View of the south end of the campus across a campus pond.

ChE *department*

UNIVERSITY OF MASSACHUSETTS

Chemical engineering at the University of Massachusetts is a vigorous program with a distinctive vision. Traditional strengths are built on within reaction engineering and separations. At the same time, we address contemporary opportunities in areas of polymeric and electronic materials. Meanwhile, we are blending new approaches to macroscale design and molecular-scale chemistry with the power of transport phenomena, creating a new perspective on chemical engineering

The University is situated in a picturesque section of New England along the Connecticut River valley. Ninety miles to the east is Boston and the coast, the Berkshires lie to the west, and New York City is about a four-hour drive to the south. Although Amherst is a small town with a population of about 25,000 residents, it has been home to a surprisingly large number of prominent citizens, including poets Emily Dickinson and Robert Frost, lexicographer Noah Webster, and sculptor Daniel Chester French.

In this scenically and intellectually rich environment, our department has grown in a relatively brief time. Between 1951 and 1966, it evolved from a small undergraduate department to a modest-sized program offering undergraduate and graduate degrees to the MS level. The first PhD degree was awarded in 1968. Since then, the program has matured into an established teaching and research department granting about thirty BS, five MS, and thirteen PhD degrees each year.

The chemical engineering department was begun within the fledgling School of Engineering in 1951 by Ernie Lindsey, formerly of Yale. It was a small program during its first ten years, with five faculty, twenty seniors each year, and no graduate program.

In 1962, John Eldridge accepted the task of forging a graduate program in chemical engineering during a time of incredible growth and change in Amherst. In the ten years between 1960 and 1970, UMass grew from 8,000 to over 20,000 students. It was a vital time when everyone was eagerly building programs, and John's persistence, optimism, and charm worked wonders for the department. In eight years he hired eleven new faculty, saw a miniscule graduate program grow to fifty-five students, and found new research funds and space.

In 1976, after fourteen years of building a program, Eldridge let the reins fall to Leigh Short. These were difficult economic times for New England, however, and Leigh left the university in 1978, leaving Jim Douglas to serve as interim head for a year while the search for a new head got under way. Jim used the opportunity to begin planning activities that brought new focus and new directions to

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the program. As a result he was appointed head of the department and remained until 1982 when Bob Laurence took over. The ten years during which Douglas and Laurence had responsibility was another period of dramatic growth. It was a period when research activity grew significantly and new faculty were taken on board. When Bob decided to step down, Mike Doherty became head.

Twenty-three years have passed since the first PhD was awarded. Since then, 132 PhDs have completed their work in chemical engineering and an additional 37 PhDs from the Polymer Science and Engineering Department have been advised and supported by chemical engineering faculty.

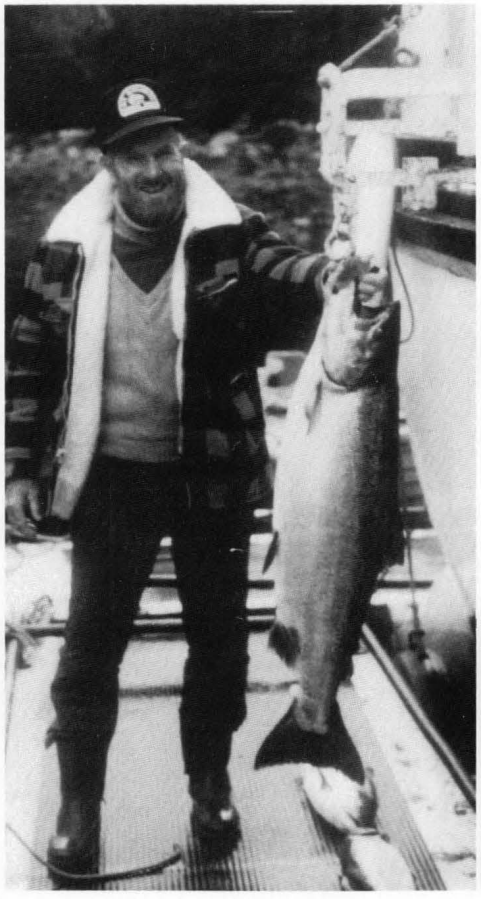
In 1966 the chemical engineering and chemistry departments played a key role in the creation of a new program—Polymer Science and Engineering (PSE), a program of international prominence. The two departments have close ties, and over the years there have been many chemical engineering students advised by PSE faculty and vice versa.

