 Requested format on paper and ink is used</td>
<td></td>
</tr>
<tr>
<td>□ 2.9 Lines are double spaced</td>
<td></td>
</tr>
<tr>
<td>□ 2.10 Item 2 is accepted in its first version</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>3. Quality of Editing</th>
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</thead>
<tbody>
<tr>
<td>□ 3.1 Existence of 100% of required text</td>
<td></td>
</tr>
<tr>
<td>□ 3.2 Existence of 80% of required text</td>
<td></td>
</tr>
<tr>
<td>□ 3.3 Existence of 60% of required text</td>
<td></td>
</tr>
<tr>
<td>□ 3.4 Mean number of words per sentence is less than 16</td>
<td></td>
</tr>
<tr>
<td>□ 3.5 Absence of grammar infractions</td>
<td></td>
</tr>
<tr>
<td>□ 3.6 Percent of sentences containing grammar infractions is less than 5</td>
<td></td>
</tr>
<tr>
<td>□ 3.7 Percent of sentences containing grammar infractions is less than 10</td>
<td></td>
</tr>
<tr>
<td>□ 3.8 Absence of superfluous words or expressions</td>
<td></td>
</tr>
<tr>
<td>□ 3.9 Percent of words with more than 4 syllables is less than 8</td>
<td></td>
</tr>
<tr>
<td>□ 3.10 Percent of sentences containing style infractions (syntax) is less than 10</td>
<td></td>
</tr>
<tr>
<td>□ 3.11 Absence of sentences without meaning</td>
<td></td>
</tr>
<tr>
<td>□ 3.12 Absence of incomplete sentences</td>
<td></td>
</tr>
<tr>
<td>□ 3.13 Existence of continuous and easily readable text</td>
<td></td>
</tr>
<tr>
<td>□ 3.14 Text conforms to the required number of words</td>
<td></td>
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<tr>
<td>□ 3.15 Item 3 is accepted in its first version</td>
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<table>
<thead>
<tr>
<th>4. Technical Level</th>
<th></th>
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</thead>
<tbody>
<tr>
<td>□ 4.1 Existence of all items requested</td>
<td></td>
</tr>
<tr>
<td>□ 4.2 Appropriate use of subtitles</td>
<td></td>
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</tbody>
</table>

| □ 4.3 Coverage of subject matter is above 90% |   |
| □ 4.4 Coverage of subject matter is above 60% |   |
| □ 4.5 Existence of correct reasoning for all items covered |   |
| □ 4.6 Existence of correct reasoning for part of the items covered |   |
| □ 4.7 Number of original ideas is above zero |   |
| □ 4.8 Number of original ideas is above three |   |
| □ 4.9 Absence of nonsense |   |
| □ 4.10 Absence of meaningless, superfluous, or false arguments |   |
| □ 4.11 Number of ideas expressed divided by number of sentences used is above 0.90 |   |
| □ 4.12 Sufficient information for reader to understand everything |   |
| □ 4.13 Correct reference to attachments and literature |   |
| □ 4.14 Item 4 is accepted in its first version |   |

<table>
<thead>
<tr>
<th>5. Quality of Calculations</th>
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<tbody>
<tr>
<td>□ 5.1 Existence of titles and subtitles in the sample calculation</td>
<td></td>
</tr>
<tr>
<td>□ 5.2 Elegant layout on the sheet</td>
<td></td>
</tr>
<tr>
<td>□ 5.3 Origin of the data is identified</td>
<td></td>
</tr>
<tr>
<td>□ 5.4 Symbols are defined</td>
<td></td>
</tr>
<tr>
<td>□ 5.5 Sequence of presentation is clear</td>
<td></td>
</tr>
<tr>
<td>□ 5.6 Equations are identified</td>
<td></td>
</tr>
<tr>
<td>□ 5.7 Results are highlighted</td>
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</tr>
<tr>
<td>□ 5.8 SI units are used</td>
<td></td>
</tr>
<tr>
<td>□ 5.9 Absence of arithmetic errors</td>
<td></td>
</tr>
<tr>
<td>□ 5.10 Complete results are presented</td>
<td></td>
</tr>
<tr>
<td>□ 5.11 Sufficient information for reader to follow and understand the calculations</td>
<td></td>
</tr>
<tr>
<td>□ 5.12 Presence of 90% of sample calculation required by subject</td>
<td></td>
</tr>
<tr>
<td>□ 5.13 Presence of 60% of sample calculation required by subject</td>
<td></td>
</tr>
<tr>
<td>□ 5.14 Item 5 is accepted in its first version</td>
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</tbody>
</table>

