

SPECIAL PROCESS CONTROL ISSUE

ADVANCED PROCESS CONTROL EXPERIMENTS

Deshpande, Laukhuf, Patke

PROCESS CONTROL EXPERIMENT: THE TOILET TANK

Thomas J. Ward

INTEGRATION OF REAL-TIME COMPUTING INTO TEACHING

M. Morari, W. H. Ray

A FULL-YEAR COURSE SEQUENCE IN REAL-TIME COMPUTING

D. A. Mellichamp

SURVEY OF PROCESS CONTROL EDUCATION IN THE U.S. AND CANADA

Dale E. Seborg

ALSO

CHE AT GEORGIA TECH

THE RATE OF REACTION: A DEFINITION OR THE RESULT OF A CONSERVATION EQUATION?

Alberto Cassano

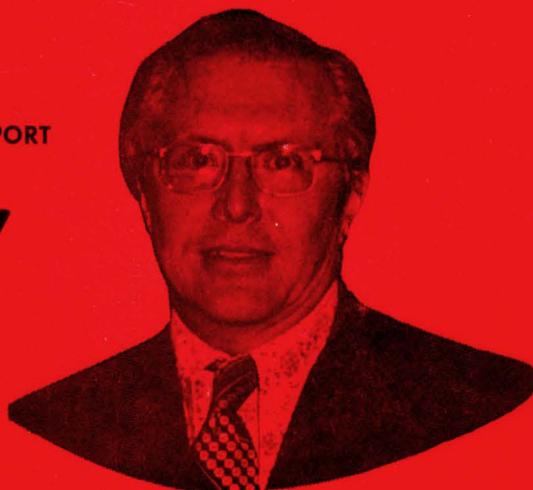
IN THE "HEAT" OF THE NIGHT

R. J. Gordon

TWO DIMENSIONAL HEAT TRANSPORT

A. Basio

ART HUMPHREY OF PENNSYLVANIA



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Atlanta's skyline is shown behind the Tower of Tech's Administration Building.

ChE department

CHE AT GEORGIA TECH

A Period of Transition

GARY W. POEHLEIN

*Georgia Institute of Technology
Atlanta, GA 30332*

LAST WINTER WHILE browsing in the campus bookstore I found a stack of T-shirts imprinted with the message "MIT—THE GEORGIA TECH OF THE NORTH." I returned two days later to purchase one for my friend Professor James Wei (MIT Department Head and a Georgia Tech graduate) only to find they had all been sold. In their place were T-shirts which bore the message "NORTH AVENUE TRADE SCHOOL" (North Avenue is the southern boundary of the campus). I decided not to buy one of the replacement shirts. It probably would not have been received with

much enthusiasm by Professor Wei.

Both T-shirt messages contained elements of truth and fiction. Georgia Tech, like MIT, has a long-standing reputation for quality engineering and scientific education. Unlike MIT, Georgia Tech is a State Institution, being part of the University System of Georgia. Four colleges (Engineering, Architecture, Sciences and Liberal Studies, and Industrial Management) offer undergraduate and graduate degrees in areas that could be described, in a broad sense, by the term "Technology." Degrees are not offered in areas such as music, English, art, history, etc. This last fact is responsible for the "trade school" label on the second stack of T-shirts. Of course, those of us associated with Tech know that this label does not reflect

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reality. Our liberal studies departments are staffed with high-quality faculty who offer a very wide range of courses to help our students obtain a broad education.

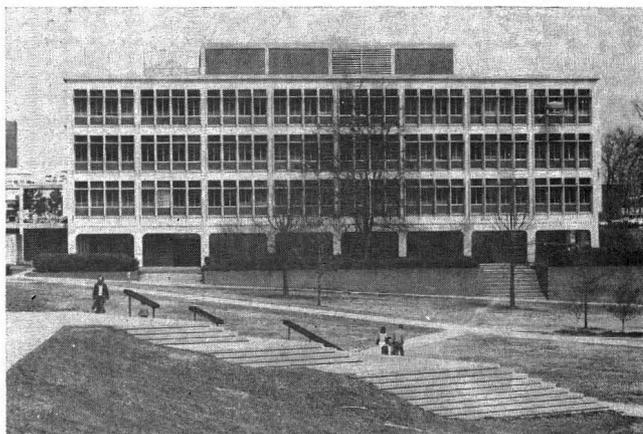
The Georgia Tech campus is located on 280 acres about 1½ miles from the center of Atlanta. With a population of about 1,750,000, Atlanta is the center of commerce in the rapidly growing Southeast. It is a dynamic, beautiful and exciting city with a very diverse population. Atlanta is an educational center with 29 degree-granting colleges, junior colleges, and universities; a center for the arts with a symphony orchestra, a ballet company, numerous art exhibits, local and imported theater groups, a wide variety of special festivals; and a center for sports, with teams in all major professional leagues.

The School of Chemical Engineering at Georgia Tech is comprised of a Chemical Engineering Division, a Metallurgy Division, and the Fracture and Fatigue Research Laboratory, an interdisciplinary research organization. Faculty and other scientific staff are listed in Table 1. The Chemical Engineering Division offers B.S., M.S. and Ph.D. degrees. The Metallurgy Division does not offer a designated undergraduate degree but does have a very active graduate program leading to M.S. and Ph.D. degrees.

The School of Chemical Engineering has been changing rapidly during the past few years. Dr. Waldemar Ziegler retired at the end of the 1977-78 academic year, several faculty have left for other positions and, unfortunately, Dr. Leon Bridger and Dr. Homer Grubb died suddenly during the past academic year. Thus much of our efforts during the past fifteen months have been involved with recruiting new faculty. These efforts have been very successful, with ten outstanding individuals accepting offers to join our faculty. Dr. Edvin Underwood was a Senior Research Scientist here prior to accepting a faculty position. Eight of the remaining nine have moved to Atlanta since April, 1979. Dr. Aryn Teja, presently at Loughborough University, will join us in September, 1980. The faculty members and their areas of interest are identified in Table 1.

GEORGIA TECH—A BRIEF HISTORY*

The Georgia Institute of Technology began as the Georgia School of Technology in 1888. The School of Chemical Engineering evolved from the chemistry curriculum. An Engineering[®] Chemistry Program was published in the 1900-1901 catalog. In addition to chemistry and chemical engineering topics, areas such as metallurgy, dyeing, me-



Chemical Engineering is housed in the Bunger-Henry Building.

chanics, electricity, minerals, and industrial processes were included in this early program. The 1929 catalog listed a B.S. in Engineering Chemistry, and the 1930 catalog indicated that a B.S. in ChE could be obtained under the Department of Chemistry.

McLaren White, whose father, Alfred H. White, was an MIT graduate and Head of ChE at Michigan, was the first chemical engineer to come to Tech. This happened during the 1920s, and Professor White was part of the chemistry department faculty. Changes toward chemical engineering were too slow to suit Professor White, so he left. The first-prize for the AIChE contest problem is named in honor of McLaren White.

The first Chief of the Chemical Engineering Division within the Department of Chemistry was

*The information presented here is condensed from a paper, "An Early History of Chemical Engineering at Georgia Tech," by Marcella M. Lusby, Unpublished (November, 1977).

The School of Chemical Engineering currently enrolls about 950 undergraduates. This figure includes freshmen who declare a major at Tech and co-op students who are on work assignments. Cooperative education dates back to 1915 at Tech. Today nearly 30% of undergraduate ChE's are in the Coop Program.