PHILOSOPHY OF THE DEPARTMENT

The large turnover of faculty during the years from 1977 to 1986 gave us an opportunity to restructure the department, and after numerous discussions we decided to try some different approaches. Although the general departmental model at that time was for each faculty member to be an expert in a single area, we decided to build groups of three to five faculty, each with a different viewpoint, who would work in the same general area. We hoped that the "creative tensions" encountered in each group would lead to novel approaches. In addition, our goal was to get members of the specific areas to engage in dialogue with members of other groups and in this way to define significant research problems at the interfaces between traditional problem areas.

All of us love to learn and love to teach. Hence, we made a commitment to integrate our research programs as much as possible with both our undergraduate and graduate curricula. That is, we would transfer research results to our undergraduate and graduate courses as quickly as possible. We would periodically revise the undergraduate and graduate courses, and when we had developed enough new material we would write new textbooks based on our ideas. The first two books to be written out of this period were Jim Douglas' book, *Conceptual Design of Chemical Processes*, and Julio Ottino's book, *The Kinematics of Mixing: Stretching, Chaos and Transport.* Readers familiar with these books will probably agree that they represent rather significant departures from traditional thinking. Other books are also currently under way.

We also decided to try to achieve a better balance between fundamental science and process engineering. Thus, we hoped to develop different approaches for solving widely recognized practical problems of importance, such as process design, polymer engineering, solids processing, and mixing problems. This effort would be balanced by programs focused on fundamentals such as kinetics and catalysis, thermodynamics, fluid mechanics, *etc.* Most of the design research at that time was focused on the computational



Department heads in action: John Eldridge and fishy friend (left); Jim Douglas in full highland dress (above); and Bob Laurence (below) who is also the varsity rugby coach.

As a statement of commitment to our teaching and scholarship, the faculty agreed to rotate the teaching of our undergraduate courses every three or four years.

problems associated with flowsheeting and optimization. We decided to focus instead on process synthesis and conceptual design. We expected that a new approach to conceptual design would provide better material to teach undergraduates than the design courses that were taught to most of us.

Traditionally we had strong interaction with the Polymer Science and Engineering Department, and several faculty had joint appointments in both departments. We had a strong support base in polymer chemistry and one of the large and rapidly growing areas of material science. We could use this support base to develop a stronger research program in polymer processing operations and the design of flowsheets for complete polymer plants. In conjunction with the Polymer Science and Engineering Department we have developed several joint courses at both the undergraduate and graduate levels. In addition, we have incorporated polymer components in many of the traditional chemical engineering courses, including the undergraduate laboratory which has an extruder, a blow molder, and a methyl methacrylate polymerization experiment.

When we considered the scales of chemical technology, which cover the spectrum of scales from molecular to continuum to unit operations and finally complete plants, it was clear that we had several faculty with strong backgrounds in transport phenomena and unit operations. Therefore, we decided to bring in faculty who would strengthen our chemistry expertise in the areas of catalysis, design of unconventional reactors (ceramic membranes and magnetically stabilized fluid beds), statistical thermodynamics and adsorption, molecular kinetics and applications in emerging areas of technology, and quantum mechanics and applications to materials.

For many years there have been growing complaints that chemical engineering students do not know enough chemistry. Even a cursory examination of the curriculum at that time indicated that the focus was limited to physics and mathematics and that we had essentially purged chemistry from the engineering courses. One of our goals became to look for ways to include some chemistry, as well as a molecular perspective, in many of the undergraduate courses.

Our research results have led to a complete restructuring of the graduate and undergraduate design courses, as well as our separations course (much of this course is now focused on the separation of multicomponent nonideal mixtures). Currently, Jim Douglas is moving much of the synthesis material down into the introductory course. The new course is a major revision of the old industrial chemistry courses. Instead of memorizing flowsheets, students are given a set of reactions that produces a product and are taught how to invent a flowsheet. The invention of a flowsheet provides a context for studying phase diagrams, vapor-liquid equilibria, and other introductory material normally covered in the first chemical engineering course. Then the students develop the material and energy balances for the flowsheets, as well as the raw material costs and the utilities costs. This approach has the advantage of solving open-ended problems from the outset, and it provides a context for the remainder of the curriculum. At the same time, Phil Westmoreland is creating a senior/graduate-level course on the "Chemistry of Chemical Engineering." His focus is teaching the use of modern techniques to estimate and correlate thermochemistry, kinetics, and physical properties based on molecular structures. Curt Conner has also developed a senior/graduate-level elective course, "Advanced Engineering Solids," which integrates structure, properties, and manufacturing processes for a variety of "high-technology" solids.

As a statement of commitment to our teaching and scholarship, the faculty agreed to rotate the teaching of our undergraduate courses every three or four years. This policy has been in existence for about a decade, and most of our faculty are now capable of teaching many of the courses in the curriculum, including the undergraduate lab! One of the great advantages of this policy is that it substantially widens the expertise of the faculty.