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<tr>
<th>6. Quality of Drawings, Graphs, and Tables</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>□ 6.1 Identification by number and title</td>
<td></td>
</tr>
<tr>
<td>□ 6.2 Correct layout on the sheet</td>
<td></td>
</tr>
<tr>
<td>□ 6.3 Requested margin on the left side or top of page</td>
<td></td>
</tr>
<tr>
<td>□ 6.4 Coordinates are identified</td>
<td></td>
</tr>
<tr>
<td>□ 6.5 Scales are stated</td>
<td></td>
</tr>
<tr>
<td>□ 6.6 Drawing aids used to draw lines and curves</td>
<td></td>
</tr>
<tr>
<td>□ 6.7 Good quality lettering</td>
<td></td>
</tr>
<tr>
<td>□ 6.8 Suitable for double reduction on a copying machine</td>
<td></td>
</tr>
<tr>
<td>□ 6.9 Presence of 90% of information required by subject matter</td>
<td></td>
</tr>
<tr>
<td>□ 6.10 Presence of 60% of information required by subject matter</td>
<td></td>
</tr>
<tr>
<td>□ 6.11 Item 6 is accepted in its first version</td>
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</tbody>
</table>
by the guide when they first receive it, and they confidently set out to write their first report. It is a common occurrence for their first report to be returned to them for rewriting, but within a short time (usually within two or three assignments) they have familiarized themselves with the system and they begin to produce excellent reports.

The scoring guide is not limited in any sense of the word—not to a specific language or to a specific environment. It is applicable in any language of instruction and may even be taken along as a guide for a junior engineer on the job. It has been called "mechanistic," which in fact it is. It has no pretensions of being profoundly philosophic. It guides students (and possibly engineers) in a very simple and modest way in the preparation of reports. It challenges them to define and attain their own degree of perfection. In this sense it represents a general philosophy of writing instruction that can be applied to any type of writing. Project reports, review reports, laboratory reports, and most technical assignments can all be easily handled with the scoring guide (tailored, as necessary, to the specific subject).

Different weights can be assigned to different items, or a total score can be used instead of averaging the six partial scores as shown in Table 2. In fact, I have tried these different approaches in the past, but for various reasons I have later dismissed them. The score sheet shown in Table 2 has emerged over the years as the most effective, expedient, and simplest method of scoring. But opinions differ, and the beauty of this system lies in the fact that it can accommodate any number of adaptations.

Various items on the guide require a personal judgment on the part of the grader. This is unavoidable. As a corrective instrument, the guide warns writers that these judgments will be made, and it allows the writers to stack the odds in their favor by paying special attention to those various requirements. The originality of the whole idea, in fact, lies in this corrective aspect of the guide.

No grade is assigned to the work until it is judged acceptable, but unfortunately, acceptability in itself is a subjective notion. (For example, how often does peer review of technical papers produce unanimous results?) The professor will establish his or her own definition of acceptability by answering and weighting the questions posed at the beginning of this article, which bear repeating here:

- Is report writing considered an essential part of engineering apprenticeship?
- Is enough time taken in teaching students how to write a report and check the feedback, or is the teaching assistant left to struggle along on his own?
- How objective is the professor when evaluating a report?
- Can the same mark for the same report be arrived at both today and a month from now?
- Is flawless composition required, or are the calculations the only thing that matter?

Although each of the items on the scoring guide calls for a personal judgment on the part of the grader, that judgment will (hopefully) remain the same in all cases and not vary from one paper to the next. For example, an "0" for items 2.7, 3.3, 4.4, or 5.9 on the guide will always render a report unacceptable to me, and students are so informed at the very beginning of the course.

**CONCLUSIONS**

No writing guide can be perfect or final, and this one is no exception. But if the philosophy behind it is accepted and it is adapted to improve your present grading system, my objective in writing this paper has been realized.

**REFERENCES**

AUTHOR GUIDELINES

This guide is offered to aid authors in preparing manuscripts for Chemical Engineering Education (CEE), a quarterly journal published by the Chemical Engineering Division of the American Society for Engineering Education (ASEE).

CEE publishes papers in the broad field of chemical engineering education. Papers generally describe a course, a laboratory, a ChE department, a ChE educator, a ChE curriculum, research program, machine computation, special instructional programs, or give views and opinions on various topics of interest to the profession.

• Specific suggestions on preparing papers •

TITLE • Use specific and informative titles. They should be as brief as possible, consistent with the need for defining the subject area covered by the paper.

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TABLES • Avoid tables and graphs which involve duplication or superfluous data. If you can use a graph, do not include a table. If the reader needs the table, omit the graph. Substitute a few typical results for lengthy tables when practical. Avoid computer printouts.

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ACKNOWLEDGMENT • Include in acknowledgment only such credits as are essential.

LITERATURE CITED • References should be numbered and listed on a separate sheet in the order occurring in the text.

COPY REQUIREMENTS • Send two legible copies of the typed (double-spaced) manuscript on standard letter-size paper. Submit original drawings (or clear prints) of graphs and diagrams on separate sheets of paper, and include clear glossy prints of any photographs that will be used. Choose graph papers with blue cross-sectional lines; other colors interfere with good reproduction. Label ordinates and abscissas of graphs along the axes and outside the graph proper. Figure captions and legends will be set in type and need not be lettered on the drawings. Number all illustrations consecutively. Supply all captions and legends typed on a separate page. State in cover letter if drawings or photographs are to be returned. Authors should also include brief biographical sketches and recent photographs with the manuscript.
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