Dr. Harold Bunger, who started at Tech around 1929. The name of the academic unit was changed to the Department of Chemistry and Chemical Engineering in the 1930s. This department was

headed by Dr. Boggs, with Dr. Bunger continuing as Chief of the ChE Division. Both Boggs and Bunger died in 1941 and the two divisions were split, forming separate departments. Professor

TABLE 1

Staff: ChE Division

Pradeep K. Agrawal; Assistant Professor; Ph.D. 1979, University of Delaware; Heterogeneous Catalysis
Charles J. Aloisio; Lecturer; Ph.D. 1970, Purdue University; Polymer Engineering and Science
William R. Ernst; Associate Professor; Ph.D. 1974, University of Delaware; Heterogeneous Catalysis; Assistant Director for Ch.E. Undergraduate Programs
Larry J. Forney; Associate Professor, Ch.E./C.E.; Ph.D. 1974, Harvard University; Aerosol and Particle Technology
George A. Fowles; Adjunct Professor; Retired Vice President, Marketing, B.F. Goodrich Co.; Plastics Pioneer
Charles W. Gorton; Professor; Ph.D. 1953, Purdue University; Transport Phenomena, Fluidization
Edwin M. Hartley; Associate Professor; Ph.D. 1973, Georgia Tech; Pulp and Paper Engineering
H. Clay Lewis; Professor; Sc.D. 1943, Carnegie Institute of Technology; Chemical Process Design
Albert A. Liabastre; Research Scientist; Ph.D. 1974, Georgia Tech; Surface Science
Michael J. Matteson; Professor; D. Eng. 1967, Technical University Clausthal (Germany); Aerosols, Particle Technology, Air Pollution Control; Assistant Director for Ch.E. Graduate Programs
John D. Muzzy; Professor; Ph.D. 1970, Rensselaer Polytechnic Institute; Polymer Engineering, Energy Conservation, Economics
Allan S. Myerson; Assistant Professor; Ph.D. 1977, University of Virginia; Thermodynamics, Crystallization, Biochemical Reactions
Clyde Orr, Jr.; Regents' Professor; Ph.D. 1953, Georgia Tech; Instrumentation and Particle Technology
Gary W. Poehlein; Professor; Ph.D. 1966, Purdue University; Emulsion Polymerization, Latex Technology; Director of the School
Ronnie S. Roberts; Assistant Professor; Ph.D. 1976, University of Tennessee; Biochemical Engineering, Mass Transfer, Reactor Design
Robert J. Samuels; Professor; Ph.D. 1960, University of Akron; Polymer Science and Engineering
A. H. Peter Skelland; Professor; Ph.D. 1952, University of Birmingham (England); Non-Newtonian Fluids, Mixing and Fluid Dynamics, Heat and Mass Transfer
Jude T. Sommerfeld; Professor; Ph.D. 1963, University of Michigan; Computer Applications
D. William Tedder; Assistant Professor; Ph.D. 1975, University of Wisconsin; Process Synthesis, Optimization and Waste Management
Amy S. Teja; Associate Professor, Ph.D. 1972, Imperial College (London), Phase Equilibria, Thermodynamics
Henderson C. Ward; Professor; Ph.D. 1953, Georgia

Tech; Transport Phenomena, Process Design, Co-Siting

Mark G. White; Assistant Professor; Ph.D. 1978, Rice University; Heterogeneous Catalysis
Jack Winnick; Professor; Ph.D. 1963, University of Oklahoma; Thermodynamics, Electrochemical Engineering, Air Pollution Control
Ajit P. Yoganathan; Assistant Professor; Ph.D. 1978, California Institute of Technology; Biomedical Engineering, Polymer Rheology
Alex Zhavoronkov; Visiting Scientist; Ph.D. 1975, Moscow Technical Institute; Aerosols

Staff: Metallurgy Division

Helen E. Grenga; Professor; Ph.D. 1967, University of Virginia; Catalysis, Corrosion, Extractive Metallurgy
Robert F. Hochman; Professor; Ph.D. 1959, University of Notre Dame; Phys-Chem. of Metals, Corrosion, Biomaterials; Associate Director for Metallurgy
John E. Husted; Professor; Ph.D. 1970, Florida State University; Mineral Engineering
Miroslav Marek; Associate Professor; Ph.D. 1970, Georgia Tech; Corrosion, Dental Materials
Pieter Muije; Associate Professor; Ph.D. 1971, Washington State University; Metallurgy, Mineral Processing
Stephen Spooner; Professor; Sc.D. 1965, Massachusetts Institute of Technology; Physical Metallurgy, Metal Physics

Staff: Fracture and Fatigue Research Lab.

Saghana B. Chakraborty; Research Scientist; Ph.D. 1974, Georgia Tech; Mechanical Metallurgy, Electron Microscopy
Albrecht Gysler; Visiting Research Scientist; Ph.D. 1965, University of Stuttgart (Germany); Microstructure-Properties Relationships
Ludmilla Konopasek; Research Engineer; M.S. 1975, Manchester University (England); Fracture and Fatigue of Materials
Fu-Shiong Lin; Research Scientist; Ph.D. 1978, Georgia Tech; Corrosion, Fatigue, and Ti and Al Alloys
T. H. B. Sanders; Research Scientist; Ph.D. 1974, Georgia Tech; Aluminum Alloy Development, Microstructure and Fatigue
Bhaskar Sarkar; Postdoctoral Fellow; Ph.D. 1979, Georgia Tech; Stress Corrosion Cracking and Fatigue
Edgar A. Starke, Jr. Professor; Ph.D. 1964, University of Florida; Fracture and Fatigue; Director of the Fracture and Fatigue Research Laboratory
Edvin E. Underwood; Professor; Sc.D. 1954, Massachusetts Institute of Technology; Physical Metallurgy, High Temperature Deformation and Stereology

Jesse Mason became Director of the Chemical Engineering Department; and Dr. Paul Weber, a chemical engineering faculty member, was named Assistant Director of the Engineering Experiment Station.

A reorganization took place in 1948 with Professor Mason becoming Dean of the College of Engineering and Dr. Weber the new Director of the School of Chemical Engineering. Dr. Weber held this position until 1955 when he became Dean of the Faculty (equivalent to the present position of Vice President for Academic Affairs), and Dr. Robert Raudebaugh from the Metallurgy Division was appointed Acting Director of the School of Chemical Engineering for the year. Dr. W. M. Newton assumed the acting director position and



The "Ramblin Wreck" Parade, a real demonstration of student creativity—weird things that move!

served for about three years until Dr. Homer Grubb was named Acting Director. The name change from "Department" to "School" was made to identify ChE as a degree-granting component of the Institute; the School of Chemical Engineering offers degrees, the Departments of English, History, etc., do not. In addition, schools are generally more autonomous than departments.

One of the reasons for the dramatic, almost three-fold, increase in ChE undergraduate enrollment at Tech during the past five years has been the number of women and minorities entering the School.

Dr. Grubb was later named Director of the School, a position he held until 1965 when Dr. Leon Bridger became the Director. During this period the Metallurgy Division developed a significant graduate program which operated partially independently of the Chemical Engineering Division. Dr. Robert Hochman came to Tech in 1959 and is currently the Associate Director responsible for the Metallurgy Division.

Dr. Bridger returned to a full-time faculty position in ChE during the summer of 1978; and Dr. Gary Poehlein was appointed Director after moving to Tech from Lehigh University. The Fracture and Fatigue Research Laboratory, headed by Dr. Edgar Starke, Jr., was also established in 1978.

UNDERGRADUATE PROFILE

APPROXIMATELY 8500 undergraduates were enrolled at Georgia Tech to start the Fall Quarter, 1979. About one-half of these students are residents of the State of Georgia. The others include representatives from every other state in the U.S. and many foreign countries. A selective admissions policy continues to produce a high-quality undergraduate student body. The 1978 freshman class had an average SAT score of 1161 comprised of an average verbal score of 533 and an average math score of 628. Georgia Tech ranks seventh in the nation in attracting National Merit Scholars and second to Harvard-Radcliffe in the number of National Achievement Scholars enrolled.