There are five major thrusts in the department: process design and control, polymer engineering, kinetics and catalysis, transport processes, and applied theoretical chemistry. Each thrust has several faculty and graduate student participants and many faculty have their feet in more than one camp. A brief discussion of these thrusts follows.

Design and Control

There is a major research effort in the areas of process design and control involving Mike Doherty, Jim Douglas, Mike Malone, Ka Ng, and Erik Ydstie. The programs have close ties with industry, including an Industry/University Center which was established in 1985. Regular meetings on campus provide students with an opportunity to meet industrial sponsors and give updates on recent research

results. The Center receives no direct government support, but contributions from the sponsors supplement and complement substantial government and industrial research funding of the individual faculty in the general area of chemical process design and control.

Research results also provide important feedback for the evolution of the graduate and undergraduate curriculum. New materials are often taught first in short courses to practicing engineers; more than thirty short courses in conceptual design and six in distillation systems have been taught in the last ten years. Some of the material is then incorporated in course offerings at the university, throughout the undergraduate program, and in the graduate process design and control courses.

Polymer Engineering

The department has a long tradition of research and teaching in polymer engineering that began in the 1960s with Bob Lenz, Bob Laurence, and Stan Middleman, who between them covered much territory from polymer synthesis, kinetics, and characterization to polymer diffusion, reactor engineering, rheology, and polymer processing. The effort was expanded significantly around 1980 with the addition of Julio Ottino, Mike Malone, and Henning Winter. They all came with backgrounds in fluid mechanics (albeit with very different perspectives), and each developed his own unique niche in the polymer business.

Today we find a wide spectrum of interests in this field. Molecular-scale phenomena such as molecular orientation are studied in order to understand the behavior of liquid-crystal polymers and the properties of blends. A variety of experiments has been designed to probe these systems, including fluorescence and light-scattering techniques. Polymer processing is studied to find the influence of the elasticity of the material on the processability and on the molecular orientation in the flow.

Several projects explore the relationship between transport and morphology in polymer blends, mixed polymer systems, and copolymers. Research in this area involves theory, experiments, and novel computer image analysis.

In recent years a novel effort has been initiated to explore the design and optimization of batch and continuous processes for polymer production. A systems approach shows interactions of process components, economic tradeoffs, and optimal flowsheet design. For teaching purposes, this approach has the attraction of identifying design problems where non-trivial transport effects (velocity gradients, diffusion, *etc.*) play dominant roles in the design calculations. For such processes, our old and friendly assumptions like "well mixed" and "plug flow" rarely give satisfactory results, especially in the finishing operations of polymer processing.

Reaction Systems

Another large research effort is directed toward a wide variety of problems involving chemical reactions. Seven faculty direct approximately twenty graduate students in problems spanning heterogeneous metal and metal oxide catalysis, chemical vapor deposition, reaction and separation by reactive distillation or with catalytic inorganic membranes, and multiphase catalysis.

There is a strong element of chemistry in these projects. Phil Westmoreland and his students measure detailed compositions of steam-cracking products and of free radicals and stable species within flames; then they interpret the reaction chemistry with reactor models involving 200 to 1000 elementary reactions. The observation of phenomena such as steady-state multiplicity and oscillations and measurement of more conventional kinetic trends provide the basis for Mike Harold's procedure of kinetic model development and discrimination for a wide class of noble-metal-catalyzed oxidation reactions. Together with Curt Conner, Harold uses Fourier-transform infrared spectroscopy to monitor surface species and catalyst structure during reaction on metal oxide catalysts. Val Haensel studies molecular rearrangement, fragmentation, and scavenging in metal-catalyzed hydrocarbon reactions.

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Interactions between reaction and transport processes are of paramount importance for chemical reactor analysis and design. The common approach used in several of these projects is the focus at the local level. Conner and Laurence observe and model reaction and transport during olefin polymerization in a fragmenting catalyst pellet. Harold and Ng are concerned with multiphase transport-reaction interactions and their impact on performance of multiphase reactors. Progress towards the development of a realistic trickle-bed reactor model exploits Ng's focus on local flow features and Harold's focus on single-pore and pellet multiphase reaction and diffusion phenomena.

In addition to the polymerization and multiphase reactor projects, several new types of reactors are being developed for use in emerging technologies. Doherty studies simultaneous reaction and distillation of components in highly nonideal liquid mixtures. Design and synthesis schemes are being developed to achieve reaction and separation in a single unit. Coupled reaction and separation is also a motivation for Harold's development of catalytic ceramic membranes. A new type of catalytic membrane reactor has been developed which segregates the gas and liquid streams and thus reduces mass transport limitations for the wide class of volatile-reactant-limited multiphase reactions. Westmoreland's understanding of plasma chemistry provides the basis for improved plasma-enhanced CVD reactors.

