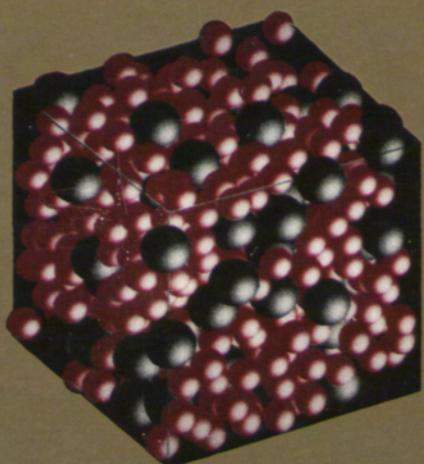
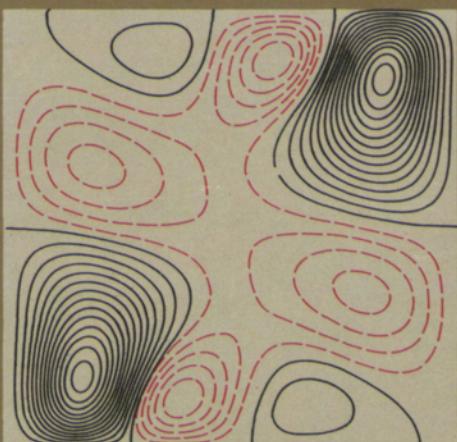
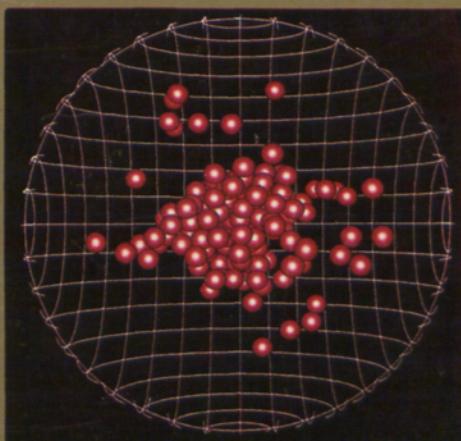
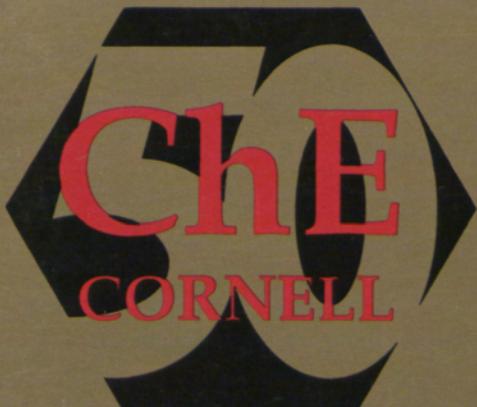


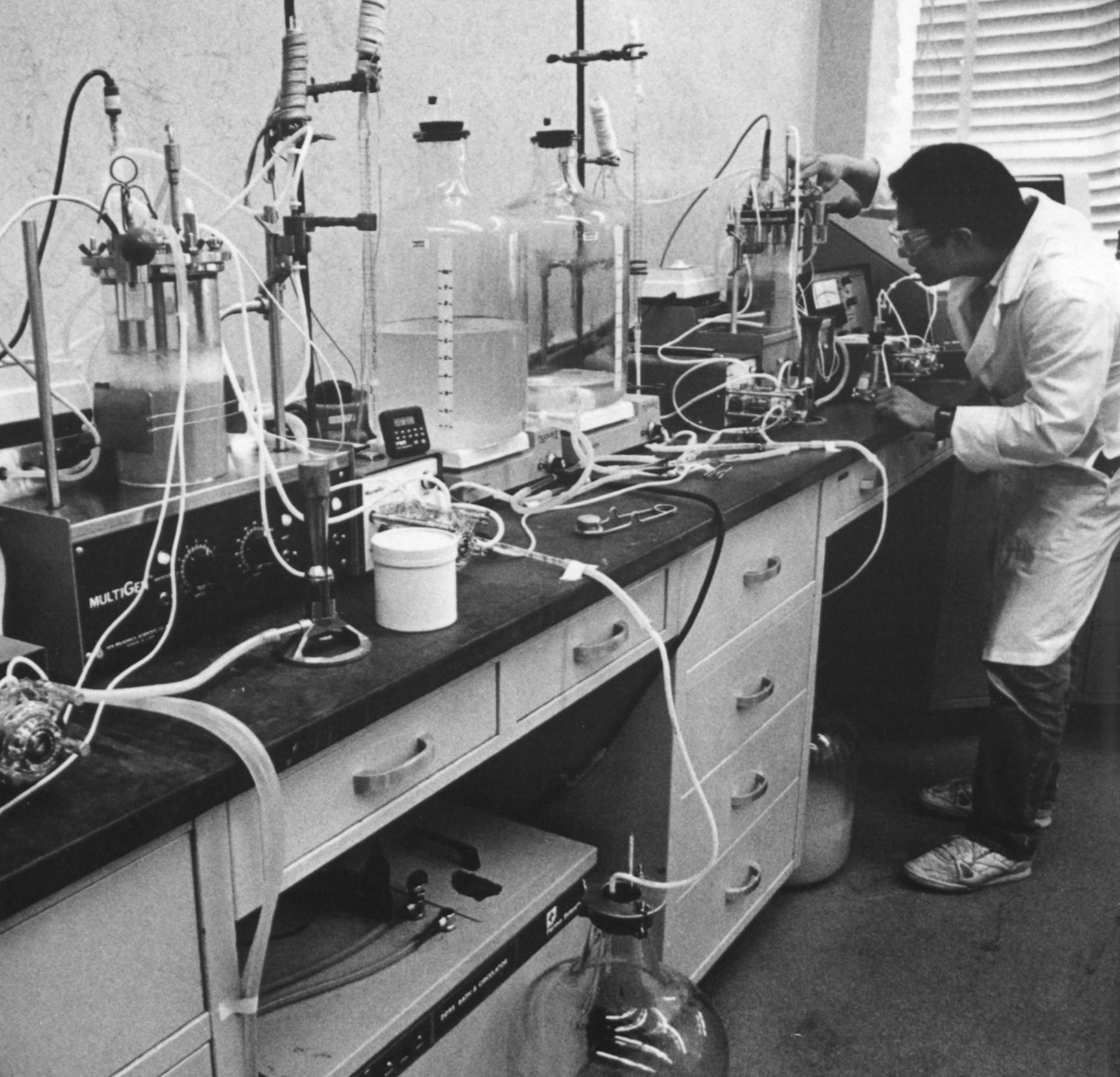
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THE CHEM. E. SCHOOL:
FIFTY YEARS OLD
AND GOING STRONG



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Opposite: In Professor Shuler's laboratory, graduate student Jeffrey Fu works with the experimental reactor for producing excreted protein by means of E. coli (see page 43).

Outside cover, clockwise from upper left: The logo for the Golden Jubilee of the School of Chemical Engineering; a "snapshot" of a drop of methane molecules in equilibrium with vapor (see page 27); an entrance to Olin Hall of Chemical Engineering; a simulation of a hypothetical "alloy" (see page 30); a "fingerprint" of a small destabilizing disturbance, part of a study of the transition from steady to periodic convection in a model system consisting of a flask of fluid-saturated porous material heated from below (see page 39).

THE FIRST FIFTY YEARS

of Cornell's School of Chemical Engineering

by Julian C. Smith

In 1938 the new School of Chemical Engineering at Cornell was small and isolated, with only a tenuous allegiance to the College of Engineering and little interaction with the rest of the university. In 1988, as it celebrates its Golden Anniversary, the school is a strong, integral part of the college and has important links within and beyond the university. This article is a brief account of how the school began, events that have taken place during its half-century of history, and directions it is taking today.

Actually, the origins of the school go back a lot further than 1938. As a recognized curriculum, chemical engineering dates back to 1930, and as long ago as 1870 there were sporadic offerings of courses in industrial chemistry. In the early 1890s, just after MIT started the first chemical en-

gineering program anywhere, Cornell offered an option in chemical engineering for mechanical engineers, but there was no support for a formal program in the engineering college. Also, most members of the chemistry department were opposed to such a program—they wanted to keep chemical engineering under their wing. But the idea was hotly debated around 1911. In that year a professional program leading to the degree Bachelor of Chemistry was established in the chemistry department, at least in part to prevent the formation of a chemical engineering curriculum.

It wasn't until 1930 that Fred H. "Dusty" Rhodes was able to set up a true program. Dusty was a Cornell Ph.D. in chemistry who had gained some industrial experience during World War I and had returned to Cornell in 1920 as a professor of industrial chemistry. From the beginning, his lectures were largely on unit operations and other chemical engineering topics, yet no one (except Dusty) wanted a full-blown program. Finally, he proposed a compromise that met with enthusiasm: a hybrid program with four years in the Department of Chemistry, leading to the B.Chem. degree, followed by a fifth year in the College

of Engineering, culminating in the degree Chemical Engineer. To almost everyone's surprise, the program flourished and grew until, in 1937–38, Dusty was able to break with Chemistry and establish the School of Chemical Engineering as part of the College of Engineering. A five-year program, integrated with the regular engineering curriculum, led to the degree Bachelor of Chemical Engineering. By then the faculty size had doubled with the appointment of Charles C. (Chuck) Winding in 1935.

A NEW BUILDING AND A WORLD WAR

For four years the new school was housed in Baker Laboratory, grudgingly given space by the chemistry department. In 1938 Oscar J. Swenson was appointed as assistant professor, and in 1941 Dusty Rhodes was named the Herbert Fisk Johnson Professor of Industrial Chemistry. During this period, Dusty and Engineering Dean S. C. Hollister persuaded Franklin W. Olin, a Cornell graduate of 1886, to give money in memory of his son for the construction of a new building. Olin Hall, the first of the new engineering buildings at the south end of the campus, was built in 1941–42 at a cost

Julian C. Smith is also the author of *The School of Chemical Engineering at Cornell: A History of the First Fifty Years*, which was published this spring by the College of Engineering as Volume I of the series Cornell Engineering Histories. The illustrated book may be obtained from the School of Chemical Engineering.

*“...as it celebrates its Golden Anniversary,
the school... has important links
within and beyond the university.”*

of \$9.64 per square foot. The school moved from Baker Laboratory in February 1943, making both the chemists and the chemical engineers happy.

During World War II, almost all the able-bodied men on campus were in the Navy V-12 program. In this program, four years of work were crammed into three years that culminated in the award of the

degree Bachelor of Science in Chemical Engineering. Professors Rhodes, Winding, Swenson, and Clyde W. Mason, who came from Chemistry to Chemical Engineering in 1941, carried enormous teaching loads, yet found time to do consulting on war-

Olin Hall was constructed in 1941-42 on this site. The view is of Central Avenue in the 1920s.



related projects. Student enrollments fluctuated wildly, rising to new heights and then dropping, in 1946, to five undergraduates and two graduate students. When the war ended, the returning veterans swelled the class sizes once again.

DEVELOPMENT UNDER RHODES DURING THE POSTWAR YEARS

After the war, returning veterans with G.I. benefits began filling up Olin Hall. Housing was scarce, so Dusty arranged for twenty students to live in Olin, under strict rules governing their behavior. By 1951 the “veteran bulge” had passed by and enrollments fell to a much more manageable level.

Swenson resigned in 1946 and three assistant professors—Julian C. Smith, Robert L. Von Berg, and Herbert F. Wiegandt—were appointed.

The 1950s were relatively peaceful. The five-year curriculum was modified substantially and graduate study and research increased a little, although the emphasis continued to be heavily on undergraduate instruction. Several more faculty members were added: Jay E. Hedrick, Raymond G. Thorpe, Peter Harriott, Robert K. Finn, and

Robert York, who was named the Socony-Mobil Professor.

During this period, a division of metallurgical engineering was developed. It had been established in 1947, and from then until 1963 the school was called the School of Chemical and Metallurgical Engineering. The first director of the division was Peter E. Kyle, who served until 1954, when he was succeeded by George V. Smith. Each of these men held the Francis Norwood Bard Professorship of Metallurgical Engineering. The faculty in the division grew from two in 1947 to eight in 1963, although undergraduate enrollments remained small. The five-year curriculum was similar in form to that in chemical engineering; in fact, in the first year they were identical.

In 1963 metallurgical engineering was combined with other disciplines to form the Department of Engineering Physics and Materials Science, and the metallurgical engineering faculty moved from Olin Hall to the new Bard Hall. The program was greatly broadened as the emphasis shifted from metallurgy to materials science and from industrial practice to research. Today, although metallurgy is a



Fred H. "Dusty" Rhodes was the founder and first director of the School of Chemical Engineering, serving from 1937-38 until his retirement in 1957.

This photograph, taken in the early 1950s, shows him with the school tie he designed and tried to get all the students to wear. The graduating seniors, that first year, presented him with a matching vest in red, black, and gold (the colors of the Golden Jubilee).

significant part of the materials science curriculum, the term "metallurgical engineering" is gone from the Cornell lexicon.

Dusty Rhodes, who started programs in both chemical and metallurgical engineering at Cornell, was a remarkable teacher. He evenhandedly dismayed and inspired his students, and showed them how much they could accomplish under pressure. His notorious report-grading system was typical: he gave one grade for technical content and one for presentation, then multiplied them and divided by 100; thus 70 for form and 80 for content meant a grade of 56. A

satisfactory score, according to Dusty, was 75. Chemical engineering was considered the most difficult course in the university.

As Cornell President Dale R. Corson wrote after Dusty's death in 1975, "Dusty Rhodes was himself no ordinary person, and he wanted extraordinary individuals as students. He wanted to teach and train superior engineers. . . . He fought for his students, he supported them. . . [and he] continued to be concerned about them after they left Olin Hall."

In 1956 Dusty Rhodes took a sabbatical leave (his only one) and retired the next year. Chuck Winding, who had been acting director while Dusty was on leave, became the second director of the school when Dusty returned the following year. Winding also assumed the Herbert Fisk Johnson professorship.

WINDING AS DIRECTOR IN CHANGING TIMES

In the early part of his thirteen-year service as director, from 1957 to 1970, Charles C. Winding was occupied with the need to adapt the school's program to changing conditions. That first year, he started a six-year professional nonthesis graduate program that led to the degree Master of Chemical Engineering. By 1960 about 30 percent of the B.Ch.E. graduates were going on to graduate school, and so Winding introduced a predoctoral honors program for undergraduates planning careers in teaching or research.

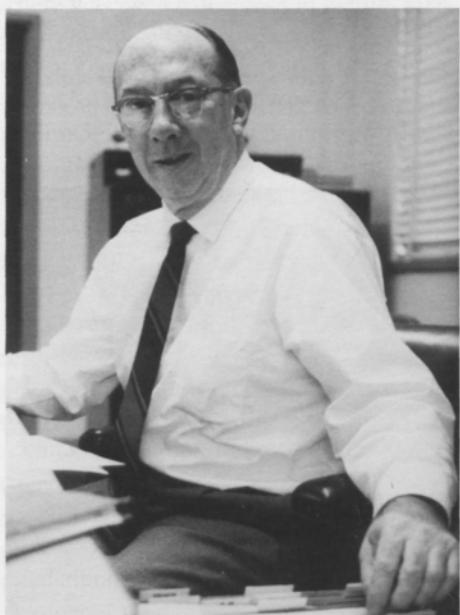
That same year the College of Engineering established the Division of Basic Studies to administer a "common" curriculum for the first two years: all undergraduates were to take the same courses as underclassmen, and then choose an upperclass major. Winding and his faculty fought hard to retain some difference for chemical

engineering students. They were successful in convincing their colleagues in other departments that chemical engineering is "different" in that it is based largely on chemistry and not on physics, and so won approval for a modified underclass program for students planning to enter chemical engineering.

Faculty members appointed during this period were Ferdinand Rodriguez, George F. Scheele, George G. Cocks, and Jean Paul Leinroth. In 1958 Clyde Mason became the Emile M. Chamot Professor of Chemical Microscopy; in 1966 he retired and Cocks took over the courses in materials and microscopy.

In 1964 there were more signs of change. A committee that I chaired suggested a complete reorganization of the College of Engineering, with new research

Charles C. "Chuck" Winding was the school's second faculty member (from 1935) and second director (from 1957 to 1970).



departments replacing the traditional schools. Also, the Engineering Policy Committee recommended abandoning the five-year baccalaureate curriculum in favor of a four-year Bachelor of Science degree program and a one-year Master of Engineering program. Both propositions were controversial. The reorganization of the college was discussed and (wisely) tabled; the four-year undergraduate program, to begin in 1965, was approved.

Although faculty turmoil diminished, student turmoil began. Increased concern over the injustices of the Vietnam war and the plight of minorities led to marches, demonstrations, mass meetings, sit-ins, confrontations, student strikes. Some incidents became ugly; there was damage from vandalism, including the setting of fire bombs. Chuck Winding did a good job of holding the school together through this trying period. Normal activity continued; for example, two assistant professors, Victor Edwards and David M. Watt, were added to the chemical engineering faculty.

Chuck Winding, although more favorably inclined toward research and graduate study than his predecessor had been, continued Dusty Rhodes' emphasis on undergraduate and professional training. This was an unpopular stance in the 1960s, in view of the general concern for increased science and research in engineering education, and the school was considered to be lagging behind in these areas.

AN EMPHASIS ON RESEARCH UNDER BISCHOFF

An "outside" committee appointed by Dean Andrew Schultz, Jr. to study the school and its activities made recommendations that led ultimately to the appointment in 1970 of Kenneth B. Bischoff, a young research-minded professor from the

"Chuck Winding, although more favorably inclined toward research . . . continued Dusty Rhodes' emphasis on undergraduate education and professional training."

Right: The third director of the school was Kenneth B. Bischoff, who served for five years beginning in 1975. Under Bischoff, the school began an effort to increase research activity.



University of Maryland, as the third director of the school.

Ken Bischoff was appointed with the expectation that he would change the direction of the school, especially in research. He did. He soon hired three young assistant professors, all excellent researchers—John L. Anderson, James F. Stevenson, and Michael L. Shuler. Bischoff also made a number of changes in the teaching programs, especially in the M.Eng. (Chemical) program, which almost inevitably led to dissension among the members of his faculty. In addition, he instituted a research honors program for gifted undergraduates interested in research and advanced study.

Attention to practice-oriented education was not neglected, however. A work-study program (part of the college's Engineering Cooperative Program) in which undergraduates gained employment experience in industry was introduced during Bischoff's tenure.

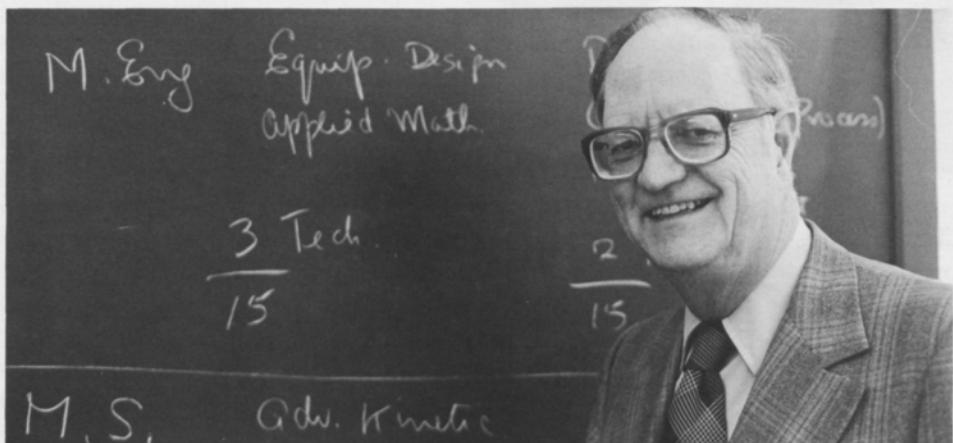
Undergraduate enrollments continued steady, with about forty students in each class. Graduate enrollments rose slowly—disappointingly so, for the pace of research had quickened and more well-qualified graduate students were needed. In 1971 job

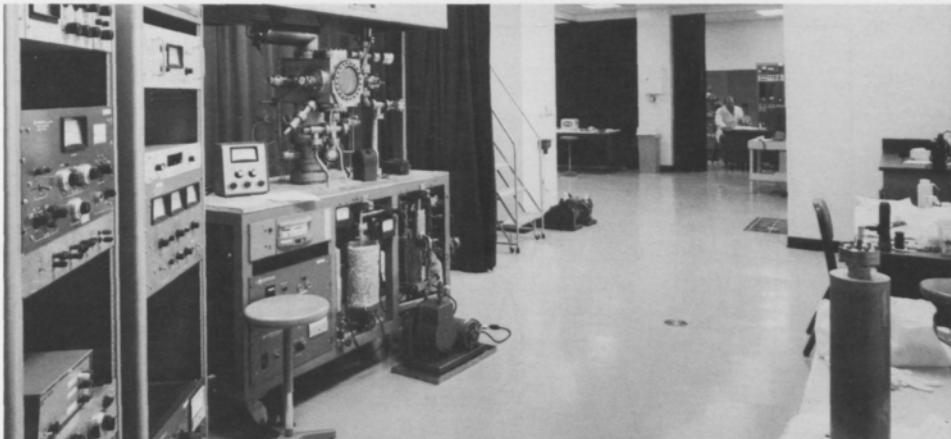
opportunities for chemical engineers were at an all-time low, but by 1975, as a result of burgeoning synthetic-fuels programs sparked by the energy crisis of 1973–74, there were more openings than people to fill them.

Professors Edwards, Leinroth, and Watt left the school between 1971 and 1973, and Professors Hedrick and Winding retired in 1975. Peter Harriott was named the Fred H. Rhodes Professor of Chemical Engineering in 1974. After six years in the dean's office as director of continuing engineering education, I returned to Chemical Engi-

neering in 1971 and became associate director in 1973 and director in 1975, when Ken Bischoff stepped down.

Below: At the school Julian C. Smith has been a student (B.Chem. '41 and Chem.E. '42), faculty member (beginning in 1945), and director (from 1975 to 1983). He also served as the college's director of continuing education for many years. He has been an emeritus professor since 1986.





Left: The conversion of a basement storage area to a "clean room" for Professor Merrill's research was the first of the continuing major renovations of the original building.

GROWTH AND DEVELOPMENT DURING THE SMITH YEARS

The eight-year period during which I served as director of the school was a time of rebuilding in the faculty and in Olin Hall. So that faculty differences could have a chance to be resolved, not much was changed during the first year. The need to augment the faculty was clear, however. There was even a decrease in faculty size, for John Anderson resigned to take a position at Carnegie-Mellon University.

A search was begun for a distinguished professor, and in 1976 it bore fruit with the appointments of two outstanding men: Keith E. Gubbins became the Thomas R. Briggs Professor of Engineering and Robert P. Merrill was named the Herbert Fisk Johnson Professor of Industrial Chemistry. They brought well-established research programs with them and began a period of rapid growth in the research activities of the school.