The School of Chemical Engineering currently enrolls about 950 undergraduates. This figure includes freshmen who declare a major at Tech and coop students who are on work assignments. Cooperative education dates back to 1915 at Tech. Chemical Engineering became involved later, and Professor Emeritus Waldemar Ziegler was the first ChE Coop graduate receiving his degree in 1932. Today nearly 30 percent of undergraduate ChEs are in the Coop Program.

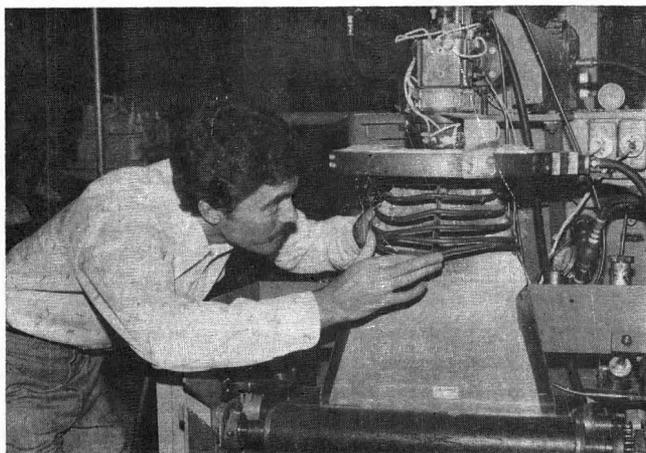
One of the reasons for the dramatic, almost three-fold, increase in undergraduate ChE enroll-

The undergraduate program in chemical engineering is quite rigorous with a good balance between theory and practice. Required courses include two quarters of transport phenomena, three quarters of unit operations, three quarters of design, as well as courses in stoichiometry, reaction kinetics, process control, etc. Engineering drawing and physical education remain as required courses.

ment at Tech during the past five years has been the number of women and minorities entering the School. These numbers have increased from near zero in 1974 to about 30 percent women and 8 percent minorities in 1979. A second significant reason for our increased enrollment has been more participation in dual-degree programs with other universities.

The undergraduate program in chemical engineering is quite rigorous with a good balance between theory and practice. Required courses include two quarters of transport phenomena, three quarters of unit operations, three quarters of design, as well as courses in stoichiometry, reaction kinetics, process control, etc. Engineering drawing and physical education remain as required courses.

Students come to Georgia Tech expecting to work hard, and most are willing to make the



Jack Childs checks the assembly of Polymer Fabric Extruder.

necessary commitment to succeed. The vast majority leave Tech with a very high opinion of the Institute and a fond feeling for Atlanta. This loyalty is clearly manifested in the fact that Georgia Tech almost always ranks first among the nation's public institutions in terms of support by alumni and alumnae.

GRADUATE PROGRAM

THE GRADUATE PROGRAM is in a period of rapid growth. The addition of ten new faculty members should provide us with the manpower necessary to improve an undergraduate program that is already quite good and, at the same time, to build a graduate program of equivalent stature. Enrollment of full-time graduate students in the Fall of 1978 was about 55. These students were about equally divided between the ChE and Metallurgy Divisions. Present graduate enrollment includes 61 chemical engineering students and 40 metallurgy students.

New graduate students entering the School of Chemical Engineering in September, 1979, consisted of 33 U.S. citizens and 9 from other countries. Thirty-six of these students are in the ChE Division and 6 in the Metallurgy Division. A continuation of this sort of success in recruiting graduate students will insure the proper development of our graduate program. We would like to achieve a steady-state graduate enrollment of about 100 ChEs and 40 Mets. with an 80/20 balance between citizens and non-citizens.

THE FUTURE

THE NUMBER OF NEW faces at our first faculty meeting in September prompted a request for round-the-table introductions. Of course, faculty on our staff last year had an opportunity to meet the new faculty during the campus visits. In fact, a number of significant working relationships have already been developed between new faculty and those continuing to serve on our staff. During a year when more than fifty interviews occurred, however, names and faces can become confused.

This introduction exercise clearly illustrates that the School of Chemical Engineering at Georgia Tech is indeed in "A Period of Rapid Transition." Prediction of the future in such an environment is surely an uncertain endeavor. Our faculty and students are very optimistic. We look forward to an exciting period in the life of an outstanding institution. □

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Art Humphrey

and Biochemical Engineering at the University of Pennsylvania

ALAN L. MYERS

University of Pennsylvania
Philadelphia, PA 19104

THE PAST ACADEMIC year served as a milestone for the field of biochemical engineering and the University of Pennsylvania. Not only did the year mark the 25th anniversary of the biochemical engineering program at the University, it was also the 25th anniversary of the leadership of the program by its founder at Penn, Arthur E. Humphrey.

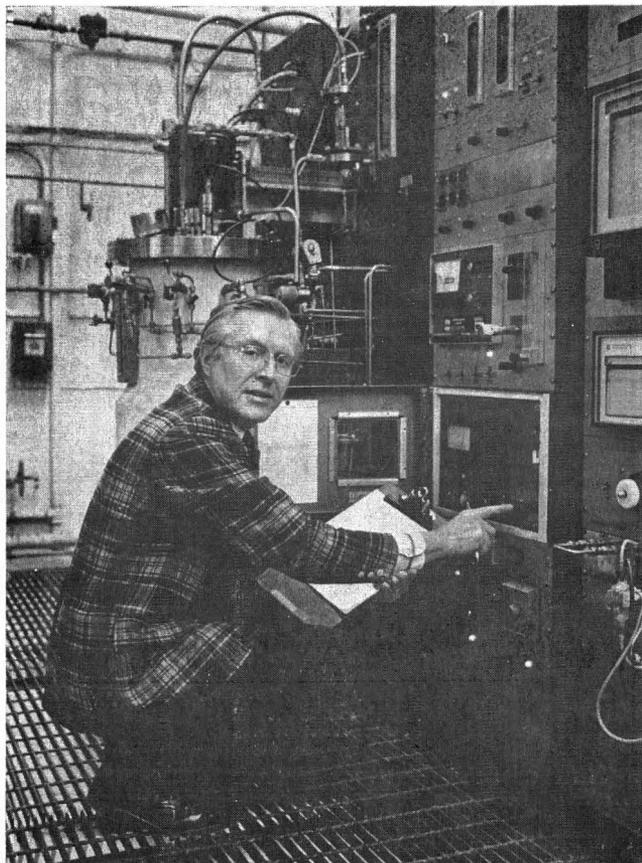
There are older and larger biochemical engineering programs in existence, but none can rival the record of Penn's program in terms of its dynamic growth and production of graduates who have gone on to become leaders in the field. To mark these achievements, the University hosted a special 25th anniversary symposium to which all the graduates of the program were invited. The "alumni" who attended participated in panel discussions on the future of biochemical engineering in the areas of food production (discussion led by Stanley Barnett), energy production (led by Charles Cooney), production of chemicals (led by Daniel Wang), and preservation of the environment (led by Larry Erickson), with a roundtable discussion on the future of biochemical engineering education led by Richard Mateles.

ORIGINS OF THE PROGRAM

IN 1953 ART ARRIVED at Penn, fresh from his PhD studies in chemical engineering at Columbia University. While working on his doctorate, he

As a scholar of biochemical engineering in general, and fermentation technology in particular, he has published over 150 technical papers and co-authored two textbooks which are regarded as the bible in their fields.