Transport Processes

Several research projects focus on problems of fluid dynamics, rheology, porous material characterization and mass transport. An underlying theme in these projects is

Continued on page 157.

DEPARTMENT: U Mass

Continued from page 125.

microstructure and morphology in both flow systems and porous materials. Winter studies structural development in well-defined flows of different classes of polymeric systems, such as phase-separating block copolymers and liquid crystalline polymers. Self-similar molecular structure is exhibited by cross-linking polymers at the sol-gel transition. Malone studies the effect of flows on the morphology and phase behavior of binary polymer blends. Computer image analysis is used for characterization and control of the process. Ng has shown by both simulation and CAT-scan analysis that the liquid distribution during flow through a bed of packing is a manifestation of local flow features involving several particles. Because of his research activities in the transport and reaction areas, his work in process design has a strong focus on the underlying physics.

The morphology of amorphous and crystalline oxides is a focus of several projects. Dynamic adsorption-desorption of liquid nitrogen or krypton, mercury porosimetry and electron microscopy are three tools used to characterize morphology. Conner and Laurence study the effects of pore size and porosity of silica-supported catalysts on the fragmentation and yield during the initial stages of olefin polymerization. In a similar vein, Conner has been collaborating with scientists at Brookhaven National Laboratories to pioneer the development of X-ray synchrotron computed microtomography and its application to characterize the morphology of olefin polymerization catalysts. Minimization of the pore size of supported microporous inorganic films and of their penetration into the macropores of the ceramic support are crucial goals in Harold's synthesis of ceramic membranes.

One of the most successful programs developed in the transport area is Julio Ottino's program in fluid mechanics and mixing. His research has raised the level of understanding in mixing to the point where, for the first time, it is possible to view many seemingly unrelated problems within the context of a single theory.

Applied Theoretical Chemistry

In many new areas it is becoming critically important to incorporate details of molecular-scale chemical physics into engineering models. The department has research efforts that address this need. Much of the work represents an emerging effort that will likely be a future core strength for the department and the profession.

Michael Cook is developing and using density functional methods for the study of point defects in materials. An important application is to electronic device materials such as silicon and III-V semiconductor alloys and compounds. He is also investigating the nature of potential-energy surfaces for free radical reactions as a means of providing a more firm foundation for kinetic models. Peter Monson's research is concerned with applications of fundamental statistical thermodynamics, especially in the context of phase equilibria and the properties of interfacial systems. He has developed new approaches to studying the influence of molecular shape and polarity upon fluid phase equilibria. This work is now being extended to prediction of solid-liquid equilibria. His group is also exploring the molecular basis of adsorption separations in terms of the nature of the intermolecular forces and the adsorbent microstructure. Fundamental theoretical studies of the molecular structure of fluid films on solid surfaces are also being carried out. Phil Westmoreland's research stands at the interface between detailed molecular theory and process reaction engineering. He co-developed Bimolecular Quantum-RRK analysis to predict rate constants and product channels for gas-phase association reactions in combustion. Westmoreland is exploiting this method in pyrolysis, combustion, and plasma chemistry while probing more complex potential-energy surfaces and intermolecular energy transfer.

THE FUTURE

As this article is being written, the department is in the middle of several new initiatives that promise to significantly improve our programs. We are a major participant in the University/Digital Equipment Corporation PILGRIM project, which is a $6 million project to design, install, and test a network of several hundred high-performance workstations in the College of Engineering and in the Computer and Information Science Department. So far the department has installed twenty workstations for research purposes and has access to a workstation classroom for teaching. Several courses will use workstation-based software to complement lecture material, including the design courses, the separations course, and the statistical thermodynamics course.

The undergraduate program continues to evolve, and it embraces a major commitment to upgrading the lab. We began converting many of the laboratory experiments to computer data acquisition and control some time ago with a generous donation of process control computers from Analog Devices (see *Chem. Eng. Ed.*, **24**, 106, 1990). Over the next two years we will design and build new experiments on crystallization, process control, and polymerization kinetics. Many of the older PCs used for on-line data acquisition and control will be retired and replaced by more modern machines. We continue to explore ways of inserting more chemistry and solid-state material into the curriculum, and two of the faculty intend to write books on these topics as that activity matures.

The department has grown into a vigorous, vibrant place in only forty years of existence, presently with eight of the thirteen faculty also at forty or under. By the time we reach our half-century in the year 2001, we hope to make our perspective a vital part of chemical engineering. ❐