Also in 1976, Professor Bischoff left Cornell to join the faculty of the University of Delaware. In 1977 Jim Stevenson left to go into industry. (He was the last of the faculty members hired between 1965 and 1972; for various reasons, all of them had

left the school.) In 1978 Robert York died suddenly of a heart attack a few months before his scheduled retirement.

The much-needed renovation of Olin Hall began in 1976 with the construction of a "clean room" for Bob Merrill's ultrahigh-vacuum studies of surface chemistry and catalysis, and the acquisition of a departmental computer facility for Keith Gubbins' research in statistical mechanics. Nine laboratories were refurbished in the east wing; the Unit Operations Laboratory was painted for the first time in thirty-eight years; and a microbiology teaching laboratory was built on the third floor. Olin Hall also got an expanded electrical system and a new roof. These changes were funded by a \$500,000 gift from the Pew Foundation, allocations from the university and the engineering college, and a grant from the National Science Foundation.

The period was one of growth in all aspects of the school's program. Undergraduate enrollments swelled to record levels, with seventy-five to eighty students in each class; for the nine years between 1977 and 1985, the number of B.S. degrees awarded annually was almost double the average number for the preceding twenty

years. More students meant heavier teaching loads for the faculty and exacerbated problems with the aging laboratory facilities. Also, the pace of research rose at a phenomenal rate, tripling in dollar expenditures between 1975 and 1979 and doubling again by 1983. Graduate-student enrollments began to rise in both number and quality after the formation of a recruitment committee chaired by Mike Shuler. Cornell Chemical Engineering became known as a leading research department.

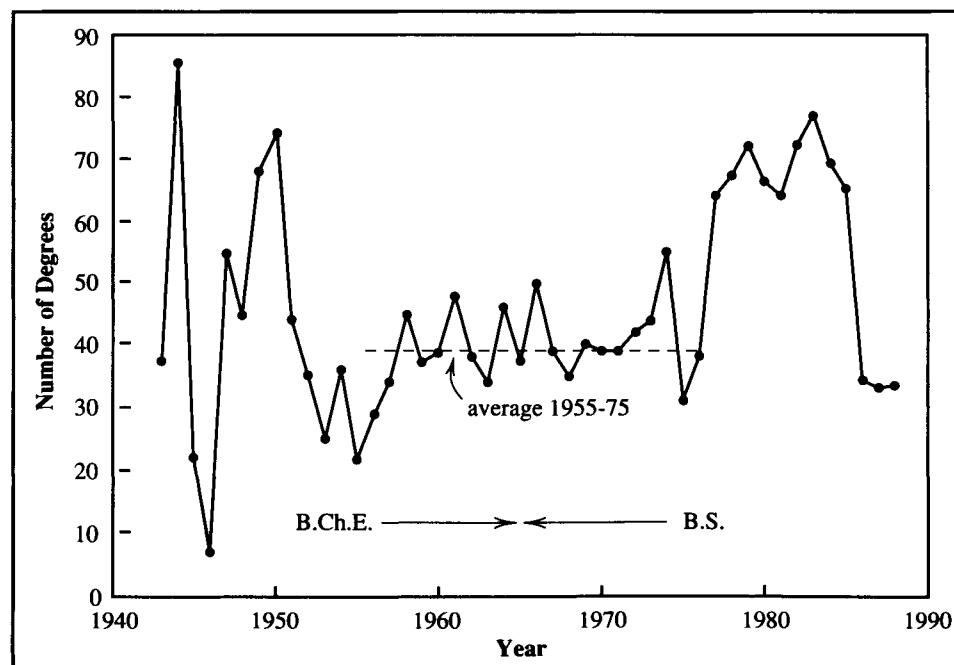
Faculty searches, which seemed to continue endlessly, led to the appointment of five assistant professors: Claude Cohen, William Olbricht, Joseph Cocchetto, Paul Steen, and Douglas Clark. In 1978 William B. Streett was appointed as a senior research associate; he was named professor in 1981 and became dean of engineering in 1985. In 1981 George Cocks retired and took a position at the Los Alamos National Laboratory. Jorge Calado of the University of Lisbon, Portugal, was named adjunct professor. Three visiting professors, all alumni of the school, came from industry to help teach undergraduate courses; they were Kenneth Karmel, Joseph Degenfelder, and Fred Vorhis.

Figure 1. Fluctuations in the number of baccalaureate degrees awarded in chemical engineering at Cornell since the beginning of the school.

An innovation was the formation of the Chemical Engineering Advisory Council. Twelve members, mostly from industry and mostly alumni, agreed to serve on this council to give advice on the needs and future directions of the school.

CONTINUED EXPANSION OF RESEARCH UNDER GUBBINS

In 1983, when I stepped down from the directorship, Keith E. Gubbins was named the fifth director of the school. He has continued the emphasis on research: annual expenditures are estimated at \$4.6 million for 1987-88, over triple the amount for 1983-84. The growth of chemical engineering research has paralleled a similar transformation in the engineering college as a whole*, though it began somewhat later. Articles elsewhere in this issue describe activities in the principal areas of research interest in the school: thermodynamics and statistical mechanics, surface science and catalysis, fluid mechanics and rheology, polymer technology, biochemi-



cal engineering, and process simulation and computer-aided design.

Developments in research and teaching were accompanied by the addition of new equipment. The original PDP 11/70 mini-computer was upgraded to a much more powerful VAX 8250; for undergraduate teaching, the Instructional Computing Facility was established in 1985 through a generous gift from the Class of 1960.

The faculty has changed a lot in the past five years. Joe Cocchetto and Douglas Clark left the school. My retirement in 1986 was followed by those of Herb Wiegandt in 1987 and Robert Von Berg in 1988. Six assistant professors were appointed: Paulette Clancy, Brad Anton, Peter Clark, Donald Koch, Athanassios Panagiotopoulos, and Daniel Hammer. In 1986 John Zollweg, a research associate, was appointed a nontenured associate professor, and Margarida Telo da Gama of the

University of Lisbon was named adjunct professor. For the past three years Helen Haller (who earned her B.Ch.E. at Cornell and was the school's first woman Ph.D.) has been appointed as a lecturer to run the unit operations laboratory and help with the process design course, and Clarence Shoch, a visiting professor, has taught process design and supervised M.Eng. design projects.

Two former members of the faculty recently died—Clyde Mason in 1983 and Chuck Winding in 1986.

Several of the school's faculty members have received national recognition in recent years—awards from professional societies have been given to Professors Finn, Gubbins, and Shuler.

In 1983 Gubbins established the position of administrative manager of the school (something I had unsuccessfully tried to do). Betty J. Bortz currently holds

*See "The Rise of Research" by J. C. Smith, *Engineering: Cornell Quarterly*, Summer 1985, pp. 26-36.

this position. There are also an executive assistant, a coordinator for external relations, an accounts coordinator, administrative aides, secretaries, a research support specialist, and two laboratory equipment technicians. The Advisory Council has been expanded to eighteen members and includes prominent individuals from several other universities as well as industrial leaders.

A new venture made possible by alumni contributions was the founding, in 1987, of the Julian C. Smith Lectureship. The first Smith Lecturer was Professor R. Byron Bird of the University of Wisconsin.

A complete renovation of the east wing of Olin Hall is now underway. Twenty-three new offices and laboratories are being created by flooring over unused space in the "high bay" of the Unit Operations Laboratory. The \$5 million needed for this has come from industrial firms and alumni, with large gifts from Harry Mattin '18 and H. D. "Ted" Doan '45. Completion of the three lower floors is scheduled for January 1989.

LOOKING BACK, MOVING AHEAD

The school has changed greatly during its first fifty years. The focus has shifted from an almost exclusive concern for undergraduate teaching to a balanced program of teaching and research. In 1937 there were seven undergraduate degrees and one advanced degree awarded in chemical engineering; in 1987 the numbers were thirty-three undergraduate and twenty-seven advanced degrees. In 1938, when the school was founded, it had three faculty members and two staff persons; in 1988 the faculty consists of twenty professors of various ranks and six others with the title of adjunct professor, senior research associ-

ate, lecturer, or visiting professor, and the support staff numbers thirteen. Research has grown from almost nothing to a very large enterprise.

Undergraduate enrollments were small until about 1940. They fluctuated wildly during World War II, stayed fairly constant from 1953 to 1975, almost doubled for nine years, and then fell abruptly in 1985 to the present level. This is reflected in the number of degrees granted (see Figure 1). Altogether there have been 2,239 undergraduate degrees and 751 advanced degrees awarded in chemical engineering.

Women students now make up a quarter to a third of the undergraduate classes, in comparison with none before 1945; they also comprise 20 percent of the candidates for advanced degrees. In graduate studies, the majority of matriculants are now seeking the Ph.D. instead of a terminal master's degree.

The original five-year baccalaureate curriculum gave way to the present four-year program in 1964, and the credit-hour requirement for a bachelor's degree has dropped from 176 in 1938 to the current 137. About half of the courses in chemistry that were once required have been replaced

by chemical engineering courses, and the original requirements in mechanical and electrical engineering, mineralogy, German, and accounting have disappeared in favor of electives.

The first fifty years of the School of Chemical Engineering at Cornell have encompassed changes that could hardly have been imagined by Dusty Rhodes when he was trying to establish a discipline, let alone a school, at the university. But throughout the years, the program must have been unusually successful, for Cornell's chemical engineering alumni are extraordinarily supportive of the school.

The story at Cornell is, of course, part of the amazing history of the profession and of the chemical manufacturing industries. Today chemical engineering is on the move, and with new industrial ventures and the growing public concern for the environment, opportunities abound for chemical engineers. Specifically what the coming years will bring to the school, our graduates, and our profession is hard to say, but as we celebrate our Golden Jubilee, we anticipate another eventful half-century.

STRONG AND LOOKING AHEAD

The School of Chemical Engineering Today

by Keith E. Gubbins and George F. Scheele

The profession of chemical engineering is undergoing rapid change and expansion into areas of new technology. The development of composite and other new materials, the manufacture of computer chips, environmental risk assessment, and biotechnology are examples of the areas in which the principles of chemical engineering are of increasing importance.

The changes present challenges to the School of Chemical Engineering, and the school, like the profession, has been undergoing change.

Over the past decade, twelve new faculty members have been added—six of them in the last two years—and the research and graduate programs have been substantially strengthened. Research expenditures have risen from a modest \$164,000 in 1977–78 to an estimated \$4.6 million in 1987–88. The number of graduate students has increased correspondingly; there are now about seventy very good students in the doctoral program.

At the same time, the undergraduate program has been adapted without compromise of its traditional strength. Our aim is to continue to provide the preparation necessary for leadership in the profession.

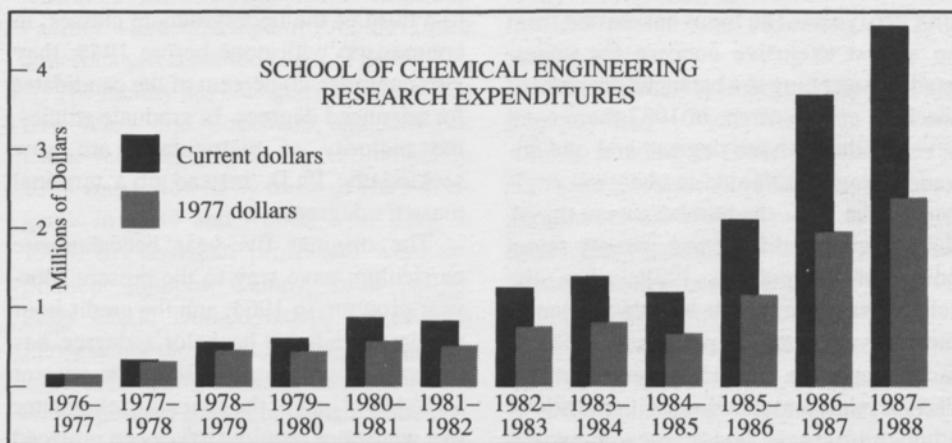
MEETING FACILITIES NEEDS: THE OLIN HALL OVERHAUL

The rapid growth in research and graduate programs, while welcome, has placed a severe strain on the school's facilities. Olin Hall, the oldest of the engineering buildings, was designed for undergraduate instruction in an era when experience in using pilot-scale equipment and in analytical chemistry was an important component of the degree program. The large high-bay area was not designed for modern teaching, which now is usually better accomplished using smaller-scale equipment. The space

was needed to provide more laboratories for research, which is highly diverse and often centers around specialized and sensitive instruments.

A major renovation of the facilities in Olin Hall is, therefore, a high priority. The first phase—a complete overhaul of the east wing of the building, to be completed in the spring of 1989—will provide twenty modern and sophisticated laboratories for teaching and research.

Figure 1. Statistics showing the rise in research activity at the school.





"The rapid growth in research and graduate programs, while welcome, has placed a severe strain on the school's facilities."



Left: The old high-bay area in Olin Hall, designed to house tall columns and large equipment, is being converted to three stories of laboratory space. The photograph, taken during the planning stage, shows Keith Gubbins and Julian Smith considering the possibilities.

The first phase of the overall program is a \$5-million renovation in the east wing. This will

provide twenty new laboratories in the basement and on the first two floors. In the second phase, new laboratories will be installed on the third floor.

Above: Signs of construction were visible on the exterior as well as inside. This was the scene outside Olin last fall.



Above: The faculty in March 1988.

Bottom row, left to right: Robert P. Merrill, Helen D. Haller (lecturer), Peter A. Clark, Keith E. Gubbins, and Paulette Clancy.

Second row: Clarence Shoch (visiting professor from Du Pont), Ferdinand Rodriguez,

William B. Streett, Robert L. Von Berg, Robert K. Finn, and Herbert Wiegandt (emeritus).

Third row: Paul H. Steen, John Rowlinson (visiting professor from Oxford University), John A. Zollweg, Daniel A. Hammer, and Peter Harriott.

Top row: Donald L. Koch, Michael L. Shuler, A. Brad Anton, George F. Scheele, Athanassios Panagiotopoulos, and Claude Cohen.

Not pictured are William L. Olbricht and Raymond G. Thorpe.

VITALITY IN AN OUTSTANDING RESEARCH PROGRAM

The research interests of the faculty reflect areas of current activity in chemical engineering today (see Tables I and II).

Since many of the research programs are multidisciplinary in nature, faculty members are active in several interdisciplinary research centers and programs on campus. These include the Biotechnology Institute and Center (Finn, Hammer, Olbricht, Shuler); the Cornell Manufacturing Engineering and Productivity Program (Clancy); the Cornell Injection Molding Program (Cohen); the Materials Science Center (Anton, Clancy, Gubbins, Merrill); the Mathematical Sciences Institute (Cohen, Gubbins, Steen); the National Nanofabrication Facility (Rodriguez); and the Center for Theory and Simulation in Science and Engineering—the supercomputer facility, referred to locally as the Theory Center (Clancy, Gubbins, Panagiotopoulos, Steen, Streett, Zollweg).

The research activities of the senior faculty members are frequently recognized by national and international awards. In the last few years:

- Robert Finn received both the Van Lanen Award of the American Chemical Society and the Food, Pharmaceutical, and Bioengineering Award of the American Institute of Chemical Engineers for his work in fermentation and microbial kinetics.
- Michael Shuler was given the Marvin J. Johnson Award of the American Chemical Society for his research in biochemical engineering.
- Keith Gubbins received the Alpha Chi Sigma Research Award of the American Institute of Chemical Engineers for his work on computer simulation of fluids, and also a Guggenheim Fellowship and a Sen-

Table I. FACULTY MEMBERS AND THEIR RESEARCH INTERESTS

A. Brad Anton	Mechanisms and kinetics of reactions catalyzed by metal surfaces
Paulette Clancy	Studies of thermodynamics and kinetics for materials-processing techniques such as laser annealing and CVD, using theory and computer simulation
Peter A. Clark	Computer-aided design, optimization, expert process-control systems
Claude Cohen	Thermodynamic and transport properties of polymers and composites, light scattering, rheology, processing
Robert K. Finn	Waste treatment, microbial kinetics, ethanol from pentoses
Keith E. Gubbins	Molecular thermodynamics of liquid mixtures, phase equilibria, computer simulation of liquids, interfacial properties
Daniel A. Hammer	Bioengineering, receptor-mediated adhesion of cells, insect-cell tissue culture, shear effects on cells
Peter Harriott	Kinetics, catalysis, and reactor design, diffusion in membranes and porous solids, air-pollution control
Donald L. Koch	Transport and rheological properties of fibrous suspensions, bubbly liquids, and porous media; applied mathematics
Robert P. Merrill	Chemistry and physics of reactive solid surfaces, catalysis, corrosion, electron spectroscopy of surfaces, atomic and molecular beam scattering
William L. Olbricht	Non-Newtonian fluid mechanics, rheology and biorheology, flow in porous media
A. Panagiotopoulos	Thermodynamic properties of dense fluid mixtures, micellar systems, conformations of biological macromolecules
Ferdinand Rodriguez	Polymerization, properties of polymer systems
George F. Scheele	Hydrodynamic stability, coalescence, fluid mechanics of drops and jets
Michael L. Shuler	Biochemical engineering, plant cells, novel biological reactors, mathematical models of cell growth, immobilized cells
Paul H. Steen	Fluid mechanics, hydrodynamic stability, applied mathematics
William B. Streett	Thermodynamic properties of fluids at high pressures, computer simulation of molecular liquids
Raymond G. Thorpe	Phase equilibria, separation processes
Robert L. Von Berg	Liquid-liquid extraction, effects of radiation on chemical reactions, saline-water conversion
John A. Zollweg	Experimental thermodynamics, interfacial phenomena, computer simulation

Table II. CURRENT RESEARCH ACTIVITIES AT THE SCHOOL

<i>Area</i>	<i>Faculty Members Involved</i>
Biochemical engineering	Finn, Hammer, Shuler
Design, process control	Clark
Fluid dynamics, applied mathematics	Cohen, Hammer, Koch, Olbricht, Scheele, Steen
Kinetics, catalysis	Anton, Harriott, Merrill
Materials, polymers	Clancy, Cohen, Rodriguez
Thermodynamics, computer simulation, separations	Gubbins, Panagiotopoulos, Streett, Thorpe, Zollweg

ior Visiting Scientist Award from the British government to support research carried out at Oxford University in 1986-87.

• Ferdinand Rodriguez, George Scheele, and Julian Smith were elected fellows of the American Institute of Chemical Engineers.

The younger faculty members have also received national recognition, accompanied by funding for research. Donald Koch just won a National Science Foundation Presidential Young Investigator Award. Brad Anton received a Shell Young Faculty Development Grant, Thanasis Panagiotopoulos and Peter Clark were each awarded a Young Faculty Grant from Mobil, and William Olbricht was the recipient of an IBM Faculty Development Award.

Faculty members have received special recognition on campus as well. The Excellence in Teaching Award at the College of Engineering has been won by several members of the chemical engineering faculty: Keith Gubbins, Ferdinand Rodriguez, George Scheele, Michael Shuler, and Raymond Thorpe (twice). In each of the first four years (1984 through 1987) of Cornell's Presidential Scholars program to recognize outstanding seniors, Thorpe was

named by one of the honorees as the professor who had been most influential. This spring Brad Anton was named by a Presidential Scholar.

MAINTAINING EXCELLENCE IN UNDERGRADUATE EDUCATION

Undergraduate enrollment, which reached record highs between 1977 and 1985 in response to an unprecedented demand for chemical engineers, has declined to pre-1977 levels, reflecting the fact that the bottom fell out of the job market in 1982. (The graph on page 8, showing the numbers of baccalaureate degrees awarded, reflects the enrollment figures.) Although the employment situation has improved markedly, there has not yet been an upturn in enrollment. Currently, the school graduates thirty to thirty-five students each year, one-third of whom continue their studies, most of them in chemical engineering, but some in medicine, business, law, chemistry, and other fields of engineering.

The undergraduate program strikes a balance between the science of chemical engineering and more empirical approaches—a blend that provides a strong base in the fundamentals and develops the

ability to apply those fundamentals to significant engineering problems. As the technologies with which chemical engineers are involved become more diverse, a strong background in the fundamentals becomes increasingly important. Courses in chemistry make up almost 20 percent of the curriculum (most other engineering programs at Cornell require only one chemistry course), and courses in mathematics and physics constitute another 20 percent. Although they are not required, courses in the biological sciences are elected by a number of students.

The chemical engineering portion of the curriculum was recently revised to provide expanded coverage of the fundamentals. Juniors take courses in fluid mechanics, heat and mass transfer, thermodynamics, and reaction kinetics. In the senior year the emphasis is on practical applications of the fundamentals: the curriculum includes laboratory courses and instruction in process design and control.

Industrial input into the undergraduate program has been strengthened in recent years by bringing in visiting faculty members with extensive experience in process design. For the past three years, for ex-

“Although the chemical industry in the United States remains strong, the decline in job opportunities in certain areas [has] spurred a review of where the profession is heading.”

ample, Clarence Shoch, who received a Cornell B.Ch.E. degree in 1951 and recently retired from Du Pont, has filled this role and also supervised several Master of Engineering design projects. Many of our undergraduates get industrial experience even before they graduate: 40 percent participate in the college's Engineering Cooperative Program.

In the continual process of curriculum revision, flexibility has been enhanced by increasing the number of electives that undergraduates can take. This has made it possible to develop three-course elective sequences in biochemical engineering and in polymeric materials. Alternatively, students can choose electives outside the field that lead to concentrations in other fields of engineering, science, or mathematics.

The educational facilities available to our students have been enhanced significantly in recent years. The Instructional Computing Facility for chemical engineering students was established three years ago with a gift from the chemical engineering graduates of the Class of 1960 to commemorate their twenty-fifth reunion. This gift was used to purchase computer hardware for students to use in course work.

Two large rooms in the basement of Olin Hall have been renovated and air-conditioned; the computers are housed in one room, and the adjacent room has been partitioned to provide space for study and the collaborative work that is an integral part of our laboratory and design courses. Students have twenty-four-hour access to both rooms. There is an ongoing effort to develop and implement graphics-oriented software for instructional use.

In addition, the school has begun a major effort to modernize the teaching laboratories, a long-recognized need. These laboratories will be located in upgraded space in the renovated east wing of Olin Hall. The experimental work will be updated also; generous support for the modernization of current experiments and the development of new ones has been provided by Theodore Ohart '29 and the College of Engineering. Two completely redesigned experiments were used for the first time last year, and three new experiments will be introduced in the coming academic year.

The undergraduate program was recently reaccredited for six years, the maximum period possible. The accreditation

report stated that “the Chemical Engineering faculty is well qualified, has a wide range of interests, and offers an effective, balanced program of teaching and research. . . . The students interviewed were bright, enthusiastic, articulate, well versed in their discipline, and very loyal to the School.”