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Art inspects the fermenter laboratory.

developed an interest in fermentation technology and subsequently took additional training in food technology at M.I.T. At Columbia, Art, along with Ernest Henley (now at the University of Houston), was the first doctoral student of Professor Elmer Gaden who was later to be cited as the "father of biochemical engineering" (in a cover story in the May 31, 1971 issue of *Chemical Engineering News*). It was through Elmer Gaden's influence that Art's interest in fermentation systems matured. Elmer had written his own thesis on "Mass Transfer in Fermentation Systems under the supervision of Arthur W. ("Pop") Hixson at Columbia, working in conjunction with a biochemical engineering team (Karow, Bartholomew, and Sfat) at the Merck Company. (It is of some interest to note that reporting of the 1945 McGraw-Hill Process Development Award, presented to Merck for its "Biochemical Engineering Development of the Penicillin Process," is apparently the first mention of "biochemical engineering" in the chemical engineering literature.)

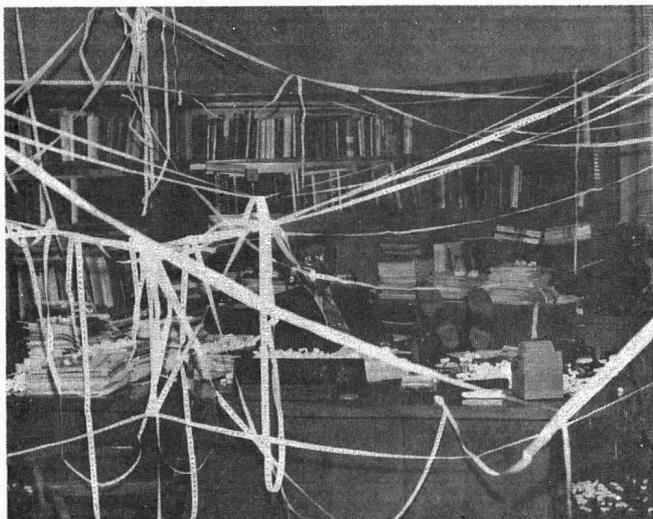
Art joined Penn's chemical engineering faculty

as an assistant professor and in the fall term of 1953 offered a new course in biochemical engineering. Since 1953 the biochemical engineering program has grown steadily, and in 1972 it was officially recognized when the Department of Chemical Engineering formally changed its name to the Department of Chemical and Biochemical Engineering.

THE MAN BEHIND THE PROGRAM

AS OVERWORKED AS THE WORD "dynamic" is in today's usage, it is nevertheless the appropriate term to characterize the founder of Penn's biochemical engineering program—Art Humphrey. Whether at work in his laboratory, or leading a faculty debate, or scaling a mountain in Guatemala, Art is possessed of energy that leaves others much younger in a race to catch up, and he inspires his contemporaries to set equally challenging goals for themselves.

In his 25 years at Pennsylvania, Art has established professional credentials that are indisputable. As a scholar of biochemical engineering in general, and fermentation technology in particular, he has published over 150 technical papers and co-authored two textbooks which are regarded as the bible in their fields, *Biochemical Engineering* (Academic Press, 2nd ed., 1976) and *Fermentation & Enzyme Technology* (John Wiley, 1979). He holds three U.S. patents and has actively consulted for more than 20 chemical companies during his career. He has served on and chaired numerous AIChE committees including the FBP



Art seems to approve of his students' efforts at office "re-decoration."

Over the years he has formed a special bond with his students, based on mutual respect, willingness to devote intense effort to a project, and in no small measure on the ability to dish out and take a practical joke.

Division, and between 1975 and 1978 was a director of the organization. He has also been a past chairman of the MC&T Division of ACS and of the Working Group on the Production of Substances by Microbial Means of the US/USSR Committee on Cooperation in Science and Technology. In addition, he served from 1971-1973 as a member of the NSF Advisory Committee for Engineering. In 1973 he was elected to the National Academy of Engineering.

Such a summary of professional activities, however, doesn't begin to capture Art Humphrey, the man, who by virtue of his enthusiasm and exuberant love for life succeeds in making people want to work together toward a common goal. Art always has a full complement of five doctoral students to work with him as advisees or, more appropriate to the man, associates. Over the years he has formed a special bond with his students based on mutual respect, willingness to devote intense effort to a project, and in no small measure on the ability to dish out and take a practical joke. For pranks he's played on his students, Art was rewarded on one occasion with the careful "re-decoration" of his office (as shown in the accompanying photograph) and on another with the clamping of a ball and chain on his leg only minutes before he was to make a presentation to the University Trustees. In Houdini-like fashion he arrived before the Trustees on time sans ball and chain.

Art is an avid outdoorsman who cheerfully ignores middle age (and some say common sense) as he pursues his interests. Having hiked the trails of much of this country, he frequently substitutes an opportunity to climb a mountain in a foreign country in place of the honorarium he would receive for lecturing there. Such negotiations have enabled him to climb Mount Fuji in Japan, Popocatepetl in Mexico, and Augua in Guatemala, among others. Last year when taking up skiing for the first time, Art found himself by mistake in an advanced intermediate class and, not having the good sense to get out of the class, "mostly fell

Collectively, this group conducts a research program amounting to \$500,000 a year, and this past year they published the program's 150th paper on biochemical problems.

down the hill" and received a National Standard Medal for downhill racing as a result. Each year Art leads a departmental canoe trip down the Delaware River, an activity he organized 16 years ago (when Bob Bird was a member of that group). The annual event now involves between 60 and 70 people, including faculty members, students, alumni, and participants from other schools. This year an eight-mile run was included as part of the trip, and he typically outpaced the younger generation—without having trained for the run.

The honesty and openness with which Art approaches every aspect of his life generates an unswerving loyalty among his associates. Never afraid to admit when he's wrong or simply doesn't know an answer, he leads people to trust that they'll "hear it straight," good or bad, in dealing with him. Add to these qualities Art's rare talent of being a good listener, and the result is an individual who is extremely effective in accomplishing the work he sets out to do. His spirit has inspired and guided the development of Penn's biochemical engineering program over 25 years, and it has set the tone with which the biochemical engineering faculty now approaches the next 25 years.

BIOCHEMICAL ENGINEERING AT PENN TODAY

ART HUMPHREY STILL heads the biochemical engineering program within the University's Department of Chemical and Biochemical Engineering, despite his heavy administrative load as Dean of the School of Engineering and Applied Science. (From 1962 until he was named Dean in 1972, he served as Chairman of the Department of Chemical Engineering.) Art and three others of the Department's 12-member faculty have the focus of their teaching and research activities in the area of biochemical engineering. At least three others conduct a significant portion of their research within the field. Collectively, this group conducts a research program amounting to \$500,000 a year, and this past year they published the program's 150th paper on biochemical engineering problems (out of a total of more than 350 scientific articles published by these individuals). Six national AIChE, ACS, and ASEE awards have

been won by members of the group, and two members have been elected to the National Academy of Engineering.

Those members of the faculty of the Department of Chemical and Biochemical Engineering who participate in the biochemical engineering program are:

David J. Graves:	enzyme kinetics
Arthur E. Humphrey:	fermentation technology
Douglas A. Lauffenburger:	cell population dynamics
Mitchell D. Litt:	bioreology
Daniel D. Perlmutter:	enzyme reactor dynamics
E. Kendall Pye:	enzyme behavior and purification
John A. Quinn:	bound membrane systems

The facilities which are used in both the research and teaching functions of the biochemical engineering program consist of four primary laboratories: the fermenter laboratory, a wet chemistry laboratory for enzyme analysis, a membrane laboratory, and a reactor laboratory.

The fermenter laboratory (pictured in an accompanying photograph) centers about a 70-liter highly instrumented fermenter that is coupled to a PDP 11/34 computer with a 96K core capacity and three discs (two fixed), a Calcomp plotter and a video screen for data acquisition and control. The facility is supported by a Nuclide Mass Spectrometer and other appropriate analysis equipment. In addition, the laboratory has a number of smaller fermenter units, including a 20-1, 14-1, two 1-1, and five 500-ml systems—most having temperature, pH, foam, and dissolved oxygen control.

ACADEMIC PROGRAMS

UNDER THE LEADERSHIP of Art Humphrey, the biochemical engineering faculty has always insisted that the academic program remain a part of the basic program in chemical engineering, allowing the "biochemical" aspects of the program to emerge from an emphasis on biological processes. Because of the emerging significance of bioconversion processes in the production of energy, food, and chemical feedstocks and as a means for controlling the environment, students are eager to investigate these problems. The faculty believes the students' eventual careers are better served by

having them pursue these interests from a solid foundation in chemical engineering, rather than by focussing exclusively on a subspecialty.

Thus, the undergraduate *biochemical engineering* student takes the standard chemical engineering curriculum, but biochemistry is substituted for one of the courses in organic chemistry, as is a biology course for the course in nuclear physics. In addition, the student will take two or three courses in microbiology, biological processes, utilization of wastes, biochemical engineering, or food engineering as his senior technical electives; and his senior research project will focus on a biological process.

Out of a senior chemical engineering class of 45 students, about 7 of them will be taking courses with a focus in biochemical engineering. Most of these students will either continue their biochemical engineering studies at the graduate level or will enter medical school.

At the graduate level the student planning a focus in biochemical engineering is also expected to take the core courses in chemical engineering—in applied mathematics, transport processes, reactor design, and thermodynamics. The student is then expected to take courses in advanced biochemistry, molecular biology, and genetics, in addition to the four basic graduate courses in biochemical engineering.

The basic graduate level biochemical engineering courses include:

Biochemical Engineering:	fermenter kinetics, design and operation
Biological Processes:	physics and chemistry of biological processes
Enzyme Technology:	behavior and utilization of enzymes
Utilization of Wastes:	waste utilization and treatment

These courses are taught by the faculty on a rotating basis, i.e., once every other year. They are frequently team-taught with the help of visiting professors and members of the University's Department of Biochemistry and Biophysics.

Students in the graduate program can develop and shape their programs to serve their own particular career emphases by selecting additional courses in areas ranging from nutrition to microbiology. They are free to select these courses from throughout the University's graduate and professional programs, including its Medical School and School of Veterinary Medicine.

At any given time, about 15 students in the chemical and biochemical engineering graduate program (which numbers approximately 50 full-time students) will be focussing their studies in the direction of biochemical engineering. Upon receiving their doctoral degrees, these individuals generally seek employment in the food production, pharmaceutical, waste treatment, and chemical process industries, or in academia.

When questioned, most of the alumni of Penn's biochemical engineering program say they consider themselves chemical engineers who have an interest in biological processes, for such is the slant of their curriculum. This may in part explain why Penn graduates have never encountered problems on seeking employment. Indeed, a recent graduate of the program looking for a position in the biochemical field received more than ten offers from firms, with several offers in excess of \$31,000 a year.

FUTURE OF BIOCHEMICAL ENGINEERING: ART HUMPHREY'S VIEW

THE FACULTY OF THE biochemical engineering program at Pennsylvania looks forward to continued growth of the program. The field is now



Over 60 faculty members and students now participate in Art's annual canoe trip down the Delaware River.

coming into its own and the opportunities are unlimited. Perhaps the enthusiasm of those active in Penn's biochemical engineering program comes across best in the words of the man responsible for its flourishing here—Art Humphrey.

“Never has the future for biochemical engineering looked so bright. This is due largely to the energy crisis and the attendant emphasis on the use of renewable resources, meaning materials of biological origin. It seems fairly evident that many of these materials will be processed by bio-

logical means, with the use of enzymes, in order to achieve low temperature, energy saving processes. The environmental crisis and the increasingly strict limits placed on the use of nitrates, phosphates, and other surface water contaminants mean that more efficient and more complicated waste treatment systems will have to be evolved. Also, wastes will be viewed in the future as valuable resources which can be treated to yield useful materials.

"Perhaps the most significant development affecting the future of biochemical engineering is the explosion of knowledge concerning genetic engineering techniques. Not only do we now possess the ability to cultivate both animal and plant tissue cells in large-scale reactor systems, but we can transfer their genetic information for making various biologically active molecules such as insulin into more easily cultivated bacterial cells by gene splicing techniques. Soon the scientist will be able to create cells with virtually any desired metabolic activity. When this comes to pass, the biochemical engineer will become active in efficiently simulating and optimizing many of nature's special reactions in stainless steel fermenters. In many ways biomass can be regarded as the crude oil of the future. Just as crude oil now serves as the feedstock of the petrochemical industry, from 'barrels of biomass' will come a number of the chemical feedstocks of the future. It would not surprise me to see biomass refineries emerging within the next decade.

"I for one will welcome the change. I believe the chemical engineering textbooks of the future will reflect this change and will include examples of biomass problems along with those from the petroleum industry. Chemical engineering is a truly broad-based discipline, and I believe it is already demonstrating its concern not just with physical and chemical changes, but with biological changes as well." □

ChE book reviews

CONTACT CATALYSIS, VOLS. 1 and 2

Edited by Z. G. Szabo, Elsevier Scientific, 1976

Reviewed by John B. Butt, Northwestern U.

This monumental two volume set is an essay of the Catalysis Club of the Hungarian Academy of Sciences with individual chapters contributed

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by thirteen different authors. In many ways the work is reminiscent of the series "Catalysis" edited by Prof. P. H. Emmett in the 1950's, and it promises to be as useful. True to the title, the entire field of contact catalysis is treated, starting with the fundamentals of solid state science, chemisorption and kinetics in the first volume, with applications concerning preparation, characterization, and catalytic reaction engineering in the second volume. The topics included are treated in quite some detail and in many instances represent current state of the art in both catalysis research and applications.

With so many different aspects of the field treated in such detail, it is difficult in a review of reasonable length to do other than cite certain parts that are of particular use to the reviewer. In this respect, there are particularly fine treatments of adsorption on solid surfaces and physical characterization methods which eclipse much existing literature. For example, the characterization methods discussed include x-ray diffraction, electron-optical methods, magnetic properties, electrical properties, adsorption, infrared and EPR spectroscopy.

Another very useful chapter deals with the preparation of catalysts. This is particularly timely now, since we have attained sufficient abilities in characterization that the long-time
Continued on page 44.

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THE RATE OF REACTION: A DEFINITION OR THE RESULT OF A CONSERVATION EQUATION?*

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A quick survey of the classical literature on chemical kinetics and reactor analysis reveals different criteria concerning the definition of the rate of reaction. Relying on historical rather than rational bases, the following "definition" has been used:

$$r_i = \frac{dC_i}{dt} \quad (1)$$

Eq. (1) was probably derived from the first physicochemical studies on rates of reaction developed in constant volume batch systems.

This "definition" has been used by Glasstone [1], Benson [2], Daniels [3], Laidler [4], Frost and Pearson [5], and Johnston [6], among others.

On the other hand, chemical engineers mainly engaged in design problems, distrusted the validity of the "definition," taking into account its inapplicability to reacting systems of variable volume. The alternative "definition" was based on the number of moles instead of concentration. The difference lies in defining beforehand an extensive rate of reaction which can then be turned into an intensive property dividing by the reaction volume.

$$r'_i = \frac{dN_i}{dt} \quad (2)$$

$$r_i = \frac{1}{V_r} \frac{dN_i}{dt} \quad (3)$$

The greater generality of expression (3) as compared to equation (1) is easily demonstratable, in either conceptual or mathematical terms.