GETTING READY FOR THE FUTURE

There has been considerable concern in the chemical engineering profession recently about what direction education and research should take. In part this stems from the desire to increase national competitiveness. Although the chemical industry in the United States remains strong, the decline in job opportunities in certain areas, such as the oil industry, that traditionally have been major sources of employment for chemical engineers has also spurred a review of where the profession is heading.

The National Research Council recently published a report, “Frontiers in Chemical Engineering: Research Needs and Opportunities,” that emphasizes the contributions chemical engineering can make to new industries and technologies.



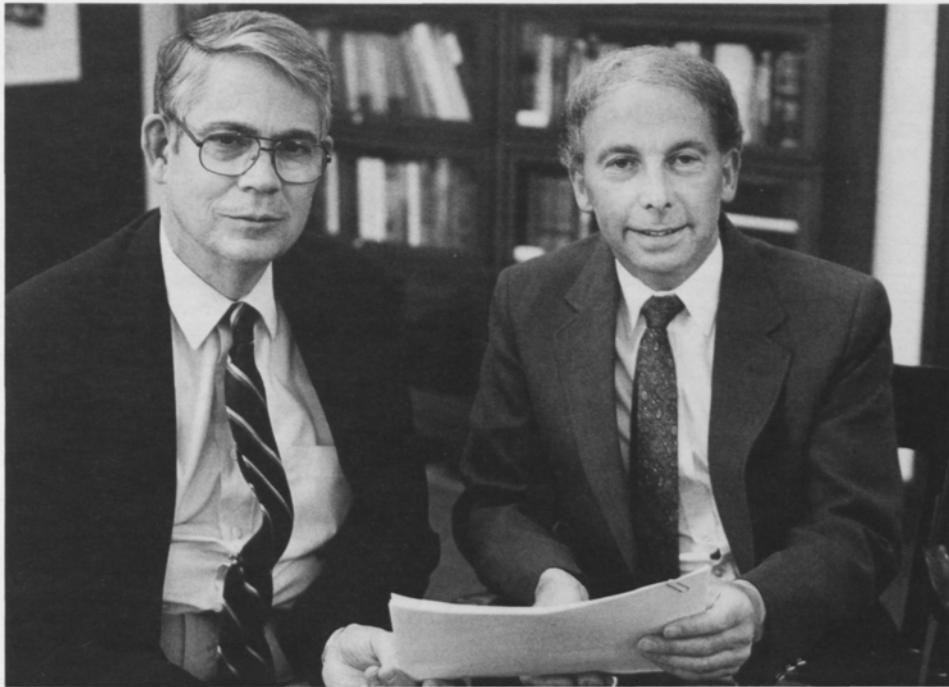
Above: Members of the Chemical Engineering Advisory Council at the October 1987 meeting.

First row, left to right: Stanford H. Taylor, AeroVironment; Bryce I. MacDonald, General Electric Company; John F. Schmutz, E. I. du Pont de Nemours and Company; David S. Laity, Chevron Research Company; William R. Schowalter, Princeton University; Leonard A. Barnstone, Exxon Research and Engineering

Company; and Andreas Acrivos, City College of CUNY.

Top row: H. Ted Davis, University of Minnesota; David S. Barmby, Sun Company; Scott C. Roberts, Shell Oil Company; L. Gary Leal, California Institute of Technology; Thomas K. Smith, Dow Chemical Company; Vern W. Weekman, Mobil Oil Corporation; and George W. Roberts, Air Products and Chemicals, Inc.

Current members not pictured are Samuel C. Fleming, Arthur D. Little, Inc.; Edward J. Holden, IBM Technology Products; W. Thomas Mitchell, Eastman Kodak Company; Larry F. Thompson, AT&T Bell Laboratories; Heinrich Tomfohrde, III, GAF Chemicals Corporation; and James Wei, Massachusetts Institute of Technology.



Keith E. Gubbins (at right), the Thomas R. Briggs Professor of Engineering, has been director of the School of Chemical Engineering since 1983. George F. Scheele (at left), a professor in the school, has been associate director since 1982; he supervises the undergraduate program, in addition to teaching and conducting research.

The upcoming fields cited in the report (prepared by Neal Amundson of the University of Houston and his committee) include biotechnology, electronic and photonic materials processing, environmental protection and risk assessment, and processes involving surfaces and microstructures.

As educators, we must equip our students to deal not only with these emerging fields, but with unpredictable future changes in technology and employment. How this can be done is a matter of intense interest and debate among members of our own faculty and nationally. An Engineering Foundation Conference on the topic was held earlier this year, and it will be the focus of a symposium to be held at MIT in October as part of that institution's centennial celebration.

ing in the fundamentals of chemistry, physics, and the engineering sciences is likely to be even more important in the future than it is now. Such an education will improve the ability of chemical engineering graduates to work with a variety of other specialists, including chemists, biologists, materials scientists, and electrical engineers.

In the immediate future, the school's goals include continuing to modernize our facilities, add faculty members of the highest quality, and improve our relations with industry. We need to upgrade and renovate the Olin Hall north wing, which contains all the offices and classrooms, the computing facilities, and some laboratories. High-priority areas for faculty recruitment are likely to be design, process control, materials, and biotechnology.

The Chemical Engineering Advisory Council has played a crucial role in the de-

velopment of the school over the past few years, and we are counting on its continued help. The eighteen members, thirteen from industry and five from academia, meet at Cornell twice a year. They have provided important advice not only on improving the school's ties with industry, but on facilities improvement, faculty recruitment, the use of computers in the undergraduate curriculum, and a number of other issues of concern to students and faculty.

As research and teaching programs expand to keep pace with new challenges, we must be able to continue offering the best possible preparation for students entering the field of chemical engineering. We intend to see to it that our school maintains its reputation for excellence and meets the demands of the 1990s and beyond.

REACTIVE SURFACE CHEMISTRY

A Fundamental Side of Applied Science

by Brad Anton

When automotive exhaust passes through a catalytic converter, a noxious mixture of carbon monoxide, oxides of nitrogen, and unburned hydrocarbons is converted to a relatively harmless mixture of carbon dioxide, nitrogen, and water. The chemical changes that occur in the catalytic converter are examples of *reactive surface chemistry*, since they result from the reactions of the exhaust gases at the surface of the platinum, palladium, and rhodium catalyst inside the converter. The pursuit of fundamental understanding of these and similar surface-reactive processes has become a requisite area of chemical engineering research today.

Recently there has been a flurry of activity in this research area, for many economically important technologies besides pollution control rely in a crucial way on aspects of the reactive chemistry of solid surfaces. For example, millions of pounds of chemical feedstocks are produced annually via *heterogeneous catalytic reactions*—reactions catalyzed at gas-solid interfaces. For manufacturing industries, engineers are called upon to develop materials that will withstand corrosive environments, and to grapple with problems of adhesion, lubri-

cation, and wear at interfaces. Progress in each of these areas demands a fundamental understanding of the reactive chemistry of solid surfaces.

Fortunately, recent and dramatic developments in theoretical and experimental techniques are bringing this understanding within reach. And fortunately for those of us at the School of Chemical Engineering who are working in this area, the multidisciplinary nature of surface chemistry has led to strong support from colleagues in other departments, as well as opportunities for productive collaborations.

Currently, two chemical engineering faculty members—Robert P. Merrill and I—are investigating the reactive chemistry of transition-metal surfaces. Our work, described briefly here, focuses on complementary aspects of the role transition metals play as heterogeneous catalysts.

THE THEORETICAL AND EXPERIMENTAL APPROACH

The clearest theoretical basis for understanding any elementary reaction event is the *potential-energy surface*, a mathematical construct (see Figure 1). This function, unique to each reaction, describes the total

potential energy of the reactant and product molecules in terms of the relative orientations of their constituent atoms. Its local minima describe relatively stable intermediates along the path of the reaction, and the troughs and saddle points represent the minimum-energy “valleys” and “passes” in molecular orientation through which the system moves as the reactants are converted to products. The detailed shape of this potential-energy function indicates the preferred products of the reaction (thermodynamics), the sequence of bond-breaking and bond-formation steps which make up the reaction (mechanism), its rate (kinetics), and how the degrees of freedom of the molecular participants—translational, rotational, vibrational, and electronic—contribute to its progress (dynamics).

Accurate computation of potential-energy surfaces for any reactions that have more than academic significance is an overwhelming task. The aim of much research in reactive chemistry, therefore, is to perform experiments that elucidate the most important features for reactions of interest. These features include the geometric and electronic structures of the reactants, intermediates, and products, and the

Figure 1. An example of a potential-energy surface. This one is for a reaction of the type $A + BC \rightleftharpoons AB + C$.

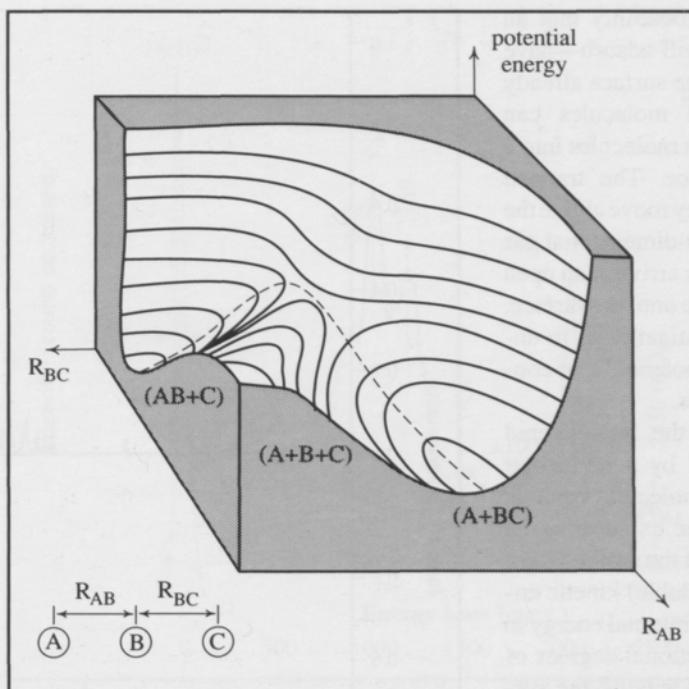
For a simple reaction like this, involving only three atoms interacting along a common line, the potential-energy surface has the general shape shown. R_{AB} and R_{BC} are the distances between atoms A and B and B and C, respectively, and height on the surface gives the relative potential energy of the three-atom system for each combination of R_{AB} and R_{BC} .

As one follows the dotted line from the lower right toward the upper left, one sees the change in orientation of the three-atom system as the A atom approaches the stable BC molecule, the potential-energy barrier for the reaction is surmounted, and the C atom separates from the stable AB product. Since this path starts and ends in the lowest parts of the reactant and product troughs and passes over the lowest part of the barrier separating them, it represents the path of minimum energy change for the reaction.

Other paths that climb the walls of the potential-energy surface would depict the participation of vibrational motion of the AB and/or BC molecules in the progress of the reaction.

details of the reaction mechanism in terms of bonds broken and formed. Also important is information about the heights and shapes of potential-energy barriers that must be surmounted as the reaction proceeds.

For the cases of interest to us—heterogeneous reactions catalyzed at gas-metal interfaces—the potential-energy surface is defined by the physical and chemical interactions between the metal surface and the reactants, the adsorbed intermediates, and the products. The role of the metal surface as a catalyst is identified by its ability, through these interactions, to provide alternate pathways with lower energy barriers than those encountered in direct reactions in the gas phase.



Much of our work involves characterizing experimentally these gas-metal interactions and interpreting them in terms of the structural and chemical properties of the catalytic surface. Successful experimentation requires techniques that can separate the various interactions and allow individual scrutiny of them. Most of our experiments, therefore, are conducted on single-crystal metal surfaces in ultrahigh vacuum (10^{-10} Torr): the two-dimensional periodicity of these surfaces affords straightforward characterization of their structures, and the ultrahigh-vacuum environment allows careful control of adsorbed reactant concentrations and surface cleanliness.

This rather ideal reaction environment allows the use of many powerful analytical techniques. For example, we use supersonic molecular beams to supply quanti-

fied fluxes of reactants to the surfaces, and we use various photon and electron spectroscopic techniques to characterize the structures of adsorbates. The combination of these techniques makes it possible to obtain incisive measurements of the quantities of interest.

THE TRAPPING MECHANISM OF ADSORPTION

An excellent example of this approach is provided by a project in which Merrill is collaborating with Paul Houston of Cornell's chemistry faculty. They are investigating the dynamics of the "trapping" of nitric oxide (NO) molecules that occurs when these molecules strike an iridium (111) surface already covered to saturation with an adsorbed layer of NO.

Measurements of the "sticking probability" for diatomic molecules such as NO

and CO—that is, the probability that an incident gas molecule will adsorb—have shown that portions of the surface already covered with adsorbed molecules can “trap” additional incident molecules into a region above the surface. The trapped molecules are mobile; they move above the adsorbed layer like a two-dimensional gas until they either desorb or arrive at an open site where they can adsorb onto the surface. The purpose of the investigation is to understand the interaction potential that controls this trapping process.

In the experiments, the NO-covered surface is “illuminated” by a molecular beam of NO. Since the molecular beam is produced by a supersonic expansion, the NO molecules arriving at the surface have a well defined (and selectable) kinetic energy, but have little or no internal energy in their vibrational and rotational degrees of freedom. The molecules leaving the surface are collected and counted as a function of their exit direction and their kinetic and internal energy distributions.

Kinetic-energy distributions are determined by measuring the time required for a pulse of molecules, produced by “chopping” the incident beam on and off, to travel a fixed distance from the surface to a mass spectrometer detector. This technique is referred to as *time-of-flight* measurement. Rotational- and vibrational-state distributions are measured by a technique called *multi-photon ionization*, in which the molecules are ionized by a tunable laser, and the ions are counted by a mass spectrometer as a function of the laser frequency. (See Figure 2.)

Results obtained so far show that the trapping probability is a strong function of both the incident angle and the kinetic energy of the arriving molecules; normal incidence and low kinetic energies are the

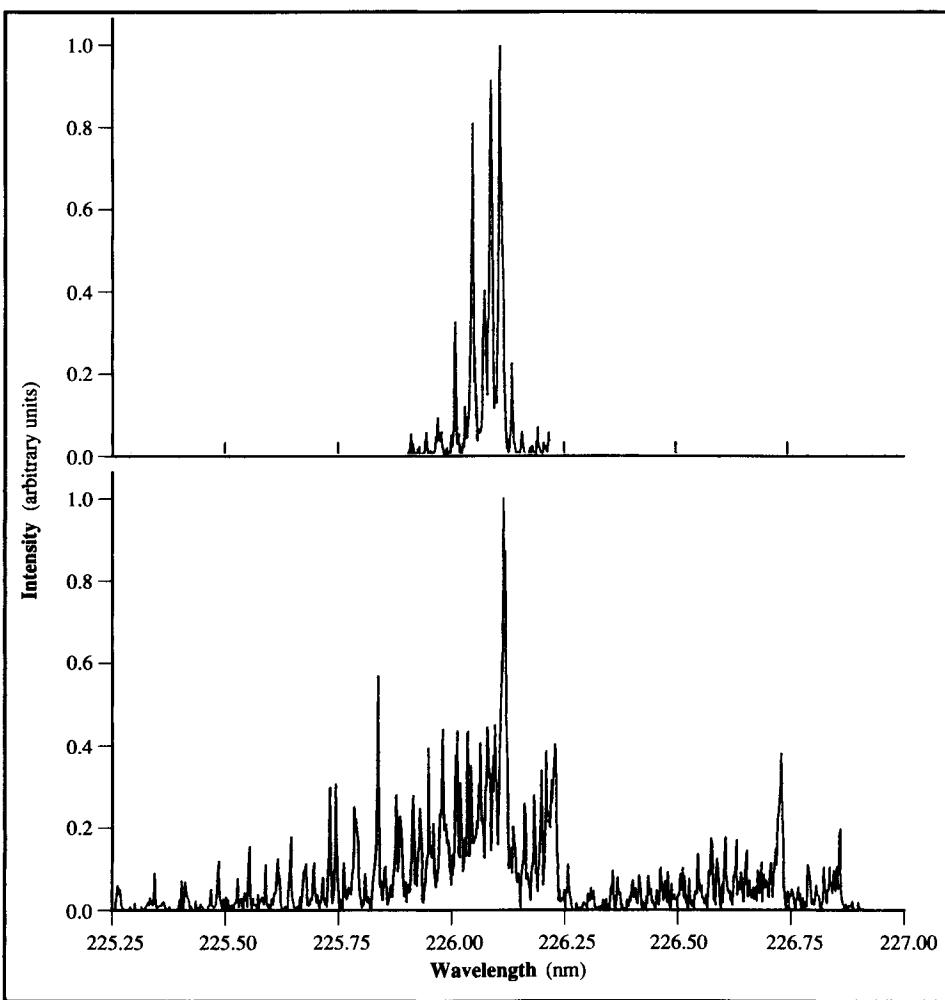


Figure 2. An illustration of the use of multi-photon ionization to measure rotational-state distributions. The spectra showing mass-spectrometer signals as a function of laser wavelength are for NO molecules scattered from an NO-covered iridium (111) surface. The fraction of NO molecules leaving the surface in each rotational level can be determined from the intensity of the peaks.

The top spectrum is for the molecular beam of NO before arrival at the surface, and the bottom spectrum is for NO molecules that have scattered from the adsorbed layer. These spec-

tra have been recorded for near-glancing incidence; therefore, trapping is not efficient and inelastic scattering dominates. The NO molecules in the incident beam show little rotational excitation and can be characterized by an equilibrium rotational temperature of 5K. The scattered NO molecules, however, show significant rotational excitation, corresponding to a temperature of about 222K. This temperature exceeds that of the surface (134K for these measurements), demonstrating the direct conversion of kinetic to rotational energy as the NO molecules scatter from the adsorbed layer.

most favorable for efficient trapping. Molecules that are not trapped scatter inelastically, transferring a significant amount (40 percent) of their incident kinetic energy either to the surface or to rotational energy.

Future experiments will include the use of a laser to excite the incident molecular beam to a higher vibrational state. The exit distributions will provide information about how the vibrational degree of freedom affects the trapping and inelastic-scattering processes.

RATES AND MECHANISMS OF METAL-CATALYZED REACTIONS

My work focuses on the mechanisms and kinetics of metal-catalyzed reactions, rather than on reaction dynamics.

For successful investigations of this kind, experimental methods are needed to determine the stable coordination geometries (the structures) of the adsorbed reactants, the intermediates, and the products. In addition, there must be methods for measuring the rates of surface chemical reactions as a function of the extent to which the surfaces are covered by the reactants. An ultrahigh vacuum apparatus for these types of measurements is now under construction in the basement of Olin Hall.

In our experiments, structural identification of stable, adsorbed species will be accomplished by means of *electron energy-loss vibrational spectroscopy*, in which a nearly monoenergetic, low-energy (10 eV) beam of electrons is focused on the surface, and the scattered electrons are collected and counted as a function of the energy they lose by exciting vibrations in the adsorbed layer. The resulting spectrum of signal intensity versus energy loss provides, in many cases, a structural "snapshot" of an otherwise unobservable adsorbed intermediate. (See Figure 3.)

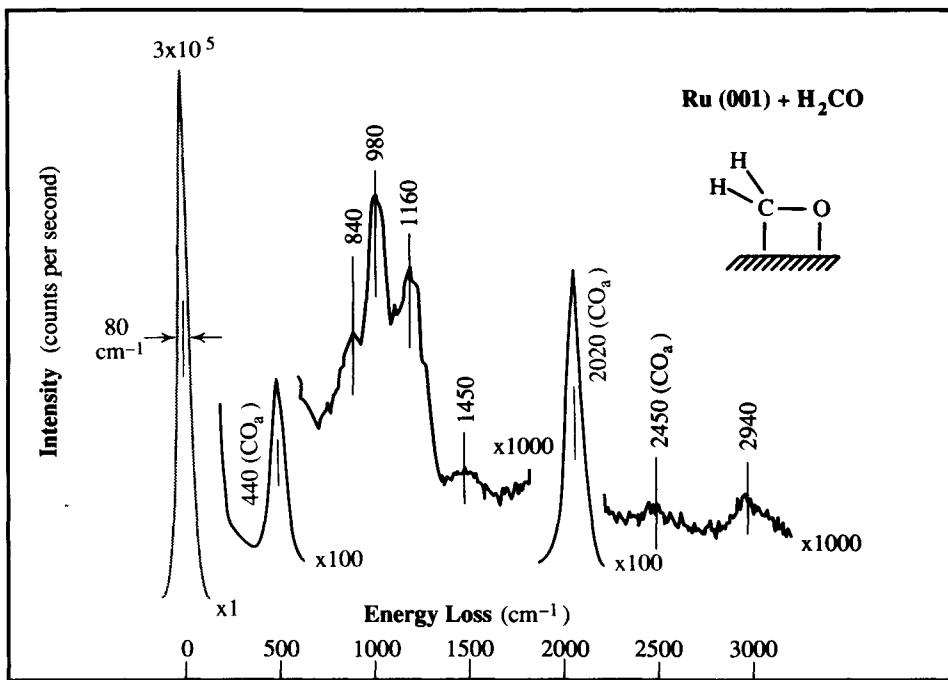


Figure 3. An electron energy-loss spectrum of a ruthenium (001) surface, recorded after adsorption of formaldehyde at 100K.

The peak at zero energy loss results from elastic scattering of electrons. The peaks at 440, 2020, and 2450 cm^{-1} indicate the presence of adsorbed CO from formaldehyde decomposition.

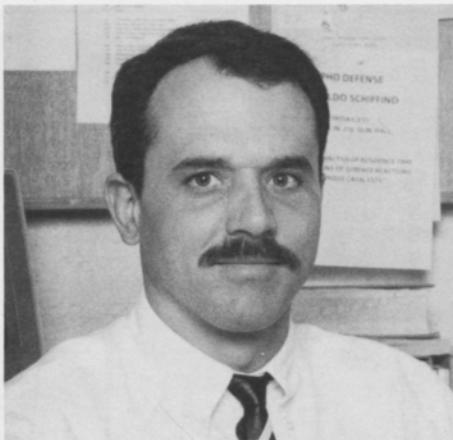
The peaks at 840, 980, 1160, 1450, and 2940 cm^{-1} indicate the presence of adsorbed formaldehyde, bonded in a side-on configuration like that shown schematically. This adsorbate is a critical intermediate in the sequence of catalytic reactions that form methanol (CH_3OH) from gaseous H_2 and CO on ruthenium surfaces.

The kinetics of surface reactions that produce adsorbed products will be quantified with time-resolved measurements of surface coverage using the energy-loss spectrometer. The kinetics of reactions that yield gaseous products will be quantified with time-dependent measurements of desorption flux using a mass spectrometer. Such information, when considered in unison, often allows the catalytic role of the metal surface to be identified in terms of chemical bonding interactions between the surface and the adsorbed intermediates.