*This paper is the result of mutually beneficial discussions on the subject with my former classmates Charles Allen and Sieghard Wanke. Any merit to this paper is theirs. Any errors in it are mine.

The "definitions" belonging to the kind provided by equation (3) can be found in books such as those written by Hougen and Watson [7], Smith [8], Levenspiel [9], Walas [10], Boudart [11], Pannetier and Souchay [12]; and with explicitly stated limitations by Kramers and Westerterp [13], by Aris [14] and Denbigh [15] as well. Many other cases could be quoted.

A good example for analysis is the "Continuous Flow Stirred Tank Reactor" (CFSTR). In this particular case the product is continuously removed at the system outlet and it becomes evident that at the steady state dN_i/dt is zero (the product being species i) but the rate of reaction is utterly different from zero. Here, as Denbigh remarks, expression (3) is not valid, either. This author tries to narrow the applicability of the "definition" (3) to processes where the only change in reactant i is due to a chemical reaction. This would exclude any other form of physical phenomena causing changes in reactant concentration. The restriction seems valid for the CFSTR and for all forms of diffusive flows. Nevertheless, it does not seem so clear for the "Piston or Plug Flow Reactor" (PFR), in which if, on the limit, dt is taken as the reacting mass average residence-time in the elementary reaction volume of length dz , equation (3) may be properly applied with some substitutions.*

This work shows the futility of arguing about the accurate "definition" of the reaction rate and

*It should be noticed that now v_z may be a function of z if changes in the number of moles take place.

**This work shows the
 futility of arguing about the
 "definition" of the reaction rate and
 the convenience of dealing with the subject
 from a different viewpoint.**

the convenience of dealing with the subject from a different viewpoint, that is, drawing the necessary equations from a more fundamental principle, as the general mass conservation equation for multicomponent systems would be.

REDEFINITION OF THE PROBLEM FOR HOMOGENEOUS REACTORS

SO FAR, IT IS obvious that the existing "definitions" seem to depend either on the author's personal likings or on the reactor to which the equations will be applied.

It seems logical to assume that any reaction rate should be a function not of the system in which it has been determined but only of temperature, pressure and concentration of the species participating in the reaction, just to mention the most commonly encountered variables affecting the rate. The reaction rate could be naturally influenced by the type of reactor—continuous or batchwise—but only up to the extent that it may affect concentrations, temperatures or pressures.

It is necessary to reconcile an expression derived from the ontological concept of the rate of reaction with a mathematical equation expressing exactly the same, involving the variables susceptible of experimental measurement.

Ontologically (and considered as an intensive property), "The rate of reaction is the change in the number of moles which takes place in unit time and unit reaction volume, due to a transformation of reactants into products."

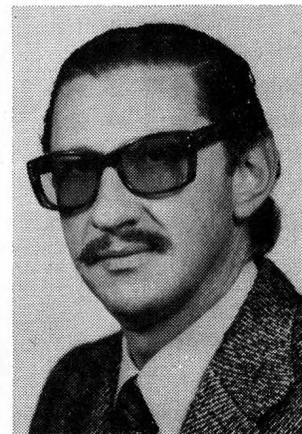
The mathematical expression of the above definition will be set equal to the kinetic equation of the chemical system under consideration; i.e. if such a definition is adequately represented by a mathematical proposition which will be called r , it is evident that:

$$r = \phi (C_1, C_2, \dots \text{etc. } T, P, \text{etc.}) \quad (4)$$

where ϕ depends on the complexity of the reacting system (order, molecularity, activation energy, etc.). It is the concern of this work to determine the adequate formulation for the left-hand side of equation (4).

The problem at issue has been partially, even though quite accurately, discussed by Petersen [16] and also singularly viewed by Amdur and Hammes [17], particularly for batch reactors. The reader may resort to the quoted references.

In many cases, experimental measurements will register not only the change in concentration but also the resultant of the chemical process of re-



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action and the physical processes of diffusion, convection and volume changes. From this point of view, all the "definitions" previously analyzed are erroneous and inaccurate, and only applicable, at best, to systems universally used but no less particular (e.g. the constant volume stirred batch reactor, etc.).

Petersen clearly points out that the left-hand side of equation (4) is a direct resultant of the experimental system employed in kinetic determinations, and that, therefore, there is no single definition which could be widely used, still less if the reacting system were non-isothermal. This statement can be effectively generalized and is the subject of the next paragraph.

SOLVING METHODS

IF THE RATE OF reaction is to be defined, the problem is usually reduced to finding the rate of change of the reacting species with respect to some independent variable (time in a batch reactor and position in many continuous reactors). The rate of change of the reacting species is generally measured considering the change in the number of moles of the said reactant or the rate of change in its concentration.

An apparent way of solving the problem would be to consider the reaction within a species material volume, instead of the generally used fixed

control volume. But it is difficult to think of a species material volume since they are not preserved [18]. If the "particles" of the material volume are elements, the difficulty is overcome at the expense of a greater complexity. Therefore, this strategy is quite troublesome.

A more adequate way of looking into the problem for an isothermal system is to consider the various mechanisms which can bring about concentration changes of a reactant within a system and, then, determine which part of these total changes is due to the chemical reaction, subtracting all contributions other than the reaction.

This means to state in detail a mass conservation balance for a multicomponent system. Generally speaking, there are two categories of phenomena through which a species concentration may vary in a fixed volume in space: (1) The species may appear or disappear by chemical reaction and (2) There is a net flow of this species through the area of this volume element. This flow mechanism, be it diffusion, forced convection or any other means of mass transport, needs not be detailed here. The description of this flow will exclusively depend on the system at stake.

The general conservation equation may be thus written [19]:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{N}_i = r_i \quad (5)$$

or in a more general way: if a_i is the stoichiometric coefficient of species i :

$$r_i = r a_i \quad (6)$$

Then:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{N}_i = a_i r \quad (7)$$

This well known conservation equation is the only general formulation for homogeneous isothermal rates of reaction that is independent of the reaction system being employed. It clearly shows that the rate of reaction is the "source" or "sink" term in the mass inventory; therefore all the remaining non-zero terms resulting from taking r out of expression (7) must be substituted into the right-hand side of equation (4).

So far, it is obvious that the existing "definitions" seem to depend either on the author's personal likings or on the reactor to which the equations will be applied.

APPLICATION TO COMMON REACTING SYSTEMS

EQUATION (7) WILL now be used to obtain the adequate expressions for some classical reacting systems. The following homogeneous isothermal systems will be considered:

- 1) Isothermal constant volume batch reactor
- 2) Isothermal variable volume batch reactor
- 3) Steady state, isothermal continuous plug flow reactor
- 4) Steady state, isothermal continuous flow stirred tank reactor

In every case, the adequate assumptions will be made in order to allow an analytical description of the flux \mathbf{N}_i so as to simplify the rate expression.

ISOTHERMAL CONSTANT VOLUME BATCH REACTOR

IF WE ASSUME THAT properties are constant in the whole volume of the reactor (especially concentration and temperature), then the divergence of the flux becomes zero since \mathbf{N}_i will be independent of position. Therefore, if $\nabla \cdot \mathbf{N}_i = 0$, equation (7) is reduced to:

$$r = \frac{1}{a_i} \frac{dC_i}{dt} \quad (8)$$

where the derivative is now total insofar as concentration will be a function of time only.

ISOTHERMAL VARIABLE VOLUME BATCH REACTOR

IF WE ASSUME THAT the expansion of volume is slow so that, as in the previous case, such properties as concentration, pressure and temperature are independent of their position within the reactor, no diffusional effects whatsoever will result, and the flow will be caused only by expansion.

In this case, by definition:

$$\mathbf{N}_i = C_i \mathbf{v}_i^*$$

but, as all species expand at the same rate:

$$\mathbf{v}_i = \mathbf{v}_j = \mathbf{v} = \mathbf{v}^*$$

the velocity of all species coincides with the global velocity of the system.

With the previous relationships, equation (7) results:

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (C_i \mathbf{v}) = a_i r$$

But, since it has been assumed that concentration is independent of position $\nabla C_i = 0$. Then:

$$\frac{\partial C_i}{\partial t} + C_i (\nabla \cdot \mathbf{v}) = a_i r \quad (9)$$

Continued on page 48.

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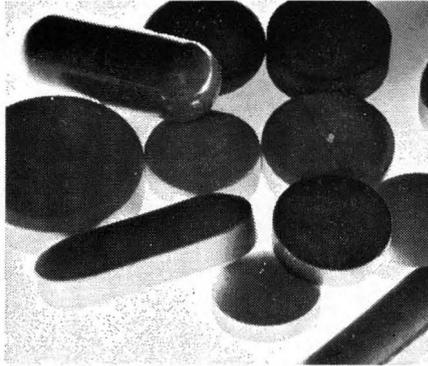
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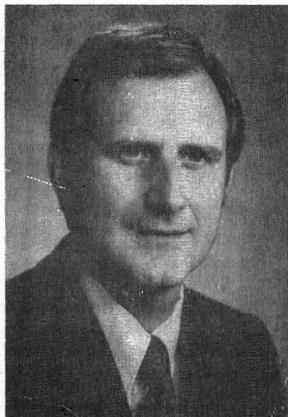
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A FULL-YEAR COURSE SEQUENCE IN REAL-TIME COMPUTING

D. A. MELLICHAMP
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THE CHEMICAL ENGINEERING program at U.C. Santa Barbara began in the mid-1960's with an intended emphasis on the process control part of the curriculum. The use of digital computers for data acquisition and control, what often is referred to as real-time computing, at that time was an object of relatively intense interest in industry. However, except for one or two schools with the financial resources to acquire an industrial-scale computer (e.g. IBM 1800), there was little opportunity for universities to give students hands-on experience with data acquisition and control computers.

The appearance of the minicomputer in the late 1960's made it possible for virtually any department to acquire or build a real-time computing facility which could be used in teaching and in research. The more recent introduction of the micro-



Duncan A. Mellichamp is Professor of ChE at the University of California, Santa Barbara, where he was initially responsible for development of the process dynamics and control program. An early interest in computers led subsequently to activities with the CACHE Real-Time Task Force (Chairman 1974-76), to the CACHE Corp. Board of Trustees (President 1977-78), to the Editorship of the CACHE Monograph series in Real-Time Computing, and to a long succession of aggravations associated with building and maintaining a real-time laboratory facility. He would like to forswear all future activities involving computers, but cannot.

processor (and microcomputer) has merely accelerated the trend of chemical engineering departments to install real-time facilities and to introduce elements of real-time computing into the curriculum.

In the past few years, the early fascination with hardware and software among real-time

TABLE 1

Topics Covered in Undergraduate Control Courses
(2 hr. lecture and 3 hr. lab per week for two quarters)

- Derivation of process dynamic models
- Transfer function models
- Open- and closed-loop systems
- Frequency-response methods for controller design
- Process applications
- Overview of advanced control methods

users has decreased to some extent, and the more important educational questions of what, where, and how to teach this new subject area are receiving more attention. Since real-time computing was and is tied to the subject of process control, it seems reasonable to explore some ideas concerning the teaching of real-time computing within that context. The chemical engineering department at U.C. Santa Barbara has developed what must be one of the most extensive teaching and research programs in real-time computing in this country (at least among chemical engineering departments); and I would like to describe it, to discuss some of the background behind its development, and to note how it is changing. To begin with, however, it might be useful to discuss the process dynamics and control program which now coordinates with the more recently developed real-time computing program.

THE PROCESS CONTROL PROGRAM

IN DESCRIBING THE PROCESS control program at UCSB, it probably is fair to say that it is a traditional one. Two one-quarter undergraduate courses are required of all seniors and the usual

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CHEMICAL ENGINEERING EDUCATION

If there is any non-traditional aspect of the undergraduate program it would be the emphasis on "practical" experiments. The associated laboratory contains several experimental units for the study of liquid level and stirred tank heating dynamics and control, pneumatic and electronic control systems, and simulation facilities

range of topics is covered. Depending on who is teaching the course, there may be more or less emphasis on process dynamics and on "advanced control" topics; nevertheless the core areas listed in Table 1 are fairly rigorously and extensively covered.

If there is any non-traditional aspect of the undergraduate program it would be the emphasis on "practical" experiments. The associated laboratory contains several experimental units for the study of liquid level and stirred tank heating dynamics and control, pneumatic and electronic control systems, and simulation facilities for other, more complex processes. The experimental units are all bench scale and designed to have time constants on the order of one to two minutes. Since individual dynamics and control experiments can be carried out in 15 to 30 minutes, a whole range of experiments (summarized in Table 2) can be run during the two quarters. Students write up their results in brief (i.e. memo) form; although theory underlies all experimentation, emphasis is on the use of theory to evaluate practical consequences such as "Will the surge tank system overflow?", "Is the catalyst mixing system adequately stirred?", etc. By the end of two quarters students will have designed and tested

TABLE 2
Undergraduate Process Dynamics
and Control Laboratory Experiments

FIRST COURSE

Liquid level system:

1. Step response
2. Pulse response

Stirred tank heating system:

3. Step response
4. Transportation lags

Stirred tank reactor (simulated):

5. Model parameter fitting
6. Steady-state optimization

SECOND COURSE

Controllers:

1. Dynamic characteristics of three-mode controllers
2. Control of 1st- and 2nd-order systems

Stirred tank heating system:

3. Frequency response
4. Closed-loop control system design

Liquid level system:

5. Closed-loop control system design

TABLE 3

Topics Covered in Graduate Control Courses
(3 hr. lecture each week, per course)

FIRST COURSE

- Derivation of models for multivariable systems
- Formulation of state space models
- Solution of multivariable system models (matrix methods)
- Modal analysis
- Design of controllers using modal theory
- Simulation and computer-aided controller design
- Discrete systems analysis

SECOND COURSE

- Sampled data systems
- Sampled data controller design (or digital control algorithms)
- Decoupling control systems
- Controllability, observability, etc.
- Optimal control: quadratic and time-optimal
- Analysis of stochastic systems
- Observers, filters and state estimators

control systems for each of the laboratory bench scale processes using: (1) theory only, (2) empirically-determined process models, and (3) on-line (loop-tuning) methods.

At the graduate level we presently offer two courses in process dynamics and control. In recent years the first course has covered both time and frequency-domain methods with emphasis on state space techniques used in conjunction with the computer for analysis and design. The course deals substantially with multivariable systems and, at least in part, parallels the undergraduate courses at an advanced level (Table 3).

The second graduate course covers advanced control topics exclusively (also summarized in Table 3). Although the graduate offerings are traditional in nature (there are no laboratory experiments at the graduate level), the rigorous yet extensive coverage of advanced materials reflects the same approach as at the undergraduate level.

THE REAL-TIME COMPUTING PROGRAM

ONE OF THE MAIN PROBLEMS in bringing new material into the curriculum is that (usually) an equivalent amount of old material will have to come out. In developing the real-time teaching program we began with four basic tenets:

1. Real-time computing instruction will be offered to both

- undergraduate and graduate students on an elective basis.
2. Real-time computing course work will supplement, not replace, existing process control course work.
 3. Real-time computing will be taught from a fundamental point of view. Students will be expected to understand basic hardware and software structures and how they are used.
 4. Lectures in real-time computing will be paralleled by a "hands-on" laboratory with appropriately-designed experiments.