These methods will be used, for ex-

ample, in a study of the catalytic partial oxidation of hydrocarbons on noble-metal surfaces. Specifically, we intend to quantify the relative reactivities of oxygen that is adsorbed atomically and "dioxygen" that is adsorbed molecularly. These forms have been shown to coexist on surfaces of platinum, copper, and silver at low temperatures. Adsorbed dioxygen appears to be identical in structure to the "peroxy" ligand of homogeneous organometallic chemistry, the unique reactivity of which provides selective synthesis routes under mild reaction conditions to many partial

“...the underlying phenomena share a common aspect: the interaction of reactive molecules with chemically active solid surfaces.”



oxidation products. By analogy, adsorbed dioxygen would be expected to show reaction selectivity that is significantly different from that of atomically adsorbed oxygen.

The motivation for this investigation comes from its relevance to a widely used commercial process for producing ethylene epoxide (C_2H_4O). About 15 percent of the ethylene produced in the United States—some two million pounds per year—is converted to the epoxide by reaction with air over a silver catalyst. Of the ethylene fed to this process, only about 80 percent is converted to the desired epoxide product, the rest being combusted to carbon dioxide and water. The mechanisms of these reactions are not fully understood. More specifically, the relative roles of atomically and molecularly adsorbed oxygen in the epoxidation and combustion reactions have not been unequivocally identified. One of the important goals of our project will be to provide the surface chemical information necessary to understand fully the reaction mechanism, with the eventual goal of improving the selectivity and yield of the commercial epoxidation process.

A GENERAL VIEW OF SURFACE SCIENCE

The projects I have described reflect only a portion of our interests and are specific to only one area of surface reactivity—the catalytic chemistry of transition-metal surfaces. The theoretical concepts and the experimental techniques can be applied successfully to a multitude of other important problems. Indeed, in recent years there has been a virtual explosion in the application of surface-science techniques in areas ranging from microelectronics and specialty materials to problems of friction and wear. The research interests of chemical engineers are expanding continually into these new and exciting fields.

Though different in application and detail, the underlying phenomena share a common aspect: the interaction of reactive molecules with chemically active solid surfaces. In all cases, technological success will follow from in-depth understanding of the basic science, and it is belief in this approach that motivates our research.

Brad Anton joined the Cornell faculty in 1986 following research in Germany as an Alexander von Humboldt postdoctoral fellow. This research was conducted at the Institut für Grenzflächenforschung und Vakuumphysik at the Kernforschungslage in Jülich.

Anton holds the B.S. degree from Virginia Polytechnic Institute, awarded in 1979, and the M.S. (1982) and Ph.D. (1985) from the California Institute of Technology.

MOLECULAR SIMULATION

by Keith E. Gubbins and Athanassios Z. Panagiotopoulos

In molecular simulation one starts from a molecular model and then calculates macroscopic properties on the basis of statistical mechanics.

The model includes a detailed description, on the atomic level, of the material to be studied, and an equation for the intermolecular forces acting between the molecules. The macroscopic properties might include the thermodynamic functions (pressure, free energy, and so on), transport properties (such as diffusion rates and viscosity), molecular arrangements or packing, dielectric and optical properties, and surface properties. The exact relationships of statistical mechanics are used in averaging over the molecular positions and motions that are possible for the particular molecules.

The approach is valuable because, except for a few simple problems, the statistical mechanical equations relating molecular and macroscopic properties cannot be solved analytically. The simulations are a way to obtain a solution using numerical methods.

Two methods are in common use: the Monte Carlo and the molecular dynamics techniques (see Figure 1).

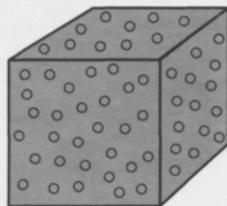
The Monte Carlo (MC) method makes use of a random-number generator to “move” the molecules in a random fashion. Statistical mechanics tells us that for a fixed temperature and density the probability of a particular arrangement of the molecules is proportional to $\exp(-U/kT)$, where U is the total energy of the collection of molecules, k is the Boltzmann constant, and T is the temperature. The random moves are accepted or rejected according to a “recipe” that ensures that the generated arrangements have probabilities given by this law. After generating a long series of such arrangements, they can be averaged to obtain the various equilibrium properties of the system of molecules.

In the molecular dynamics (MD) method, the molecules are allowed to move naturally under the influence of their own intermolecular forces. The positions and velocities of each molecule are followed in time by solving Newton’s equation of motion (force equals mass times acceleration, a second-order differential equation) using standard numerical methods. The macroscopic properties are calculated by averaging the appropriate function of molecular positions and velocities over time.

These two techniques have several features in common. One is that highly accurate results can be expected, provided that the simulation runs are carried on long enough and that the number of molecules is large enough. In practice, the results are limited by the speed and storage capacity of current supercomputers. Typically, the number of molecules in the sample simulated can range up to a few thousand or tens of thousands; the real time simulated in MD is of the order of a nanosecond.

In order to minimize boundary effects in such small samples, it is customary to use periodic boundary conditions; that is, the sample is surrounded on all sides by replicas of itself, so that when a molecule moves through a boundary and so out of the sample, it is automatically replaced by a molecule moving into the sample through the opposite face of the box. (Anyone who has played Pacman, Asteroids, or similar video games is familiar with this periodic-boundaries trick.)

Although molecular simulation can be successfully applied to a wide range of problems, difficulties can arise with some applications because of the storage or speed limitations. Examples include ionic



$N \sim 100 - 10,000$
Periodic Boundaries
Prescribed Intermolecular Potential

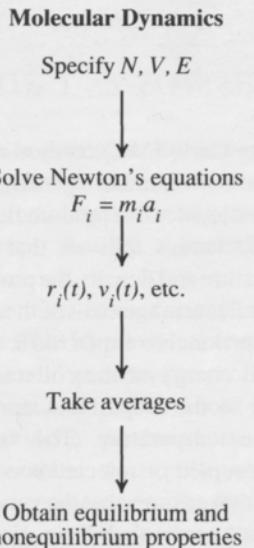
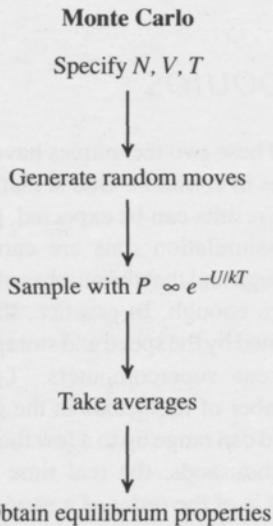


Figure 1. Two methods of molecular simulation. Typically, both treat a sample of N molecules in a box of volume V (here shown as being of cubic shape).

In the Monte Carlo method it is common, but not necessary, to choose N, V , and temperature T as the independent variables, and to keep these fixed during the simulation. Molecules are moved randomly, generating a new molecular arrangement with the intermolecular potential energy U . These new arrangements are accepted or rejected in such a way that those accepted occur with the probability distribution that is required by the laws of statistical mechanics.

In molecular dynamics the energy E , rather than the temperature T , is fixed. The molecular positions r_i and velocities v_i (and also orientations and angular velocities) for each molecule i are followed in time.

fluids—such as plasmas and electrolytes—in which the range of the intermolecular forces is very large, necessitating a large number of molecules. Difficulties arise also with substances in which long-range fluctuations occur: substances very near critical points and those exhibiting certain surface phenomena. Long-time phenomena are also apt to make simulation difficult.

There are not only common features, but also significant differences between the MC and MD methods. MC is easy to program and can be easily adapted to different

conditions; it is adaptable, for example, to studies of mixtures at constant pressure or of adsorption at constant chemical potential. MD is more difficult to program, and since energy must be conserved, it is less easily adapted to different conditions. However, MD has two important advantages over MC: it can be used to study time-dependent phenomena and transport processes, and the molecular motions can be observed and photographed easily using computer graphics.

Since 1976 Cornell has had an active program in applying these techniques to problems of chemical engineering interest (see the table). Calculations are carried out on supercomputers on campus or at one of the other national centers. Advanced computer-graphics methods are used to observe molecular motions, behavior near surfaces, polymerization, and other phenomena. The potential of molecular simulation as a tool has expanded rapidly with improvements

SUBJECTS OF SIMULATION STUDIES AT CORNELL

- Phase equilibria in liquid mixtures
- Fluid droplets
- Fluids in porous materials
- Ionic and associating liquids
- Liquid crystals
- Colloids and surfactants
- Surface phenomena

Figure 2. Possible steps in the Gibbs method for simulating the properties of fluids. The schematic illustrates the initial system configuration and three steps: (a) particle displacement; (b) volume change; and (c) particle transfer. Variables are defined as in Figure 1.

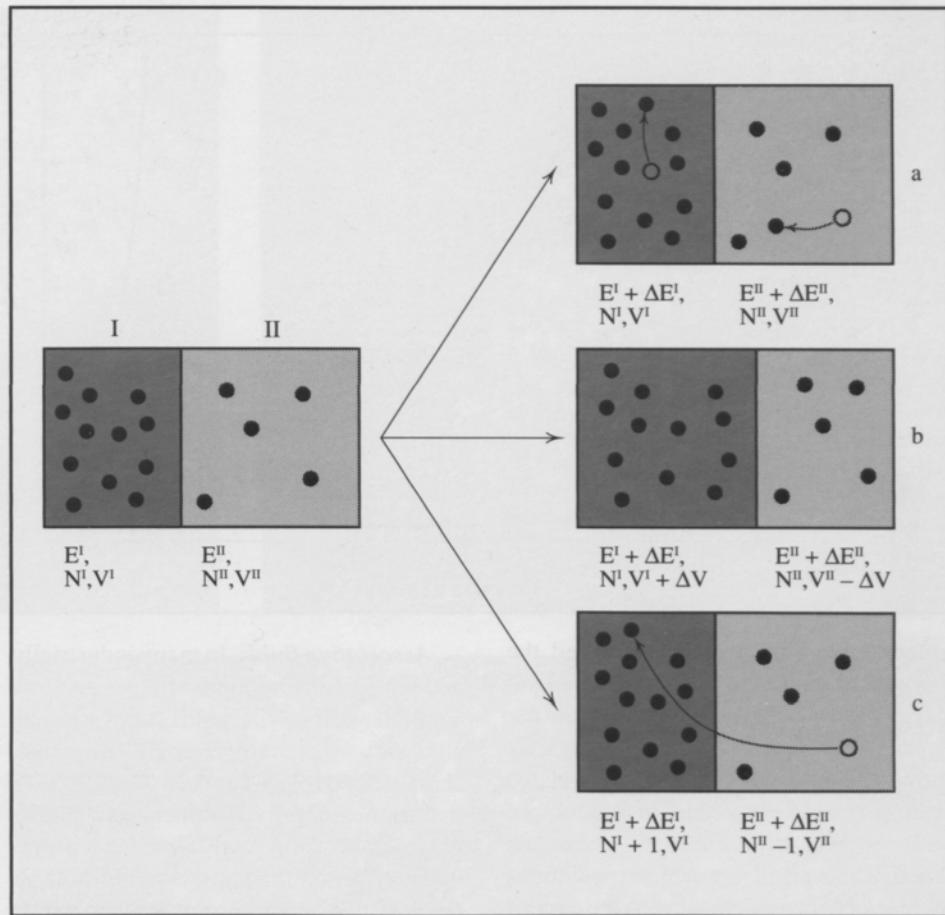
in speed and availability of supercomputers, and these trends are expected to continue for the next decade.

PHASE BEHAVIOR OF COMPLEX SYSTEMS

Many phenomena of industrial and scientific importance involve equilibria between two (or more) phases with different properties. Traditional chemical engineering operations, such as distillation or liquid-liquid extraction, are based on the ability to set up and operate a two-phase system with desirable partitioning characteristics. Emerging technologies, such as membrane-based separations or chromatographic techniques, are based on the same principle.

In addition, phase separations play a fundamental role in phenomena ranging in scale from the microscopic to the cosmic. Studies in molecular biology are at one extreme; at the stellar-dimensional end of the scale are studies of such phenomena as demixing in planetary atmospheres, and the equilibria of dense plasmas in the solar interior.

From a theoretical point of view, the problem of predicting phase partitioning from knowledge of the intermolecular forces is especially difficult because it involves systems with many degrees of freedom, for which no exact solutions are possible. In recent research at Cornell, molecular-simulation predictions have been carried out successfully in several areas:



Phase-coexistence properties of fluids. The first molecular-simulation technique specifically tailored for determining these properties was developed. This "Gibbs method", as we refer to it, involves performing a Monte Carlo simulation in two distinct regions of space. The two regions are not considered to be in physical contact (therefore, no interfaces are present). Conventional boundary conditions (spatially periodic) are applied for each region separately. As diagrammed in Figure 2, three types of perturbation are performed:

(a) Random displacement steps in each re-

gion separately. These steps ensure equilibration within each region.

(b) Random changes of the volume of each region. The changes result in equality of the average pressure for the two simulated regions.

(c) Transfers of molecules from one region to the other. The transfers ensure equality of the chemical potential of all components present in the two regions.

Phase diagrams of fluids at high pressures. The Gibbs methodology has also been used to predict phase diagrams of fluids at extreme conditions of pressure or

Figure 3

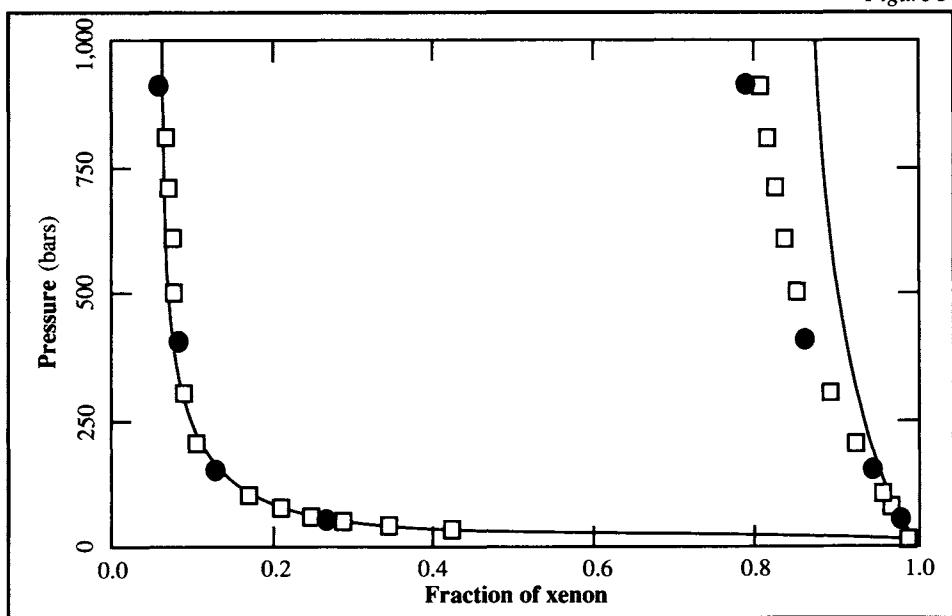


Figure 3. Phase diagram for the system neon-xenon at 223 degrees K. The points in color represent Gibbs ensemble Monte Carlo calculations; the points in black represent experimental data; the solid lines represent the predictions according to perturbation theory.

Figure 4. Molecular-dynamics simulation of the condensation of a mixture of argon (red) and krypton (yellow) atoms in a capillary, showing the vapor and liquid phases. The capillary radius is five molecular diameters. When averaged over time, the meniscus is approximately hemispherical.

Figure 5. "Snapshot" of a drop of methane molecules in equilibrium with vapor.

Figure 6. Simulation of the adsorption of model surfactant molecules on a liquid water surface (the red molecules). The yellow segments represent a polar group in the surfactant molecules.

temperature. This research achieved the first exact calculation of the phase-separation behavior of a system for which the forces between the molecules are exactly known. Figure 3 shows a typical calculated phase diagram for a mixture of two components of very different size—neon and xenon. The a priori simulation predictions are in excellent agreement with the experimental results—a significant improvement over previous theoretical calculations.

Phase diagrams of ionic systems. Exact predictions for phase separation in ionic systems are currently of great interest. Ionic equilibria are relevant to work with dense plasmas, bioseparations, and many industrial separations involving electrolytes. However, theories for the behavior of such systems lag significantly behind the corresponding theories for nonionic systems because of the extremely strong Coulombic interactions. Predictions of equilibria in molten salts and colloidal suspensions are in progress at Cornell.

Associating fluids. In many industrially and biologically important fluids—such as alcohols, carboxylic acids, and aqueous solutions—there are strongly attractive, short-ranged forces between the molecules that cause long-lived dimers and higher polymers to form, and these have a dramatic effect on the phase equilibria. Over the last two years, promising molecular models and theories for these fluids have been developed, and we are now testing them with the aid of computer simulation.

THE VALUE OF SIMULATION IN SURFACE STUDIES

A great variety of surface phenomena are important industrially. For example, adsorption is utilized for separations and purification, and the addition of surfactants is used to promote wetting and reduce surface tension; processes such as adhesion and lubrication depend on surface properties; and surface phenomena are responsible for the desired properties of colloid

materials and microemulsions. Experimental studies are very difficult to carry out, however, and so are theoretical studies, since surface phenomena are poorly understood at the molecular level. Molecular simulation, therefore, is playing an increasingly important role.

Engineers have often used classical thermodynamics as a guide to interpreting equilibrium surface phenomena, but this approach has led to errors when applied to systems in which the number of molecules is very small. Examples are drops and bubbles, fluids in pores, and colloids. One of the goals of the simulations we are doing is to determine where such classical methods break down, and to suggest more reliable prediction methods. We are working with several kinds of systems:

Fluids in microporous media. When a gas is confined inside a small pore, as in a catalyst particle, an adsorbent, a membrane, or one of a number of geological formations, its behavior is very different

Figure 4

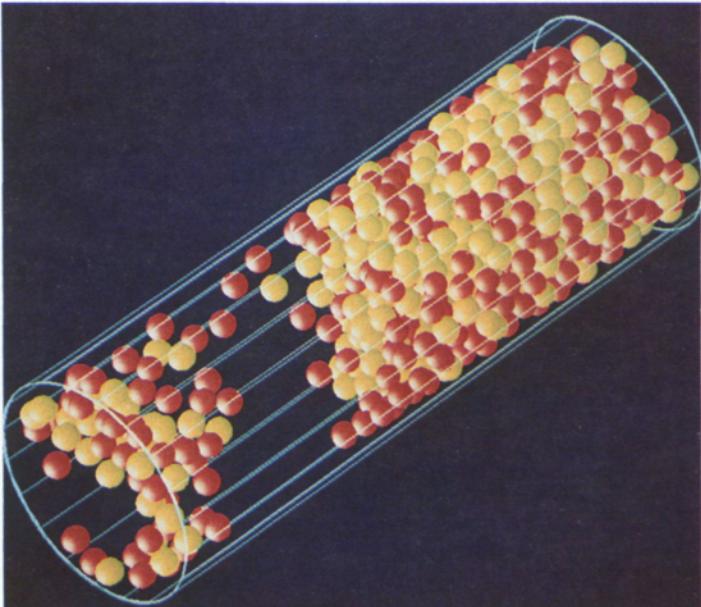
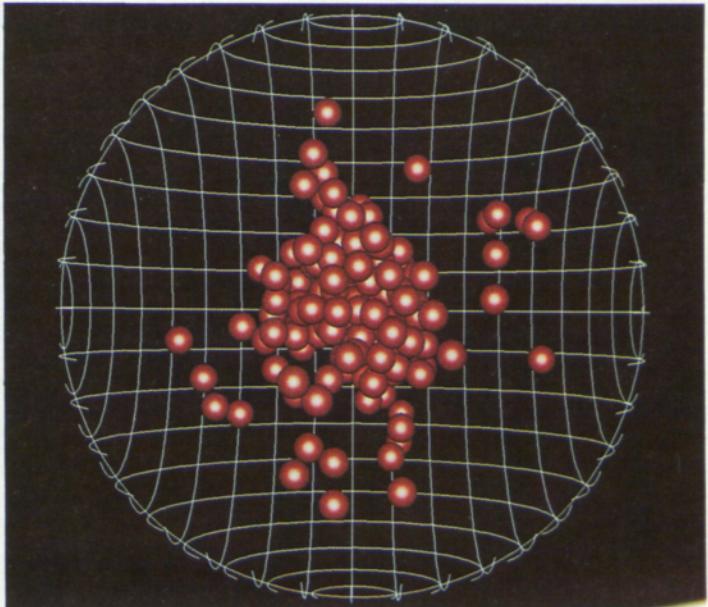


Figure 5



from that of the bulk gas. The large differences occur because of the strong intermolecular interactions between the fluid molecules and the wall. They lead to a rich variety of new phase transitions, adsorption effects, wetting phenomena, and layering on the walls.

Molecular simulation (see Figure 4) is being used to help understand these phenomena and how they are related to the underlying intermolecular forces. The long-term aim of this work is to design adsorbents and membranes that will give improved performance for specific applications in chemical processing.

Droplets. The properties of small droplets are important in nucleation phenomena, air pollution, and separation processes such as gas adsorption and liquid extraction. For sufficiently small droplets, the curvature of the surface has a strong effect on these properties, and classical thermodynamic treatments have been proposed to describe these changes. Experi-

Figure 6

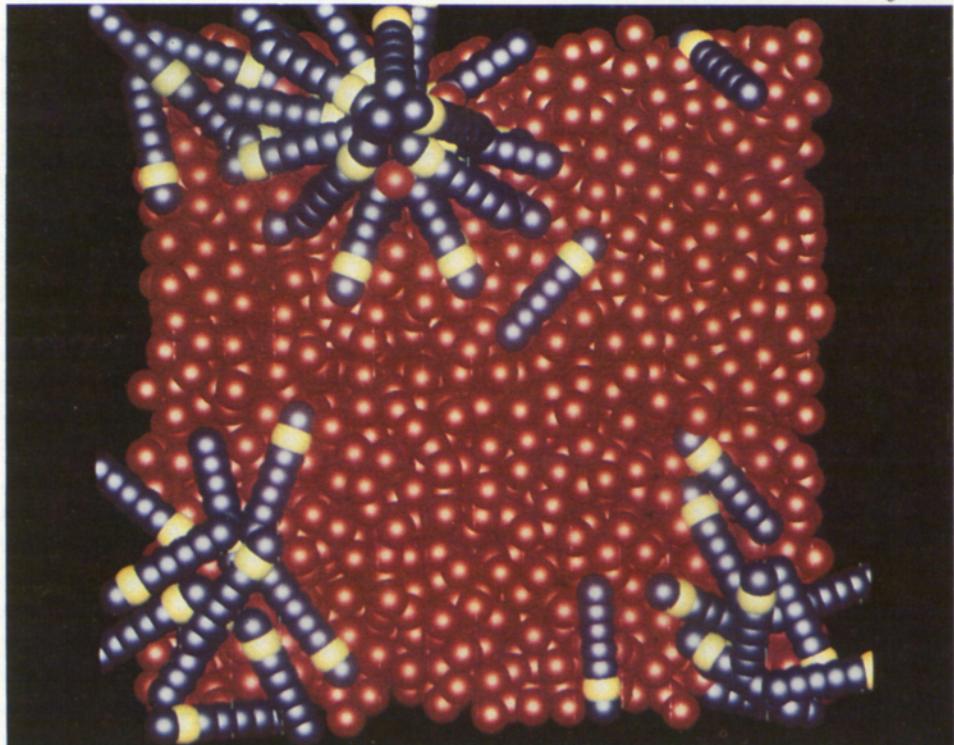


Figure 7

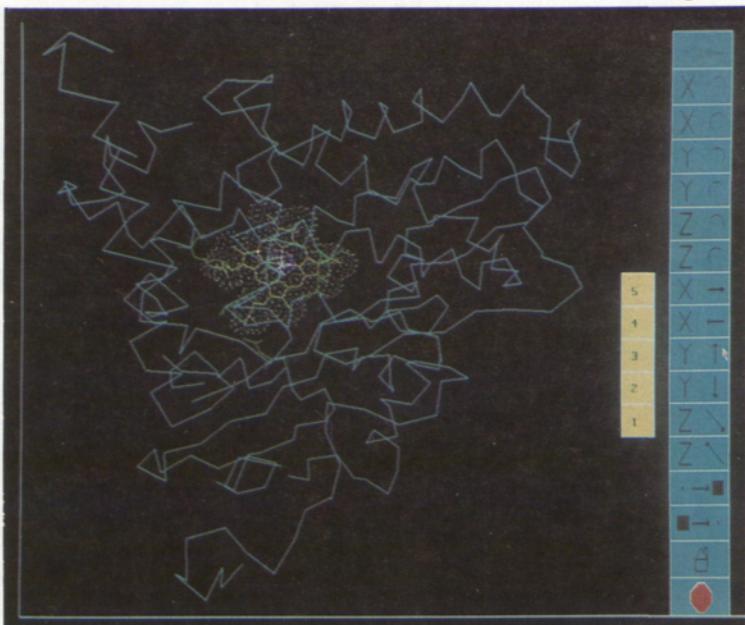


Figure 7. The three-dimensional structure of the protein Cytochrome P450, displayed on the school's IRIS graphics workstation. The user can rotate, zoom, and translate the structure using the menu and a "mouse" pointing device. (Model by T. Poulos and J. Kraut.)

physics, molecular biology, and state-of-the-art computing technology. Our work focuses on one aspect of the protein-folding problem: that of predicting, from their molecular structure, the stability limits of small globular proteins in solution. In the experimental part of this work, the thermodynamic parameters (enthalpy, volume, entropy, and heat-capacity changes) that characterize the transition from folded to unfolded form are being measured. The theoretical studies aim at developing novel simulation techniques to predict stability from detailed atomistic models for the protein and its solvent environment.

WHY MOLECULAR SIMULATION HAS A PROMISING FUTURE

Molecular simulation provides a way of predicting the properties of materials at a level of detail not possible with any other technique. The methods of molecular simulation can be applied to a very wide range of physical systems, and—unlike many theoretical methods, which are applicable only in a narrow range of systems and forces—can handle any type of interaction between molecules.

Progress in the field depends primarily on two factors. One is the increased availability of very fast computers with advanced capabilities for visualization and accompanying improvements in the languages to make them easy to use. The other factor is the development of conceptually new theoretical methods to extend the scope of molecular simulation to properties and phe-

ments are very difficult to carry out with such small systems, however, so molecular simulation is valuable (see Figure 5).

Our molecular simulations have shown that for simple fluids of nearly spherical molecules, such as methane, the thermodynamic approach breaks down for drops that are twenty molecular diameters or less across. For fluids comprising more complex molecules, such as water or electrolytes, the thermodynamic treatment breaks down for somewhat larger drops and must be replaced by molecular simulation or rigorous molecular theories. For such small drops, surface tension ceases to be a useful concept because of the small number of molecules involved.

Surfactants. Molecular simulation is being used to investigate the relation between molecular properties and surface activity (see Figure 6). The goal is to design improved surfactants for use in tertiary oil recovery and a variety of industrial proc-

esses. Small concentrations of surfactant molecules can reduce the surface tension at fluid-fluid or fluid-solid interfaces almost to zero, but the molecular mechanism involved is poorly understood at present.

STABILITY OF PROTEINS IN SOLUTION

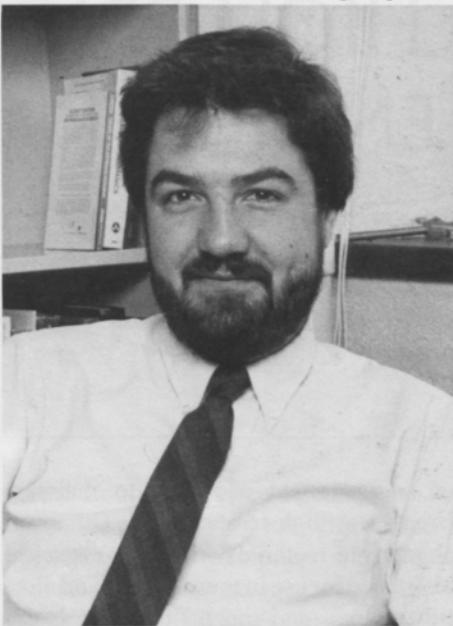
To be functional, enzymes in living organisms need to have a well defined three-dimensional arrangement of their constituent units at different organizational levels (such as secondary, tertiary, or quaternary structure). An example of a three-dimensional structure of a complex protein, hemoglobin, is given in Figure 7, which was taken on one of the school's IRIS-3100 high-performance graphics workstations.

Predicting the folding pattern of proteins from their chemical structure (sequence of constituent amino acids) is currently a very active area of research that is interdisciplinary, combining protein bio-

Gubbins



Panagiotopoulos



nomena not suitable for conventional molecular dynamics or Monte Carlo methods.

At Cornell we are making major contributions in both areas. The Theory Center, one of the five national supercomputer centers, provides the latest in computing and graphics technology. Research at the School of Chemical Engineering addresses the second central issue—the development of new methodologies and their application to the study of a wide range of physical phenomena.

Molecular simulation is a new and rapidly expanding field, and at Cornell we are in the forefront of the advance.

1958 and the Ph.D. in 1962. Before coming to Cornell, he held postdoctoral and faculty positions at the University of Florida. He has held visiting professorships at Imperial College (London), the University of Guelph, the University of Kent, the University of Oxford, and the University of California at Berkeley. In keeping with his interdisciplinary approach to research, Gubbins is a member of Cornell's graduate fields in chemistry, applied physics, applied mathematics, and the history and philosophy of science, as well as in chemical engineering. He has coauthored two monographs on the statistical mechanics of liquids, and serves on the editorial board of Molecular Physics.

Athanassios Z. Panagiotopoulos came to Cornell as a postdoctoral associate in 1987 and was appointed an assistant professor of chemical engineering the following year. He received his undergraduate education at the National Technical University in Athens, Greece, and earned a doctorate at the Massachusetts Institute of Technology in 1986. Before coming to Cornell, he spent a year in postdoctoral study at Oxford University, England.

“Molecular simulation provides a way of predicting the properties of materials at a level of detail not possible with any other technique.”

Keith E. Gubbins, the Thomas R. Briggs Professor of Engineering and director of the School of Chemical Engineering, was educated at the University of London, earning the B.S. degree in

MATERIALS: A HIGH-PRIORITY AREA IN CHEMICAL ENGINEERING RESEARCH

by Claude Cohen

Research on materials is an area of national priority today. New materials and methods of production are especially crucial in the emerging high-technology industries, for the manufacture of products from electronic devices to superconducting machinery parts, but will also be vital in more traditional areas, such as the automobile, the aerospace, and the plastics industries.

Chemical engineers have a large role in this burgeoning field, along with chemists, materials scientists, mechanical engineers, and electrical engineers. This role is exemplified at Cornell, where several chemical engineering faculty members and their students are involved in cross-disciplinary materials research. Examples of work in three different areas are presented here.

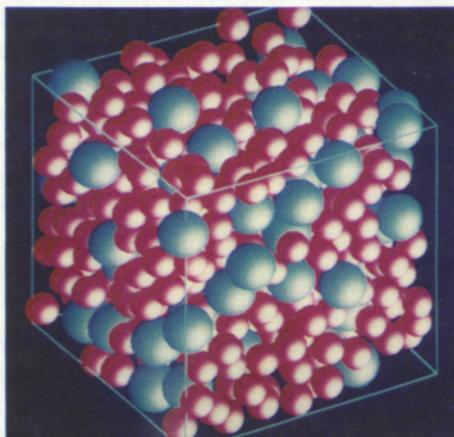
RAPID SOLIDIFICATION OF MOLTEN METALS

Metals that are rapidly solidified from the molten state are known to exhibit electrical, chemical, and mechanical properties quite different from their slowly cooled counterparts. Commercial products based on these special properties include superalloy materials used in high-performance gas turbine engines; these must be capable

of being forged and able to maintain strength at high temperatures. Other examples are materials with high electrical resistance for use in transformers and electric motors, and magnetic materials for efficient, reasonably priced magnets.

Present-day use and processing of molten metals is still largely an art based on experience and empirical knowledge. A more scientific approach—one taken by Professor Paulette Clancy—is to find out how microscopic behavior affects the structure and physical properties of such materials. Research along a specific tech-

Figure 1a



nological line is conducted by Professor Paul Steen and his group. They are focusing on rapid solidification by melt-spinning, a process that involves fluid dynamics, heat transport, and phase change in the molten metal.

Clancy's group is using computer-simulation based on statistical mechanics to study the melting and freezing characteristics of materials under both equilibrium and nonequilibrium conditions (see Figure 1). Currently, these researchers are examining how materials "doped" with impurity atoms behave under the conditions of rapid

Figure 1b

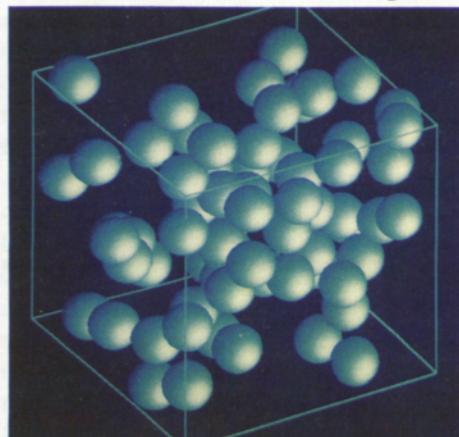


Figure 2

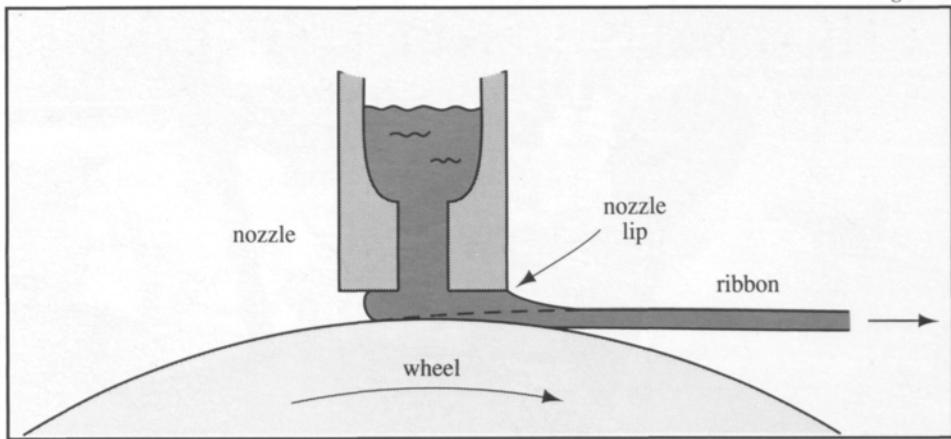


Figure 2. Planar-flow melt-spinning, one of the processes available for rapid solidification of molten metals.

In this process the nozzle that forms the jet of molten metal is brought so close to the rapidly rotating chilled wheel that the nozzle itself interferes with the flow, making a gap with nearly parallel walls. This creates the "planar flow", which produces a thin metal ribbon that is spun off the wheel at velocities on the order of 10 meters per second.

thermal processing. They can model the influence of a directed source of energy—such as a laser beam—on a solid surface, and “observe” how the material melts and then resolidifies when the energy source is removed.

The rapidly moving solid/liquid interface is influenced by the nature of the dopant, and vice versa; the researchers are identifying the mechanisms involved and the extent to which they occur. Also, they are trying to find out why the dopant is incorporated into the regrown solid to a far greater extent under these highly non-equilibrium conditions than would be ex-

pected from equilibrium calculations. To mimic the process, they have devised new nonequilibrium computer-simulation methods based on molecular dynamics.

Clancy collaborates closely with Michael O. Thompson of the materials science and engineering faculty, whose work includes laser-processing experiments. Their research groups are planning to study aluminum-lithium alloys of interest to aircraft-construction firms, and investigate doped semiconductors such as arsenic-silicon and gallium-silicon.

In his work on melt-spinning processes, one of Steen's goals is to place on a scientific basis the design and operation of a variant called *planar-flow melt-spinning* (see Figure 2). Melt-spinning achieves relatively high cooling rates (10^6 degrees Celsius per second) and offers the economic advantage of a continuous process. The planar-flow process has good overall stability, but although it is used commercially, its potential has not been realized.

Studies undertaken by Steen's group in collaboration with Dr. Ho Yu at Alcoa include experiments with the molten metal system; experiments with a Newtonian liquid in a model system are planned. Re-

Figure 1. Results from the simulation of a hypothetical “alloy” consisting of 85 percent A and 15 percent B. A and B are simple spherical components, differing only in size; the B atoms are 50 percent larger than the A atoms. The temperature for the simulation is roughly half the melting point; the pressure is around zero.

In Figure 1a, both A (red) and B (blue) components are solid, forming a solid solution. Figure 1b represents the atomic configurations of just the B particles; it shows the considerable segregation of B particles toward each other, heralding the possibility of a phase separation within the solid solution.

sults obtained with the model system will help elucidate the fluid dynamics, which can dominate the process. The project also includes theoretical analyses of the fluid dynamics, heat transport, and phase change.

Progress made so far includes showing that for a range of technologically realistic conditions, the process behaves in certain aspects much like the well-known extrusion and slot-coating techniques for coating surfaces with liquid films. Complications added by the heat-transfer and solidification front in planar-flow spinning have introduced new features that have also been measured and predicted.

The ultimate goal is an understanding of the influence of this process on the macro- and microstructure of rapidly solidified metals—an understanding sufficient to “engineer” specific material properties in the end product.

UNDERSTANDING THE PROCESS OF CHEMICAL VAPOR DEPOSITION

Silicon is an abundant element, but it never occurs naturally in the form required to make a semiconductor device. What is needed is a thin film, and in the microelectronics industry one of the key methods for forming such a film is chemical vapor deposition (CVD). Although many kinds

Right: Professor Rodriguez (at left) explains the operation of the equipment for a study of reactive-ion etching to his colleague Claude Cohen. A laser interferometer is used to measure the rate at which a reactive gas is etching a polymer film.

The apparatus was built by graduate student Bernard Dembs with help from IBM. Additional state-of-the-art equipment is available at Cornell's National Nanofabrication Facility.

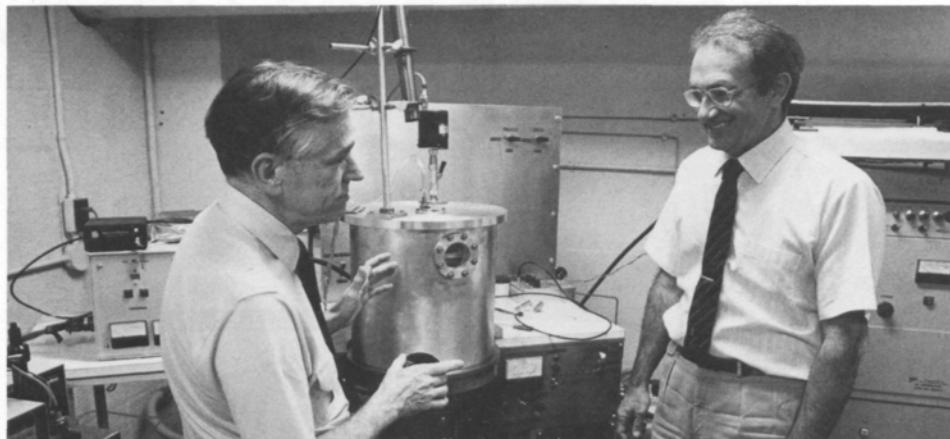
of materials can be formed by CVD, this is the most common industrial application.

Two Cornell chemical engineering faculty members—William L. Olbricht and Paulette Clancy—are directing research that is providing useful information about what goes on in CVD and how operating conditions could be improved.

In the CVD process, a gas containing silicon is heated to produce a series of chemical reactions that cause silicon atoms to deposit as a film on a solid surface (called a substrate). Conditions can be controlled so as to produce the exact properties required for a specific device; even small variations in properties such as film thickness, composition, and surface morphology make a difference.

To understand how process conditions such as reactor temperature and pressure, composition of the gas phase, and the rate of gas flow affect the quality of the film, engineers and physical chemists analyze CVD processes in terms of thermodynamics, chemical kinetics, transport phenomena, and crystal growth. At Cornell Olbricht's group is studying reaction mechanisms and heat and mass transfer in CVD reactors, and Clancy's group uses computer simulation to relate the microstructure of the growing film to its electronic properties.

Tom Lin, a graduate student working with Olbricht, is analyzing a CVD reactor



built by IBM researchers to grow amorphous silicon films from hot silane (SiH_4) gas. A model describing the mass transport of chemical intermediates yields predictions of growth rates that can be compared to measured rates in the actual reactor. The model provides information that eventually can be used in scaling up the laboratory reactor for use in manufacturing.

An important issue in the design of a CVD reactor is the relative importance of heterogeneous reactions (those that occur on the solid surface) and homogeneous (gas-phase) chemical reactions. Olbricht and Lin have proposed a simple diagnostic CVD reactor consisting of two closely spaced substrates in a very-low-pressure chamber. This could be used to examine the influence of different reaction pathways on film growth. A theoretical analysis suggests that measurements of variations in the growth rate across a wafer surface could be used to test proposed chemical reactions in the hot gas and to estimate the surface reactivity of intermediate species.

Another approach, used by Clancy's group, is to simulate the CVD process on a computer. An atomic-level description of the intermolecular forces for all the species

present is combined with the solution of Lagrangian equations of motion to describe the time evolution of the system and obtain values for thermodynamic, structural, and kinetic properties from appropriate ensemble averages. Even very simple models can be quite revealing about the likelihood of reaction mechanisms. In the modeling, particles are introduced into a vacuum at a chosen flux. These particles will descend to the surface, acted upon by the intermolecular forces between themselves and between them and the surface. The "decision" to form chemical bonds with nearby atoms will depend on the proximity, orientation, and strength of multiple bonding sites available on each molecule.

With simulation methods such as these, it is now possible to predict the fraction of species in a gas that are associating. Extensions of the technique are expected to yield further information on surface bonding sites and chemically reacting species. Such information will help define the mechanisms by which film growth proceeds, identify the diffusional characteristics of the surface prior to bonding, and assess the effect of operating conditions on the properties and quality of the film.

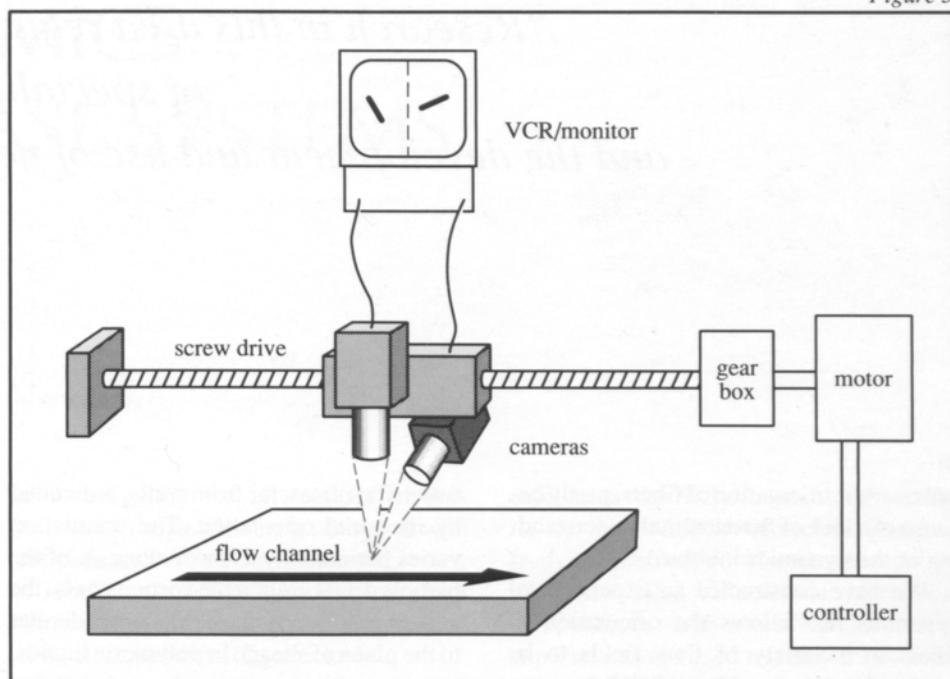
Figure 3

POLYMERS FOR PROCESSING MICROELECTRONIC DEVICES

The "micromanufacture" of integrated circuits for computers and communications systems requires polymers with special properties; their development is an area of research of particular interest to Professor Ferdinand Rodriguez.

Microlithography can be thought of as the process of producing small (micro) patterns (graph) in stone (litho). The various steps of etching, doping, metallizing, insulating, and connecting spots and lines on a single-crystal silicon wafer are accomplished on thin (1-micrometer) layers of polymer. First, polymer is selectively irradiated to make it more soluble or less soluble, and then part of the polymer film is dissolved away, leaving behind a "stencil" through which the underlying surface becomes available for alteration. The microlithographic process is often repeated ten or more times. When the etching—or other appropriate step—has been completed, the polymer film is removed, the surface completely covered by a new layer of polymer, and the next step carried out. The finished product has all the tiny transistors, wires, and other circuit elements needed for a functioning device.

In the Cornell research on photoresists, Rodriguez is collaborating with Professor S. Kay Obendorf, head of the Department of Textiles and Apparel and a member of the Fiber Science Program. Their joint project has major funding from the Office of Naval Research. The emphasis of this work has been on patterns created by scanning electron beams, although x rays and deep ultraviolet radiation are also used. They and their students are producing polymer systems with enhanced sensitivity to radiation, with controlled dissolution properties, and with superior resistance to



corrosive plasma etchants. A promising system now being studied is a combination of a host polymer (for adhesion and dimensional stability), a multifunctional monomer (for sensitivity), and an organometallic compound (for enhanced resistance to an oxygen plasma).

COMPOSITE POLYMERS AS STRUCTURAL MATERIALS

At the other end of the polymer-product scale are structural parts for products such as automobiles and appliances. The development of composites for this kind of application is the area in which I am currently working in conjunction with the Cornell Injection Molding Program.

Polymer composites containing short inorganic or organic fibers have great technological promise because of their superior mechanical properties and the ease with

Figure 3. An apparatus for tracking and recording the motion of a fiber in a polymeric liquid. This experimental equipment is used in research on fiber-filled polymers for the manufacture of molded structural parts.

Two special video cameras mounted on a carrier monitor the orientation of a particle as it travels in a pressure-driven flow between two parallel plates. The cameras follow a specific fiber in the fiber-filled polymeric solution by sliding over a ball-screw drive. The images are recorded and viewed on a high-resolution monitor of a video camera recorder.

which they can be processed. Fiber-filled polymer composites are stronger than unfilled thermoplastics, and they can be molded the same way.

We are studying the orientation of the fibers, since this can strongly affect the mechanical properties of a molded part. In practice, designers have only limited con-

“Research in this area requires the cooperative effort of specialists in various disciplines, and the development and use of new tools and techniques.”

trol over the orientation of fibers, partly because of a lack of fundamental understanding of the dynamics involved.

We have constructed an experimental apparatus that allows the orientation of fibers in a variety of flow fields to be rendered visible (see Figure 3). Video cameras record the three-dimensional orientation of naturally buoyant rod-like particles as they travel through a flow channel, and the dynamics of the fiber orientation are analyzed from the recorded images.

One of the ways we have used this apparatus is to study the effect the channel wall has on fiber orientation. We have been able to simulate the conditions in a mold cavity and elucidate the interaction between a single fiber and the cavity wall.

Another effect, overlooked by previous investigators, is the importance of the nature of the liquid in which the fibers are suspended. So-called Newtonian liquids, which are made up of small molecules, have a very different effect than polymeric fluids, which are made up of very long flexible chain-like molecules. In Newtonian liquids, such as water, glycerin, alcohols, and other common organic solvents, the orientation of a single fiber flowing be-

tween flat plates, far from walls, is dictated by its initial orientation. The orientation varies periodically as the major axis of the particle orbits around the vorticity axis (the axis of rotation of the fluid, perpendicular to the plane of shear). In polymeric liquids, however, our experiments have shown that the viscoelastic properties of the long chain-like molecules dramatically influence the orientation of the fibers. The initial orientation of a fiber far from a wall is quickly lost as the particle orients its major axis along the vorticity axis.

Our current research is focused on the effect of fiber-fiber interactions on orientation. Since short-fiber composites contain up to 10 percent by volume of fibers, such interactions must also play a major role in the final distribution of fiber orientation.

Understanding and measuring all these factors—interaction between fiber and wall, the viscoelastic nature of the liquid, and fiber-fiber interaction—will allow the development of techniques for predicting and controlling fiber orientation. Since oriented fibers are, in effect, process-induced structures, the ability to control their orientation provides a way of actually influencing the properties of the material.

A NEW THRUST IN CHEMICAL ENGINEERING RESEARCH

As the programs reviewed here demonstrate, materials engineering and processing is an active area of chemical engineering today. And because there is so much need for new and improved materials, it is a thrust that is bound to continue.

Research in this area requires the cooperative effort of specialists in various disciplines, and the development and use of new tools and techniques. For the researchers, the cross-disciplinary approach, the intellectual challenge, and the chance to contribute to important achievements add up to an exciting opportunity.

Claude Cohen is a professor of chemical engineering. Before coming to Cornell in 1977, he earned a B.S. degree at the American University in Cairo (1966) and the Ph.D. at Princeton University (1972), and was a Katzir-Katchalsky fellow at the Weizmann Institute in Israel and a research associate at the California Institute of Technology.

At Cornell he is associated with the Injection Molding Program and is a member of the graduate fields in materials science and engineering and in chemical engineering.

FLUID DYNAMICS IN MULTIPHASE SYSTEMS

by Donald L. Koch

The flow of fluids in multiphase systems has always been a major consideration for chemical engineers. Most of the operations in a chemical plant, for instance, involve transporting heat and material among liquids and solids by means of fluid motion. But today chemical engineers are expanding their expertise beyond the plant doors.

Here at Cornell our school's research programs in this area involve studies that fall outside the traditional realm of chemical engineering: blood flow in capillaries, the transport of contaminants in groundwater, the dynamics of geothermal reservoirs, enhanced oil recovery, the processing of fibrous composites, melt-spinning processes, and the growth of silicon crystals.

WHY PREDICTIONS OF TRANSPORT PROPERTIES ARE DIFFICULT

Even when the physical properties of the individual solid, liquid, and gas phases that constitute a suspension or a fluid in a porous medium are well known, predicting transport behavior presents fundamental challenges. These include:

- understanding the dynamics and stability of liquid/liquid and liquid/gas interfaces;

- investigating the interactions of particles and drops with each other and with the pore walls in a porous material;
- obtaining macroscopic descriptions of suspensions or porous media that contain very large numbers of particles;
- discovering the dynamic behavior of such macroscopic systems.

SUSPENSION FLOWS IN SMALL CAPILLARIES

In some problems of suspension mechanics, the most important hydrodynamic interactions are between the particles and the surrounding boundaries of the flow. When a suspension flows through a medium composed of small pores whose diameters are comparable to the size of the particles, the motion of the particles is influenced by nearby pore walls.

This is precisely the situation encountered in blood flow through the body's network of capillaries, where oxygen is transferred from red cells—the particles in this case—to the surrounding tissue. The capillary diameters are so small that the red cells nearly fill the vessel cross section. Experiments show that the number of red cells per unit volume is much smaller in

capillaries than in the larger blood vessels. At our school, Bill Olbricht's group is studying the motion of cells at capillary junctions called bifurcations. Numerical computations and scaled-up laboratory experiments are used to study trajectories of simple models of blood cells as they flow through fabricated structures that simulate capillary junctions. The results are useful in interpreting physiologists' in-vivo and in-vitro experiments, in which some of the important hydrodynamic variables cannot be measured.

Another example of suspension flow in small pores is the movement of oil drops through a porous matrix. This is of fundamental importance in the technique for enhancing oil recovery by "flushing out" oil trapped in porous rock. Large blobs of oil are forced through the pores by the flow of a second, immiscible fluid—water. Olbricht's group uses scaled-up and actual-scale experiments to study the motion of immiscible fluids in small pores. The experiments help determine conditions under which hydrodynamic forces would cause oil drops to break into smaller drops and so affect the efficiency of a recovery process.

COALESCENCE, BREAKUP, AND INTERFACE STABILITY

An important process affecting the properties of suspensions is the coalescence of two drops or bubbles to form a single body. In slow flows, two drops coalesce when a steady force pushes them together for a sufficiently long period of time. The process is illustrated in the sequences of photographs in Figure 1, which were taken as part of a study directed by Olbricht. In the capillary, the steady force results from the increased hydrodynamic drag experienced by the larger leading drop because of the capillary wall.

George Scheele's research group has conducted experimental studies of larger drops coalescing at higher flow rates. In these experiments the inertia of the drops and the surrounding fluid played an important role. The drops were propelled toward one another and, depending on their relative velocities, coalesced into a single drop or rebounded like a pair of elastic balls.

In still another project, my first graduate student, V. Kumaran, is engaged in a theoretical study of the dynamics of two bouncing bubbles.

Paul Steen's group is investigating the stability of interfaces between two immiscible phases. One important technological application of this work is to the "float-zone" method for growing silicon crystals. In this method, a cylinder of silicon is

melted and then resolidified into a nearly perfect single crystal. The diameter of the wafers that can be produced with this technique is limited, however, by an instability of the molten silicon bridge. While most forces, including gravity and surface tension, tend to destabilize a liquid bridge (see Figure 2), experimental and theoretical evidence suggests that certain pressure and shear forces are stabilizing. Through analysis coupled with experiment, the Cornell researchers have uncovered conditions that optimize this stabilization.

MACROSCOPIC PROPERTIES OF SUSPENSIONS AND POROUS MEDIA

Practical engineering calculations of the transport processes occurring in suspensions and porous materials, which possess complicated interphase boundaries, are possible only when a reliable macroscopic description of the multiphase system is available. One would not attempt to determine the macroscopic dynamics of a gas or liquid by calculating the motion of each individual molecule; likewise, it is generally impractical to determine the motion of each individual particle in a suspension. A theoretical description of the macroscopic transport behavior of a suspension may be derived through a kinetic theory that takes as its starting point the dynamic interactions between two or more particles moving through the suspending fluid.

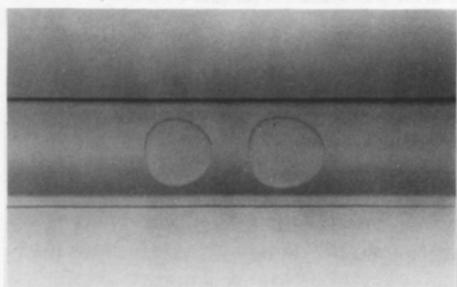
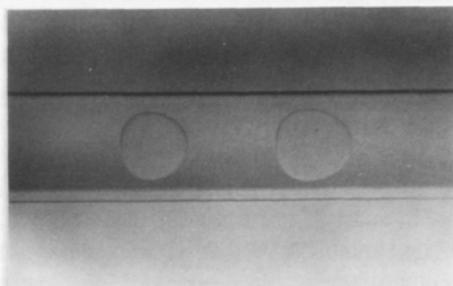
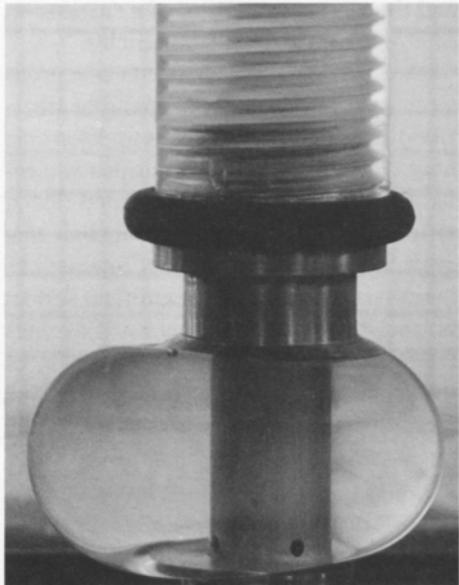


Figure 1. Photographs showing the interactions that precede the coalescence of two liquid drops flowing through a small pore. (From a 1987 article by W. L. Olbricht and D. M. Kung in Journal of Colloid and Interface Science.)

Figure 2. The "beer-belly" instability that may be exhibited by a column of liquid destabilized by surface tension. (Another instability that arises under different conditions causes the column to break into a series of droplets; this can be observed in a stream of tapwater.)

In the photograph a rotund axisymmetric column of liquid is surrounded by an immiscible liquid with a closely matched density; the inner liquid is bounded by an interface. The central rod aligns the endplates and allows inner fluid to be added through the holes near the bottom plate. (From a 1986 article by M. J. Russo and P. H. Steen in Journal of Colloid and Interface Science.)

Figure 2



Below: The pressure-driven flow of two immiscible liquids through a glass capillary is observed by graduate student Raymond Aul with the aid of a microscope and a video monitor. The work is applicable to an industrial process for enhanced oil recovery from porous rock. The capillary, simulating a pore in the rock matrix, is 50 micrometers in diameter.

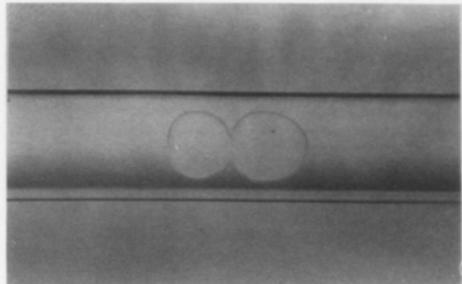
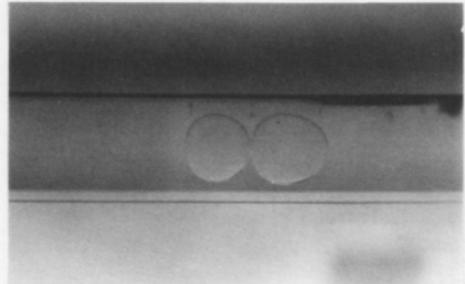
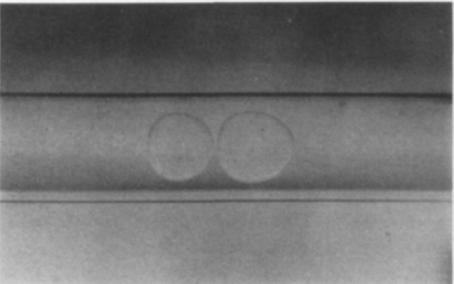
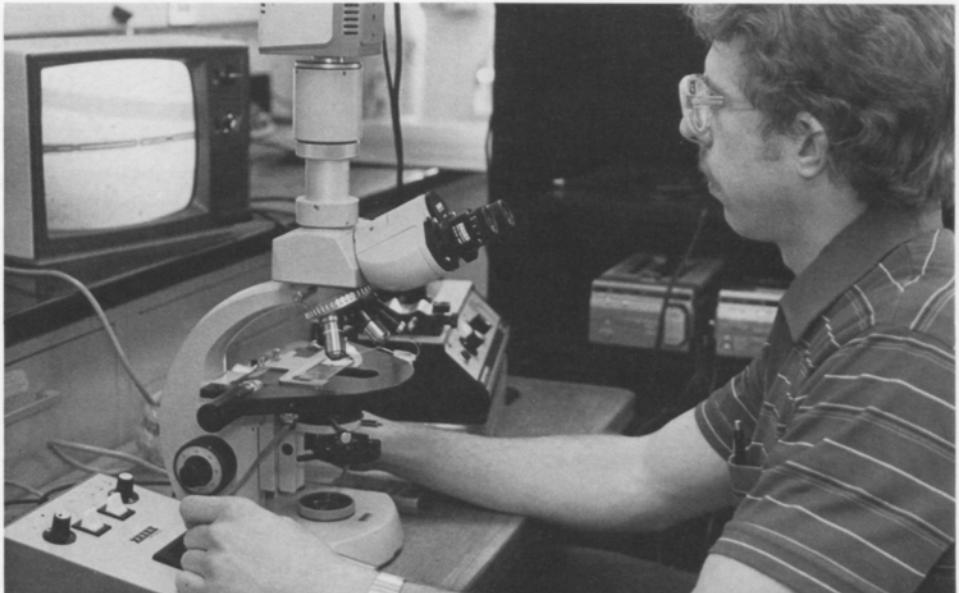


Figure 3

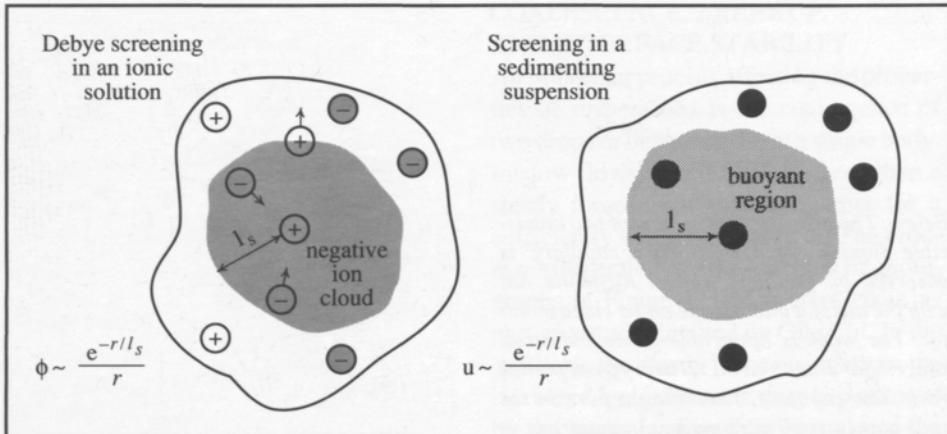


Figure 3. The mixing behavior of a suspension, considered in a manner analogous to the behavior of ions in solution.

A fundamental difficulty in describing the mixing behavior of a suspension arises from the slow decay (expressed as r^l , the reciprocal of distance) of the velocity disturbance, u , caused by a sedimenting particle. As a result of this slow decay, the motion of a particle in a suspension is affected by other particles that are very far away.

The sketch on the left illustrates how Debye and Hückel, in 1923, resolved a similar difficulty resulting from the long-range electrical interactions among ions in a solution. A positive ion attracts negative and repels positive ions, giving rise to a negatively charged ion cloud. This negative ion cloud leads to screening of the electrical potential ϕ caused by the positive ion.

The sketch on the right illustrates an analogous mechanism, in which the velocity caused by a sedimenting particle is screened by a region of buoyant suspension. According to the theory proposed by D. L. Koch and E. S. G. Shaqfeh, the region of buoyant suspension around a particle results from a deficit of neighboring particles. Such a deficit, the theory indicates, arises from interactions among groups of three sedimenting spherical particles. The researchers are currently seeking an experimental confirmation of the screening phenomenon.

The particles and fluid in a flowing suspension typically undergo a randomly fluctuating motion that is induced by the motion of the surrounding particles. A major question in suspension mechanics is under what circumstances the effects of such a motion on the macroscopic mixing and flow properties of the suspension may be expressed in terms of a hydrodynamically induced effective diffusion coefficient. Typically, for particles larger than one micrometer in diameter, this hydrodynamic mixing is much more rapid than molecular diffusion. Figure 3 illustrates the complex interplay between the structure and the mixing properties of a suspension of sedimenting, spherical particles.

A basic suspension-mechanics problem, important in the processing of fiber-filled composite materials, is to determine how the fluid motion in a suspension affects the orientations of suspended fibers. Of particular interest are suspensions that are sufficiently dense so that interactions between the fibers have a significant effect on their orientations. Figure 4 illustrates the results of a theoretical investigation of the orientation of fibers flowing through a fixed fibrous matrix. In this study, which I

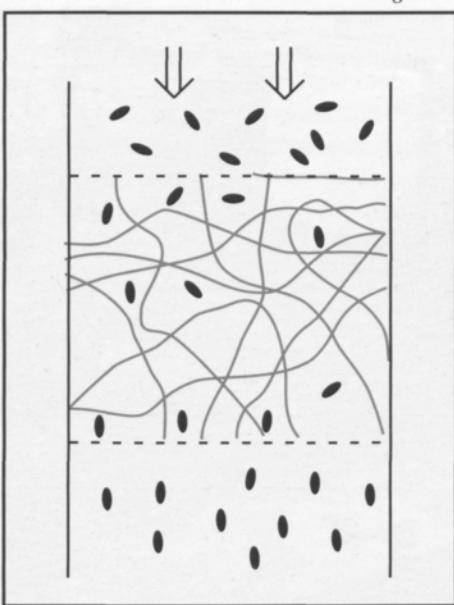
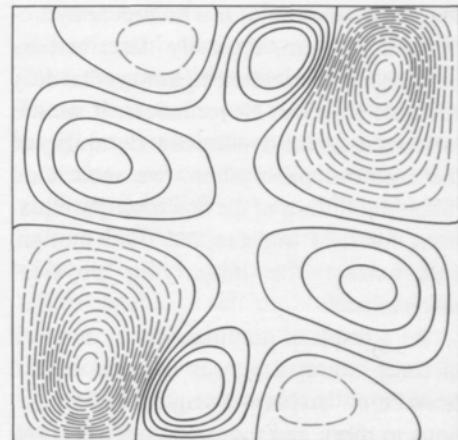
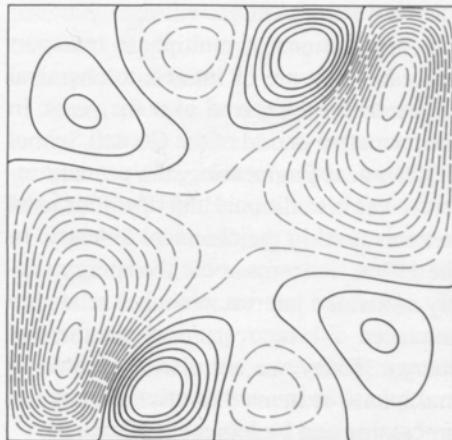
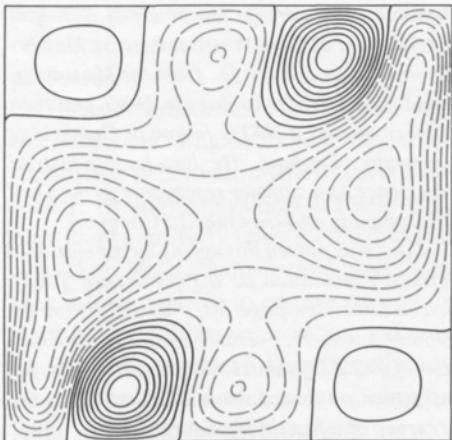
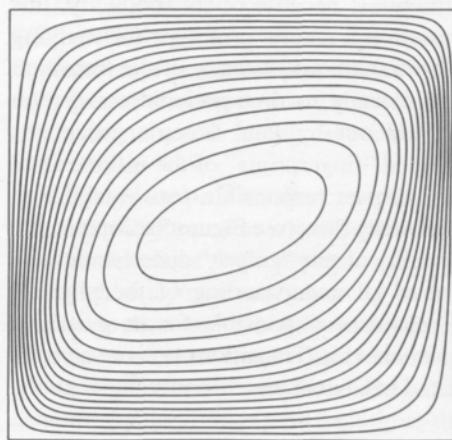
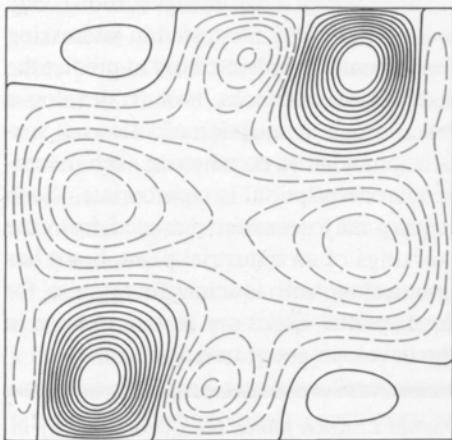
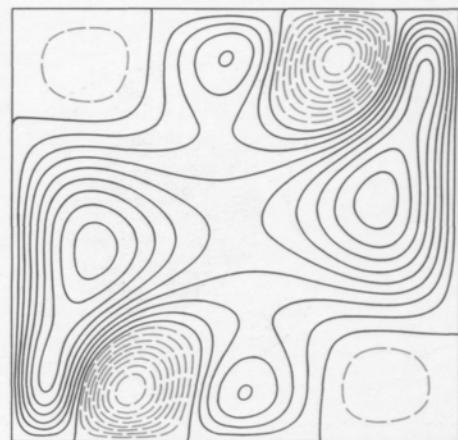
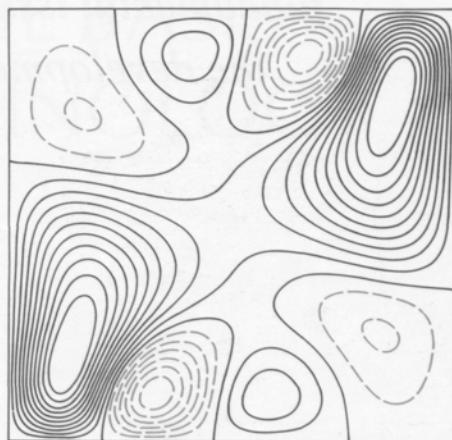
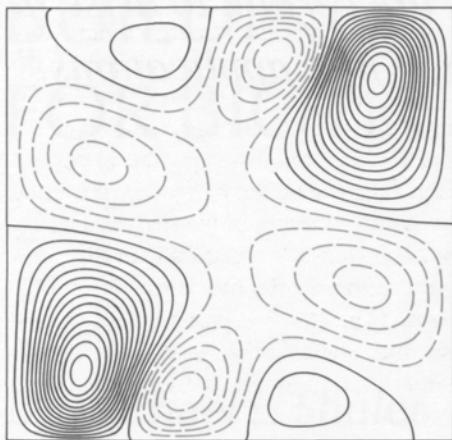


Figure 4. The strong alignment of suspended nonspherical particles that occurs when the suspension flows through a fixed fibrous material (such as steel wool). This phenomenon was discovered in a theoretical study and has been confirmed experimentally. The strong particle alignment cannot be explained by the effects of the mean flow. (From a 1988 article by E. S. G. Shaqfeh and D. L. Koch in Physics of Fluids 31:728.)

Figure 5. A study of the transition from steady to periodic flow of a fluid in a porous medium.

The center illustration shows the streamlines of the steady macroscopic fluid motion in a box of fluid-saturated porous material heated from below. The heat flux is at the point at which the transition to oscillatory flow occurs. The illustrations around the outside show the destabilization that occurs as a result of infinitesimal disturbances; the progression of the disturbances is shown (clockwise) at intervals of $1/8$ of one period. Solid lines represent a surplus and dotted lines a deficit in clockwise circulation. (From a 1988 article by P. H. Steen and C. K. Aidun in Journal of Fluid Mechanics.)

Figure 5



“... fundamental issues are certain to arise in the development of new applications.”

conducted at Cornell in collaboration with E. S. G. Shaqfeh at AT&T Bell Laboratories, we discovered that the fibers become strongly aligned. This phenomenon was confirmed by experiments, conducted in Paul Frattini's laboratory at Carnegie-Mellon University, in which a light-scattering technique was used to probe the anisotropy of the suspension.

FLOW DYNAMICS ON THE MACROSCALE

A suspension of particles in a fluid, or a fluid flowing through a porous material, often displays complicated spatial and temporal behavior: it is a nonlinear hydrodynamic system, typically described by nonlinear conservation equations that defy accurate solution. Nevertheless, if we are to understand the dynamics and stability of the macroscopic system, we must find reliable solutions of the macroscopic equations for heat transfer and fluid motion, and extract the underlying physical mechanisms.

As a result of nonlinearity, a container of fluid-saturated porous material heated from below displays a sequence of transitions to more and more complicated flow

structures; because of its simplicity, this system is a natural prototype for studying flow transitions. A study of the transition from steady to time-periodic convection carried out by Paul Steen's group has yielded “fingerprints” of the infinitesimal disturbance responsible for destabilizing the steady flow (see Figure 5). Capture and scrutiny of this “culprit” disturbance have led to an understanding of the physical mechanism responsible for its existence and behavior. Transitions to more complicated behaviors are currently under study.

THE CHANGING FOCUS OF THE RESEARCH

The applications of multiphase transport processes that are of interest to chemical engineers have evolved over the years. In the formative period of the Cornell School of Chemical Engineering, the primary interest was in traditional unit operations and reactors used in the chemical industry. In the 1970s, concerns about the energy supply motivated interest in studies related to enhanced oil recovery and geothermal energy. Today we are also interested in multiphase systems that arise in material processing and biological applications.

The approach has changed, too. Today we are especially interested in addressing fundamental problems: how to predict the stability of interfaces, how to develop a macroscopic description of a flowing suspension, what to do when no such macroscopic description is appropriate. Such inquiry may seem far removed from the workings of an industrial plant, but it has practical as well as scientific interest, for fundamental issues are certain to arise in the development of new applications.

Donald L. Koch joined the Cornell faculty in January 1987 as an assistant professor of chemical engineering. He received B.S. and B.A. degrees at Case Western Reserve University in 1981 and a Ph.D. from the Massachusetts Institute of Technology in 1986, and then spent a year as a NATO fellow at Cambridge University, England. He has had industrial experience as a summer researcher at the Shell Oil Company and the Gulf Oil Company.

Koch was named this spring by the National Science Foundation as a Presidential Young Investigator (see page 50). He also won the 1988 Francois N. Frenkiel Award of the Division of Fluid Dynamics, Physics of Fluids, for his paper on sound-wave attenuation in the presence of a fractal boundary.

BUILDING THE BASIS FOR BIOTECHNOLOGY

by Michael L. Shuler

We can now manipulate life at its most basic level—the genetic. For thousands of years people have practiced genetic engineering at the level of selection and breeding. But now it can be done in a purposeful, predetermined manner with the molecular-level manipulation of DNA. We now have a tool to probe the mysteries of life in a way unimaginable twenty years ago.

With this intellectual revolution emerge new visions and new hopes: new medicines, semisynthetic organs grown in large vats, abundant and nutritious foods, computers based on biological molecules rather than silicon chips, superorganisms to degrade pollutants, and a wide array of consumer products and industrial processes.

These dreams will remain dreams without hard work. Engineers will play an essential role in converting these visions into reality. Biological systems are very complex and beautifully constructed, but they obey the rules of chemistry and physics and they are susceptible to engineering analysis. Living cells are predictable, and processes to use them can be rationally constructed on commercial scales. Doing this is the job of the biochemical engineer.

A LITTLE BIOLOGY FOR ENGINEERS

To make bioprocesses work, the biochemical engineer must understand some things about the nature of biological molecules and cells.

Enzymes are proteins that catalyze specific chemical transformations; almost all cellular reactions are enzyme-mediated. Although enzymes are generally much more selective and rapid than inorganic catalysts under the same conditions, they are also much more sensitive. They can denature (undergo change in their three-dimensional shape) and, as a consequence, lose their activity at high temperatures or extremes of pH, salt concentration, or other external conditions.

Every protein is a polymer of amino acids, and the interactions between side groups (forming, for example, hydrogen bonds, disulfide bridges, salt bonds, or configurations resulting from hydrophobic-hydrophilic interaction) determine the shape and activity of the molecule. Of course, the primary sequence of amino acids is critical to such interactions and to the final activity of the molecule.

The exact sequence of amino acids in

each protein is determined by a sequence of nucleotides on a DNA molecule. The portion of the DNA that encodes the information for a particular protein is called a *gene*. The DNA uses an alphabet of four “letters” (each letter is a particular chemical) to write three-letter “words” (called *codons*); sixty-four words are possible. Each word stands for a particular amino acid or for “start” or “stop”. The code is essentially universal—the word specifying a particular amino acid is the same in humans as in the simplest bacterium—and the universality of the code has important implications for genetic engineering.

The chromosome (DNA) contains not only genes, but sequences of DNA that allow the genes to be read (or transcribed). These sequences are called *promoters*; many promoters are regulated by small molecules and can be turned on and off.

To genetically engineer cells we need a *vector*. For bacteria, a small circular piece of DNA, called a *plasmid*, is used. A plasmid is capable of self-replication and may be present at high copy numbers (sometimes one hundred or more copies per cell). For animal cells, viruses are often modified for use as vectors.

*"Engineers will play
an essential role
in converting these
visions into reality."*

HOW TO GENETICALLY ENGINEER A CELL

Here is a very simplified description of how a cell may be genetically engineered. Suppose the object is to produce an animal hormone. A gene that encodes the information for the protein structure of the hormone can be synthesized chemically if the structure is known, or made from a copy of the message used by the cell to make the protein, or obtained by cutting the DNA from the animal's cell and isolating a fragment with the desired gene.

With a copy of the desired gene in hand, it is possible to cut the vector DNA at specific predetermined sites, insert the desired gene, and "glue" the insert into the vector. The recombinant DNA segments are an example of *recombinant DNA*. A host cell can then be "transformed" by insertion of the vector into the cell. If everything has been done correctly, the host cell with the recombinant DNA will manufacture the foreign protein (the hormone) at very high levels. The high-level production in the recombinant system makes the commercial production of the hormone feasible.

The high-level production can be done effectively on a large scale only if there is a good understanding of how the cell will respond to external stimuli and how those stimuli might be manipulated in a bioreactor. Without this knowledge there is no usable product. Establishing the basic understanding of the system is one of the jobs of the biochemical engineer.

BIOCHEMICAL ENGINEERING RESEARCH AT CORNELL

Cornell is fortunate to have had a significant presence in biochemical engineering for more than thirty years. Only a handful of other chemical engineering departments

can make such a claim. A solid base has been laid for a strong program in biochemical engineering, and it has become a significant part of the school program.

Currently, Professors Bob Finn, Dan Hammer, and I head projects that constitute the core effort, and there are important interactions with Professors Thanasis Panagiotopoulos and Bill Olbricht. A wide variety of work is underway, much of it multidisciplinary. Cornell's Biotechnology Institute has played an important role in fostering cooperative work in bioprocess engineering.

USING *E. COLI* IN GENETIC ENGINEERING

One example of Cornell work in bioprocess engineering is a project that Professor David Wilson of the Department of Biochemistry and I began five years ago. At the time, we envisioned a continuous process for producing high levels of a desired protein using the common gut bacterium *Escherichia coli*.

E. coli is the world's best characterized and understood organism. Important advantages in using it are that the location on the chromosome of many of the cell's genes are known, and many mutants are available. *E. coli* is an ideal host organism for genetic engineering because it allows very complex, sophisticated manipulation of the cell's genetic information.

E. coli is not ideal as an industrial organism, however. When a foreign protein is made in *E. coli*, several things can go wrong. Sometimes enzymes called *proteases* that are inside *E. coli* destroy proteins that appear foreign. In other cases, the protein forms insoluble complexes, called *inclusion bodies*, inside the cell. Proteins in inclusion bodies are misfolded and have no biological activity, and resolubilization of

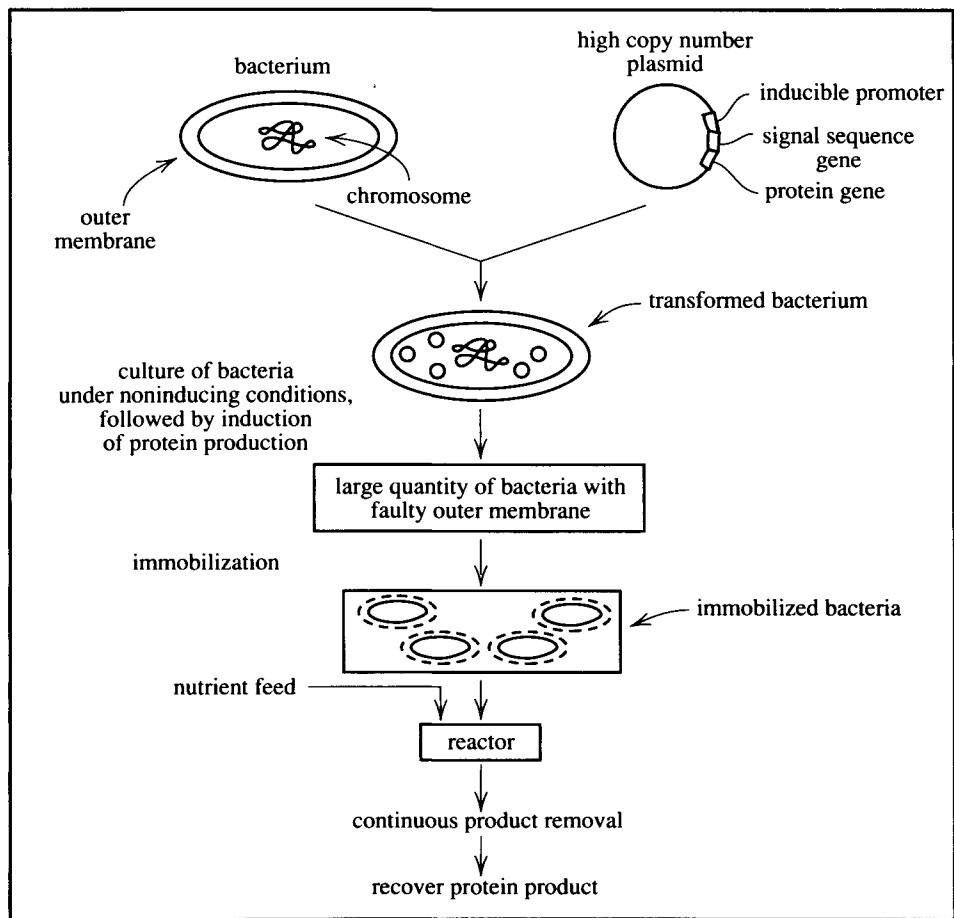


Figure 1. A general scheme for producing a plasmid-encoded protein using genetically engineered *E. coli*. The membrane of the host cell is made "leaky" so that the protein can be excreted into the extracellular fluid. Cell immobilization potentially allows the use of a continuous, high-cell-density bioreactor.

tein. It has two membranes: an inner one and an outer one beyond which proteins cannot pass. Proteins having a *signal sequence* (a leader of specific amino acids) can pass the inner membrane and reside in the space between the inner and outer membranes, or they can be incorporated into the outer membrane. Our idea was that if the outer membrane could be disrupted slightly, then excess proteins might be excreted. Of course, massive disruption of the outer membrane would lead to poor growth or cell death.

TOWARD REACTORS FOR PROTEIN PRODUCTION

Realizing these constraints, we proposed and developed a process concept for producing protein by means of *E. coli* (see Figure 1).

We genetically engineered the organism by introducing into the cell a plasmid with a strong regulated promoter (the tac promoter), allowing the transcription of a gene for the target protein with a signal sequence attached. Then we found a combination of circumstances in which a leaky outer membrane can be induced as a result of turning on the overproduction of the target protein.

If cells with leaky outer membranes were entrapped or retained within a reactor, there is the possibility that they could be continuously supplied with a stream of nutrients and that high levels of the target protein could be recovered from the efflu-

such a protein to convert it back into an active form is often difficult.

Another problem is that cells that produce large quantities of protein from the recombinant DNA grow more slowly than those without foreign DNA because a large portion of the cellular resources must go to the target protein. The target protein is of no use to the host cell. In a large population of cells there are some that shed the modified plasmids, and the plasmid-free cells—and also those in which target protein synthesis has been turned off—can outgrow

and displace productive cells. This prob-

lem of *genetic instability* becomes more severe as the reactor size is increased. We have developed an approach that circumvents these problems with *E. coli*. The key is to recognize that if the target protein were excreted outside of the cell, the complications of protein degradation and inclusion-body formation might be avoided. Further, if the protein outside the cell were target protein only, and it were present at high concentration, the cost of recovering and purifying it could be greatly reduced.

Normally, *E. coli* does not excrete pro-

*Figure 2. Electron microscope images of an *E. coli* culture. Plasmid-containing *E. coli* entrapped in calcium alginate beads were cultured in a fluidized-bed reactor. At Day 1 the cells were homogeneously distributed. After ninety days in the reactor, pockets containing high concentrations of cells had formed. (Photograph and electron microscopy by John Telford of the Section of Biochemistry, Molecular and Cell Biology at Cornell.)*

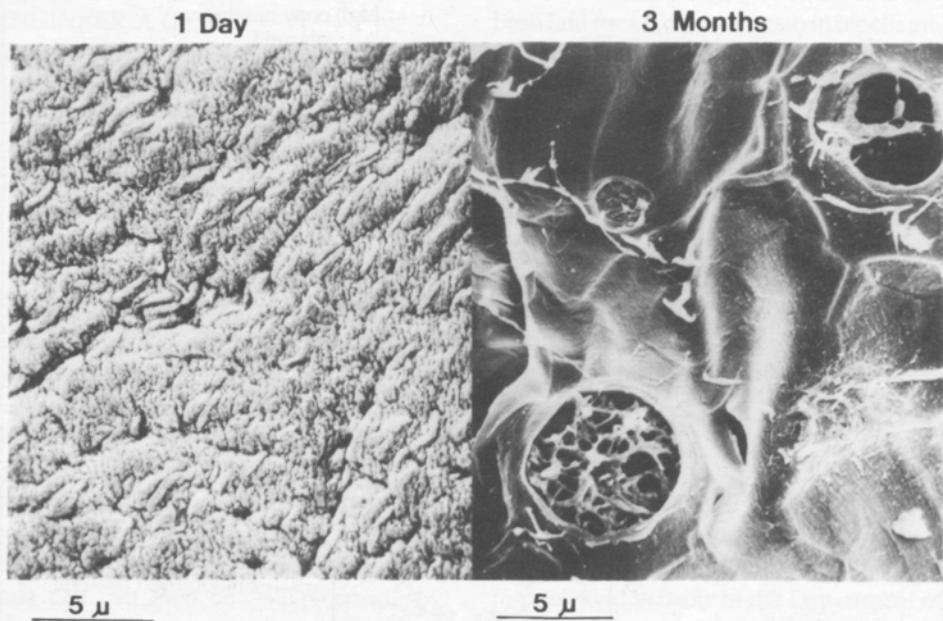
ent. Ideally, such a continuous reactor system would enable us to suppress rapid cell growth and channel all the cellular resources into making the target protein.

Such a system is probably not completely attainable, but we have made important progress toward this ideal. With the production of β -lactamase as a model system (β -lactamase is used in treating allergic responses to penicillin), we have obtained high-level production (over 35 percent of the total protein as the target protein). Over 90 percent of the target protein was excreted, and the excreted material had high purity—often above 85 percent. We have achieved concentrations in excess of 1 gram per liter.

Although we have successfully operated the system as a continuous unit for up to nine hundred hours, it has proven difficult to sustain maximum productivity levels throughout this period. Currently we are focusing on obtaining a better understanding of how the cellular regulatory systems are interacting with the operating strategy for the bioreactor.

OTHER POSSIBILITIES FOR PROTEIN PRODUCTION

The system has been used for proteins in addition to β -lactamase. For example, the production of a growth factor to speed wound healing is now being studied. Al-



though the system has not yet been optimized, the rate of formation of this small protein is impressive—in terms of the number of molecules produced, it is slightly less than 50 percent of the rate achieved in β -lactamase production. About 40 percent of the protein is excreted with essentially no cell destruction.

This system has the potential of greatly reducing the cost of production of many proteins. A difficulty, though, is that proteins produced by bacteria (such as *E. coli*) do not undergo modifications in a manner identical to the way in which the human body modifies proteins, and this may be significant if they are to have therapeutic value.

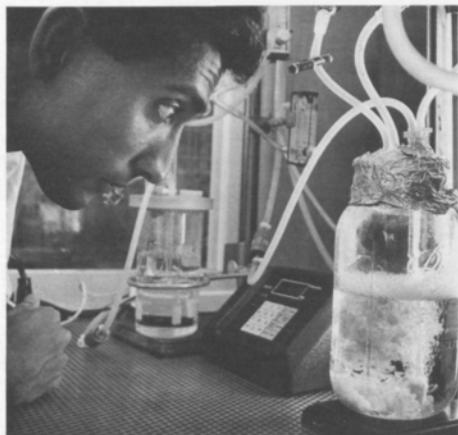
An alternate protein-production method avoids this problem. The method uses a system comprising insect cells (grown in tissue culture) and a baculovirus. If the baculovirus is genetically engineered

to produce a target protein, cells infected with the modified virus become highly efficient protein producers. Furthermore, proteins made in such a system undergo glycosylation (addition of sugars), phosphorylation, and other modifications that occur in human cells, and therefore might be useful as therapeutics when post-translational modifications are required. In fact, high protein-production rates and potential safety advantages may make the insect cell–baculovirus system more attractive than systems based on mammalian cell culture.

At Cornell we are interested in developing more effective and easily scalable reactors for this system. (By scalable we mean that the performance of a larger unit can be readily predicted from data on the operation of a smaller unit.) Currently, a team consisting of two chemical engineers and two biological scientists has initiated



Above: In research on insect-cell tissue culture, graduate student Olotu Ogonah inspects samples from the bioreactor to check on how the cells are growing. A special inverted phase-contrast microscope is used to provide good imaging of the cells.



Left: Graduate student Bobby Bringi is experimenting with plant-tissue cultures for eventual production of pharmaceuticals. One substance of interest, for example, is an anti-cancer agent found in periwinkle. Initially, the growth of tobacco shoots is being studied as a model system.



Above: The equipment in Professor Shuler's laboratory includes shaking tables for plant-tissue culture and facilities for growing plant tissues and organs (such as roots and shoots). In his thesis research, graduate student Tom Hirasuna is developing methods for producing natural pigments.

BIOCHEMICAL STUDIES NOW UNDERWAY AT CORNELL

Production of proteins from recombinant DNA

Biodegradation of hazardous chemicals

Computer modeling of cellular growth and product formation for bacteria and animal cells

Culture of plant cell tissue and organs for the production of food ingredients and medicinals

Membrane-based bioreactors

Heavy-metal adsorption onto biofilms

Exploration of shear effects using liposomes

Structure-function relationships in biological macromolecules

Development of surfaces that promote cell spreading and cell performance in bioreactors

Mathematical modeling of dynamic cell-substrate interactions

Modeling and manipulation of cell agglutination

Cell-separation techniques

work on this project. The team members are Hammer and I from Engineering and Bob Granados and H. Alan Wood from the Boyce Thompson Institute for Plant Research (which is located on campus). A more basic understanding of the effects of shear and adhesion on cell physiology needs to be developed. Novel bioreactor configurations that decouple aeration and agitation are being explored.

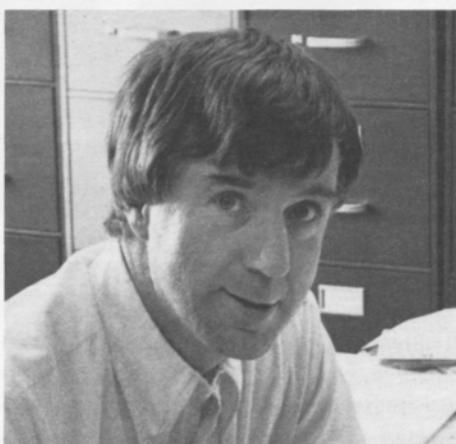
FUTURE ADVANCES IN BIOTECHNOLOGY AT CORNELL

In addition to these projects on the production of proteins from recombinant DNA, many other problems are under study at Cornell (see the table). The topics illustrate the wide variety of important problems that involve biochemical engineers today.

As we look forward, it is clear that a more complete understanding of cellular regulation and genetics will foster the rational application of engineering principles to exploit cellular systems and their components. The potential applications are numerous, and Cornell biochemical engineering will be in the forefront of many of the developments.

An example of an area in which we

anticipate a great deal of future activity is the manipulation of cell-surface receptors. Many physiological responses in mammalian, plant, and insect cell systems are modulated by surface receptor molecules. These receptors bind with complementary molecules (*ligands*) found in solution, and thereby generate an intracellular signal. Receptor-ligand interactions control nutrient metabolism, virus uptake, cell growth and cell differentiation, cell-cell communication, and the production and secretion of intracellular products. Since cell growth, product formation, and product secretion



are important elements in successful bioreactor operation, manipulating receptor molecules is one approach to improving bioprocesses. Examples might include the development of inexpensive substitutes for the costly and exotic growth factors that now must be added to animal-cell cultures.

In addition, receptors are important in cell adhesion, which in turn is important to many biomedical and biotechnological problems, from cancer-cell metastasis (spread of cancer cells throughout the body) to cell-separation processes in cancer treatment using bone-marrow transplants or lymphokine-activated killer cell (LAK) therapy. At Cornell we will focus on gaining a more fundamental understanding of receptor-mediated cell adhesion and using this understanding to propose novel therapies.

This example illustrates the significance of research in biochemical engineering, as well as the potential for growth in our program here at Cornell. It is one of many projects we intend to develop as we move toward converting the promises of biotechnology into reality.

Michael L. Shuler, professor of chemical engineering, came to Cornell in 1974 after earning the B.S. degree at Notre Dame University and a Ph.D. at the University of Minnesota. He has been active in the development of the Biotechnology Institute and Center, and is a member of the graduate fields in food science and in microbiology, as well as in chemical engineering.

He has been a visiting scholar at the University of Washington and the Coburn Lecturer at the University of Delaware. In 1986 he received the Marvin J. Johnson Award of the Microbial and Biochemical Technology Division of the American Chemical Society. He is the founding editor-in-chief of Biotechnology Progress.

REGISTER

■ The new dean of the faculty at Cornell is *Walter R. Lynn*, a professor of environmental engineering, who was elected by his colleagues for a three-year term that began July 1. He has been director of the university's Program on Science, Technology and Society, and will continue to work with that program as well as with the School of Civil and Environmental Engineering.

During his twenty-seven years at Cornell, Lynn has served as director of his school, as director of the Center for Environmental Research, and as a member of Cornell's board of trustees.

■ *David Caughey*, a professor of mechanical and aerospace engineering, has been chosen as acting director of Cornell's Center for Theory and Simulation in Science and Engineering, a national supercomputer center.

Caughey replaces Cornell physics professor Kenneth Wilson, the center's first director, who has accepted a position at Ohio State University.

A specialist in fluid dynamics, transonic flow, and computational aerodynamics, Caughey was active in establishing the center and is a major user of the facility.

■ Two engineering faculty members were awarded honorary Doctor of Science degrees this spring. *James W. Mayer*, the Francis N. Bard Professor of Materials Science and Engineering, was honored by the State University of New York. *Jack E. Oliver*, the Irving Porter Church Professor in Engineering in the Department of Geological Sciences, received his honorary degree from Hamilton College.

Mayer's citation read, in part: "You have created a revolution in nuclear physics and materials science. . . . You invented a solid state detector of nuclear particles [that] led to modern CAT-scan technology. . . . Your pioneering work laid the foundation for the integrated circuit industry. . . . You have also distinguished yourself as a humane and compassionate teacher. . . ."

Mayer, a Cornell faculty member since 1980, holds seven patents, is co-author of five books and co-editor of three books, and has published more than four hundred papers. He has received many professional honors, including election to the National Academy of Engineering.

Oliver was cited as "among the pioneers in testing the theory of plate tectonics. . . . the greatest geological discovery of our time."

Since then, the citation continued, "you have been at the forefront of studies of deep continental structure. . . . You have risen above the mundane to urge an imaginative, innovative and comprehensive global plan for the exploration of the solid earth."

Oliver came to Cornell as director of the geological sciences department in 1971. Currently he is director of the Institute for the Study of the Continents and a leader of the Consortium for Continental Reflection Profiling. He is a member of the National Academy of Sciences, a fellow of three professional societies, and has received numerous other honors and awards.

■ *William L. Maxwell*, the Andrew Schultz, Jr. Professor of Industrial Engineering, was among twelve senior members of the Institute of Industrial Engineers who received the institute's Fellow Award at the annual meeting this spring. The international organization has some 42,000 members.

Maxwell has been on the faculty of the School of Operations Research and Industrial Engineering since 1960. He is a specialist in the design and operation of manufacturing facilities.

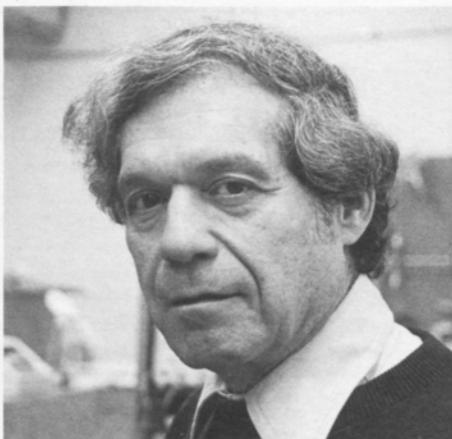
Conway

■ *Harry D. Conway* of the Department of Theoretical and Applied Science and five of his colleagues on the college faculty have retired as professors, emeritus.

Conway was educated at the University of London, earning two degrees in applied mechanics—the B.Sc. degree in 1942 and the Ph.D. in 1945. Subsequently, he spent several years at Cambridge University, England, where he served as a demonstrator in the Engineering Laboratories of Cambridge University and as assistant director of studies at St. Catharine's College, and earned a master's degree in engineering. He was awarded the Sc.D. degree from Cambridge in 1970.

Conway came to Cornell in 1947. He was a Guggenheim fellow at Imperial College, London, in 1953–54, and a National Science Foundation senior postdoctoral fellow at the same university in 1960–61. He was the Julius F. Stone visiting professor at Ohio State University in 1958–59.

Conway's specialties are structural mechanics and lubrication. He has published nearly two hundred papers in these and related fields, and has served as a consultant to a number of companies, notably IBM.

Hart

He plans to teach a course in the fall and will continue his research. Currently he is working with Che-Yu Li of the materials science and engineering faculty on a cooperative project sponsored by the Semiconductor Research Corporation.

■ *Edward W. Hart*, a professor in both the Department of Materials Science and Engineering and the Department of Theoretical and Applied Mechanics, retired this summer after twelve years at Cornell. Previously he was on the research staff at the General Electric Research Laboratory in Schenectady, New York.

Hart received the B.S. degree from the City College of New York in 1938 and the Ph.D. in theoretical physics from the University of California at Berkeley in 1950.

He has carried out an active research program in several areas of materials science and the mechanics of materials, most recently in the deformation of metals and crack growth in ductile materials.

Honors he has received include election as a fellow of the American Physical Society, the 1982 Humboldt Prize of the Alexander von Humboldt Foundation, and the U.S. Navy's Meritorious Civilian Service

Kim

Award. He has been the Battelle Visiting Professor at Ohio State University and a visiting professor at the Technical University of Braunschweig, West Germany.

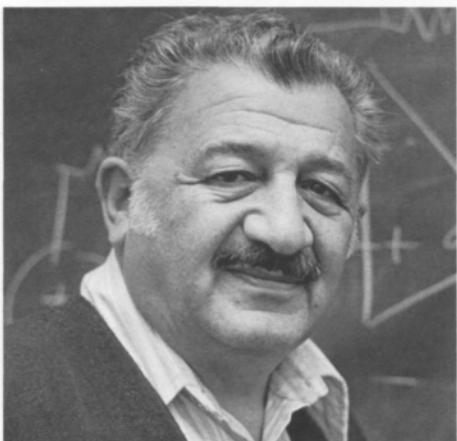
Hart will spend the calendar year 1989 at the Kernforschungszentrum (Nuclear Research Center) in Karlsruhe, West Germany, conducting research and serving as a consultant.

■ *Myunghwan Kim*, who became an emeritus professor of electrical engineering this summer, will return to his native Korea this fall as a special assistant to the president of the Korean Institute of Technology (KIT). He plans to work with the Cornell College of Engineering to establish ties in education and research between Cornell and the KIT.

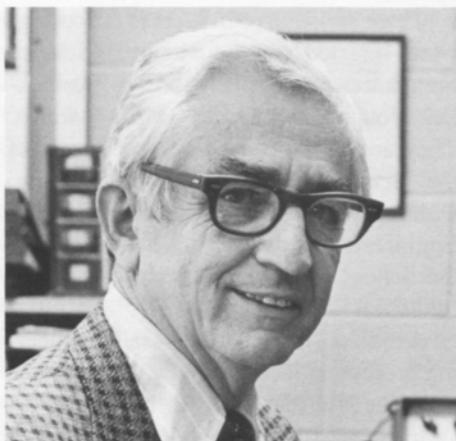
After serving in the Korean army from 1950 to 1954, Kim came to the United States as an exchange student. After receiving the B.S. degree from the University of Alabama in 1958, he did graduate work at Yale University, where he was a Danforth fellow. He received the M.E. degree in 1959 and the Ph.D. in 1962, and then joined the Cornell faculty.

A specialist in bioelectronics and con-

Nichols



Phelan



Von Berg



trol theory, Kim has maintained an active research program. In 1968-69 he held a postdoctoral position at the Jet Propulsion Laboratory. He has also held visiting positions in biology at the California Institute of Technology and at Cornell's Section of Neurobiology and Behavior. He has been a consultant to the Guidance and Control Laboratory of the United States Army Missile Command, and at the National Cancer Institute.

During recent leaves in Korea he worked at the National Center for Health Care Technology, conducted seminars at several universities, worked on VLSI digital design at the Korean Advanced Institute of Science and Technology, and served as a consultant to educational and industrial groups.

■ *Benjamin Nichols* became professor, emeritus, of electrical engineering at the end of the 1987-88 academic year. He had been on the Cornell faculty since 1946.

Nichols is also a Cornell alumnus—he received the B.E.E. degree in 1946 and the M.E.E. in 1949. He studied at the University of Alaska for a Ph.D. in geophysics, awarded in 1957.

Nichols has had special interest in educational policies and techniques. At the college he served at various times as assistant dean in charge of the Division of Basic Studies, as a curriculum committee member, and, most recently, as associate director of the School of Electrical Engineering.

He was a member of the former University Senate, and served as chairman of its executive committee.

During his years at Cornell, Nichols has served as a consultant to the Stanford Research Institute, the U.S. Office of Education, Educational Services, Inc., TRW, and the Massachusetts Institute of Technology.

He has also been active in community affairs, and is currently on the Ithaca City Council.

■ After almost forty years on the Cornell faculty, *Richard M. Phelan* became professor, emeritus, of mechanical and aerospace engineering in January.

A specialist in feedback control systems, he has combined consulting activities with teaching; he has worked mainly with the environmental test group at the Lawrence Livermore Laboratory, where he spent several sabbatical leaves. He has

published three widely used books, *Dynamics of Machinery*, *Fundamentals of Mechanical Design*, and *Automatic Control Systems*.

Phelan received the B.S. degree in mechanical engineering from the University of Missouri in 1943. Before beginning graduate study at Cornell, he served as a machinist in the Seabees, taught navigation at Notre Dame's Midshipmen's School, and worked in engineering design at a California naval base. He received the Cornell degree of Master of Mechanical Engineering in 1950.

■ *Robert L. Von Berg*, a Cornell faculty member in chemical engineering since 1946, became professor, emeritus, this summer.

Von Berg studied at the University of West Virginia, receiving the B.S. degree in 1940 and the M.S. in 1941. He was awarded the Sc.D. degree from the Massachusetts Institute of Technology in 1944. Before joining the Cornell faculty, he worked at E. I. du Pont de Nemours and Company.

His recent research has been concerned with a freezing process for the desalination of water, and in the use of gamma radiation

for controlled chemical conversions. He was a member of the graduate faculty in nuclear science and engineering, as well as in chemical engineering.

He has spent sabbatical leaves at Dow Chemical, as a NATO fellow at the Delft Technical Institute in The Netherlands, at the Los Alamos Scientific Laboratory, and as a visiting professor at universities in Australia and New Zealand.

He is now teaching for a six-month period at the University of Canterbury in Christchurch, New Zealand, and plans to return to Ithaca in January.

■ A Cornell structural engineering professor, *Thomas D. O'Rourke*, has been selected to receive the 1988 Walter L. Huber Civil Engineering Research Prize of the American Society of Civil Engineers. The prize, one of the most important awarded by the ASCE, recognizes people "of early accomplishment who can be expected to continue fruitful careers in research."

O'Rourke specializes in soil-structure interaction, underground structures, and geotechnical instrumentation.

Three other faculty members of the School of Civil and Environmental Engineering have been recipients of the prize: Philip Liu in 1978, Fred Kulhawy in 1982, and Gerhard Jirka in 1983.

■ Richard I. Dick, the Joseph P. Ripley Professor of Engineering, received the 1987 Outstanding Publication Award of the Association of Environmental Engineering Professors. This is the second time Dick has received the medal, which has been awarded only four times.

Dick is a specialist in water and wastewater treatment, and sludge treatment and disposal.

■ Three assistant professors at the college were selected by the National Science Foundation this spring to receive Presidential Young Investigator (PYI) Awards. They are *Venkatachalam Anantharam* of the School of Electrical Engineering, *Donald L. Koch* of the School of Chemical Engineering, and *Joseph S. B. Mitchell* of the School of Operations Research and Industrial Engineering.

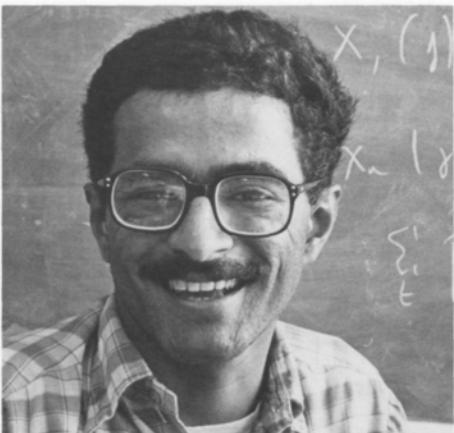
A total of twenty-one Cornell engineering professors have received these awards since the program began in 1984.

Each award carries a five-year research grant from the NSF plus funds to match industrial grants for a total of up to \$100,000 a year. The purpose is to help young researchers develop their programs and encourage them to remain at universities.

Anantharam, a Ph.D. from the University of California at Berkeley, has been at Cornell since 1986. A specialist in the mathematical analysis and design of distributed communication networks, he is a member of the graduate fields in statistics and in mathematics as well as in electrical engineering.

Koch came to Cornell in January 1987 after completing doctoral studies at the Massachusetts Institute of Technology and spending a year as a NATO fellow at Cambridge University, England. His research concerns the orientation of fibers in suspensions, a factor that affects the properties of composite materials.

Mitchell came to Cornell in 1986 after working at the Hughes Artificial Intelligence Research Center for five years. He received his Ph.D. from Stanford University in 1986. In his research, Mitchell is focusing on optimization problems in computational geometry—seeking, for example, to find the shortest paths for mobile robots.

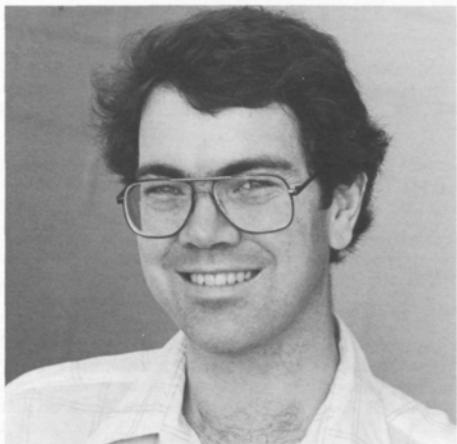


Koch



Mitchell





■ *Clifford R. Pollock* is the recipient of this year's Excellence in Teaching Award, which is sponsored by the Cornell Society of Engineers and the student honorary Tau Beta Pi. It carries a \$2,000 prize.

Pollock, an associate professor of electrical engineering, was selected on the basis of student nominations; more than a thousand students participated in the polling. Pollock was cited for his responsiveness to students' needs, and for clear presentation of complex material.

In 1984 he received a Presidential Young Investigator Award in support of his research.

■ Also awarded this spring were three Dean's Prizes for Excellence in Teaching. The recipients, announced by Dean William B. Streett, are *Kenneth C. Hover*, associate professor of structural engineering; *Joseph S. B. Mitchell*, assistant professor of operations research and industrial engineering; and *Mary Sansalone*, assistant professor of structural engineering. Each received a cash award of \$1,500.

Mitchell also was chosen this spring for a PYI award (see the story on the facing page.) *Hover* won a PYI award in 1986.

■ *James J. Bisogni, Jr.*, associate professor of environmental engineering, was awarded the Chi Epsilon Professor of the Year Award at the School of Civil and Environmental Engineering.

Bisogni, whose specialty area is water quality engineering, has been on the faculty since 1972.

■ Six engineering students were among the Cornell seniors chosen this spring as Presidential Scholars. They were presented certificates by President Frank H. T. Rhodes at a convocation in May.

Also on hand at the ceremony were educators who had been named by the students as the most influential in their academic development. Each student designated one Cornell faculty member or administrator and a high school teacher.

The engineering seniors, their major fields, and the faculty members they named are: *John P. Bayne, Jr.*, mechanical and aerospace engineering, and Associate Professor *Zellman Warhaft*; *Valerie L. Beattie*, electrical engineering (who also had a major in English), and Assistant Dean *John C. Belina*; *Stephen T. Bernt*, electrical engineering, and Associate Professor *David F. Delchamps*; *Faith A. Brown*, operations research and industrial engineering, and Professor *Lionel Weiss*; *Brian C. Hall*, applied and engineering physics (who also had a major in mathematics), and Professor *Anthony W. Knapp* of the mathematics department; and *Randall W. Verhoef*, chemical engineering, and Assistant Professor *A. Brad Anton*.

This was the first year since the Presidential Scholars program was introduced in 1984 that high school teachers have been invited to attend the ceremony. Among the twenty-five who came, at the university's expense, was *Beverly Griffith*, Randall

Verhoef's mathematics teacher. She travelled from Glendora, California.

Presidential Scholars are recognized for being in the top 5 percent of the senior class and, in the words of President Rhodes, for having "demonstrated exceptional intellectual drive, energetic leadership abilities, and a commitment to contribute to the betterment of society."

■ Engineering students took the top two prizes in a special essay contest sponsored by the Mobil Corporation and open to all students at Cornell.

John Field, a doctoral candidate in computer science, won the \$2,500 first prize for his essay, "America's Engineering Crisis: Conventional Wisdom vs. Commitment." In the essay, he advocates commitment to long-term strategies and the development of a cultural climate in which engineering and the sciences can develop "independently of the latest techno-shock."

The second-place winner, who received a \$1,000 prize, is *Douglas O'Neill*, an undergraduate in civil and environmental engineering. In his essay, "Incineration and the Garbage Crisis," he points out that the use of landfills as the major means of solid-waste disposal is doomed and that the United States should make specific plans for alternative strategies, incorporating recycling and incineration. He discusses ways of handling various hazardous wastes, and calls for the adoption of government policies for their disposal.

Karen Varley, an M.S. candidate in plant genetics, won the third-place prize of \$500. She wrote on the decline in the number of engineering students.

The winning essays were selected by a committee of Mobil staff members from sixty-five entries.

FACULTY PUBLICATIONS

Current research activities at the Cornell University College of Engineering are represented by the following publications and conference papers that appeared or were presented during the three-month period January through March 1988. (Earlier entries omitted from previous Quarterly listings are included here with the year of publication in parentheses.) The names of Cornell personnel are in italics.

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Aneshansley, D. J., R. C. Gorewit, L. R. Price, D. C. Ludington, and R. A. Pellerin. 1988. Stray voltage effects on machine milking. Paper read at Milking Systems and Milking Management Symposium, 13–14 January 1988, in Harrisburg, PA.

Myers, S. P., T.-T. Lin, R. E. Pitt, and P. L. Steponkus. 1988. Cryobehavior of immature bovine oocytes. *Cryo-Letters* 8:260–75.

Pitt, R. E. 1988. Theory of particle size distributions for chopped forages. *Transactions of the ASAE* 30:1246–53.

Pitt, R. E., and M. B. McGehee. 1988. *The rewetting of partially dried grass swaths by rain.* Departmental report no. 1. Penicuik, Midlothian, Scotland: Scottish Centre of Agricultural Engineering.

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Ryan, T. A., J. Myers, D. Holowka, B. Baird, and W. W. Webb. 1988. Molecular crowding on the cell surface. *Science* 239:61–64.

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Clark, P. A., and A. W. Westerberg. 1988. The bilevel program in chemical process design. Paper read at Spring Meeting, American Institute of Chemical Engineers, 6 March 1988, in New Orleans, LA.

Gubbins, K. E. 1988. The role of computer simulation in studying phase equilibria. Paper read at Collaborative Computational Project no. 5: Meeting on Industrial Applications of Molecular Simulation, 6–8 January 1988, in London, England.

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Jackson, G., W. Chapman, and K. E. Gubbins. 1988. Phase equilibria of associating fluids. Paper read at 67th Annual Convention, Gas Processors Association, 14–16 March 1988, in Dallas, TX.

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Peters, P. E., R. S. Schiffino, and P. Harriott. 1988. Heat transfer in packed-tube reactors. *Industrial and Engineering Chemistry Research* 27:226–33.

Ray, N. G., and M. L. Shuler. 1988. Development of a single cell model for mammalian cells. In *Bio-process engineering colloquium*, ed. R. C. Dean, Jr., pp. 536–44. Singapore: World Scientific.

and R. M. Nerem, pp. 71–74. New York: American Society of Mechanical Engineers.

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Wiegandt, H. F., A. Madani, and P. Harriott. 1988. Ice crystallization developments for the direct-contact process. *Desalination* 67:107–26.

Woods, G. B., A. Z. Panagiotopoulos, and J. S. Rowlinson. 1988. Adsorption of fluids in model zeolite cavities. *Molecular Physics* 63(1):49–63.

■ CIVIL AND ENVIRONMENTAL ENGINEERING

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Agrawal, R., D. Teneketzis, and V. Anantharam. 1988. *Asymptotically efficient adaptive allocation schemes for controlled IID processes: Finite parameter space. Pts. I and II*. Communications and Signal Processing Laboratory reports no. 235 and 254. Ann Arbor, MI: University of Michigan.

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Opposite: Lighting the lake on Independence Day is a local custom at Cayuga Lake near Cornell. At dusk flares are lit on boats and all along the shore. The scene here is at Stewart Park in Ithaca.