We have followed these principles substantially down to the present day; hence a few words of discussion might be appropriate: Tenet 1 arose out of an early realization that many chemical engineers, not just a few, will be involved with on-line

. . . . the ratio of "outsiders" to chemical engineers was about 30/70 in this second year; through the last academic year it has been more like 70/30, with the number of chemical engineering students relatively constant at 12-15.

process computing as part of their professional careers. Tenet 2 was based on a natural reluctance to tamper with established control courses, in particular to remove some significant amount of material so as to introduce lectures on real-time computing. Tenet 3 might well be open to argument but has its parallel in the controls area: twenty years ago many people felt that control theory was not chemical engineering; probably no one today would argue in favor of a control course based totally on an empirical approach. Our experience with chemical engineering students is that they do not, in general, like to spend time on computer fundamentals; nevertheless those who do find that practical applications are much easier to understand and are able to transfer their knowledge to other real-time systems much easier. Tenet 4 will need no explanation.

Historically, we began our real-time course offerings with a one-quarter graduate seminar in Spring 1972 and followed it immediately in the Fall of that year with a senior-level elective course open to graduate students. Development of the course and the associated laboratory were underwritten by the National Science Foundation through two grants totalling almost \$100,000 over a three and one-half year period. In the Fall of 1973 the course was elected by about twice as many chemical engineering students (ten). Several electrical engineering students also took

the course; in fact the ratio of "outsiders" to chemical engineers was about 30/70 in this second year; through the last academic year it has been more like 70/30 with the number of chemical engineering students relatively constant at 12-15. In the past three years we have had to restrict enrollment because of the limitation in our real-time laboratory facilities.

One of the interesting developments that came out of the real-time computing course resulted from the large number of student requests for sequel courses in the same area, but covering more advanced topics. Many of the requests came from electrical engineering or computer science students who claimed that there were no equivalent applications courses within their own departments. Additional requests came from some of our own students, both undergraduate and graduate, who planned to work in the process computer control applications areas. The real-time field naturally divides into three applications areas: (1) single process/single computer, e.g. the topics covered in our first course, (2) multiple processes/single computer (multitasking or multiprogramming applications), (3) multiple processes/multiple computers (multiprocessing or networking). So far as the author can determine, it generally is the case that the real-time instruction offered by most computer science departments is (a) non-existent, (b) concerned only with on-line systems, e.g. airline reservation systems, (c) theoretically- rather than practically-oriented, e.g. concerned with hypothetical job scheduling problems in a multiprocessor environment. Condition (c) holds on our campus; hence in order to accommodate student requests we decided to add two additional courses to our offerings to cover substantially multitask programming and operating systems for real-time applications, and networking and digital computer control systems.

Several points are worth noting here concerning the decision to expand the real-time computing course to a full-year sequence:

- Some of the specialized computer-oriented material we now teach is outside the area of expertise of most chemical engineering faculty even though the applications-oriented material is not. We have avoided potential problems somewhat by using a Teaching Associate, a Ph.D. candidate in computer engineering, to share teaching responsibilities and to supervise the laboratory. In the four years we have offered the full sequence, several students working on joint research projects involving the real-time laboratory facilities have been supported financially in this way and have

contributed significantly to the development of our teaching and research program.

- Attenuation of students enrolled in the sequence historically was relatively high, running 40-50% per quarter. Hence by the third quarter the enrollment might have dropped from approximately 40 to about 10; most students continuing through the entire sequence have been our own graduate students, chemical engineering undergraduates who have accepted jobs involving a process control starting assignment, computer science undergraduates, and undergraduate or graduate electrical engineering students with an interest in computer applications.
- Chemical engineering students who have taken the real-time sequence along with the required courses in dynamics and control have relatively little difficulty finding employment in process-control-related areas. Several process-oriented companies now recruit process control engineers actively at Santa Barbara and, if statements from recruiters can be believed, would have hired about twice as many students for control work last year if they had been available.
- The mixing of chemical engineering students who have relatively little computer background (in general only experience in programming a higher-level language, i.e. FORTRAN) together with computer science students who have little or no experience with physical equipment never was totally satisfactory. The distribution of abilities in any particular prerequisite subject area is invariably bimodal: e.g. ChE students will have relatively little background in binary arithmetic and logic (computer science students will feel they have mastered the subject); the reverse situation is true in the area of physical measurements and measurement errors. This situation led to major problems in the introductory course where so much of the lecture material must cover topics which will appear to be elementary to a computer science major.

This year, for the first time, we have not permitted computer science students to take the introductory course. The entire sequence has been rearranged somewhat to reflect these new developments. These actions represented an attempt to return the first course to what it originally was—an introduction for chemical engineers. At the same time we hoped to retain a reasonable enrollment of “outside” students in the two following courses. This hope did not grow out of any purely altruistic motivations; rather the presence of outside students furnished the department with a claim on the additional teaching staff resources necessary for us to offer such an extensive program. Also, in a rapidly changing field such as real-time computing, the presence of relatively advanced computer science students in our courses has kept the discussions lively and the lectures more nearly “state-of-the-art.” The success of these changes is now apparent as will be noted in the sequel. In any case, this rather lengthy descrip-

TABLE 4

A First Course in Real-Time Computing

(3 hr. lecture and 2 hr. lab per week)

- Introduction to BASIC and to real-time BASIC
- Structure of real-time systems
- Measurements, transducers, and signal handling
- Number systems and computer arithmetic
- Introduction to computer architecture and hardware
- Input/output systems: ADCs and DACs
- ISA FORTRAN
- Device controllers and device drivers

tion of the development of the real-time sequence is intended to motivate the description of the present courses which follows immediately.

Real-Time Computing Courses. There is no “traditional” first course in real-time computing; we have, after much experimentation, settled on coverage of the topics listed in Table 4. From the table it can be seen that we spend considerable time on computer fundamentals; number systems and digital arithmetic, digital logic and hardware, computer architecture, interfacing, assembly language programming, interrupt handling, etc. We also spend time on some topics which have long since been dropped from most process control courses; measurements and measurement errors, transduction, signal transmission, etc. In a first course of this sort the emphasis is on single process/single computer systems and the coverage must, unfortunately, be light. Our purpose is to develop a basic understanding of all the elements in a real-time system, how these interact, and how they comprise the whole.

Our purpose in teaching this course has not been to treat real-time computing as an isolated subject area but to teach it so that the material can be integrated into the control courses, at least into the undergraduate process dynamics and control laboratory. Since the introductory real-time course is taught in Fall quarter and precedes the two-quarter sequence in dynamics and control, students normally are in a position to make immediate application. Those students who have elected to take the real-time course are “permitted” to run all of their dynamics (data logging) and control experiments using one of the real-time computers. Although this normally requires more work of the student—outside reading, programming, debugging programs, etc.—our experience shows that they often take this oppor-

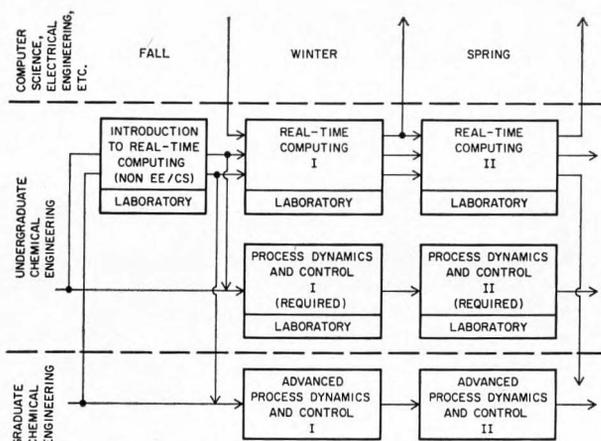


FIGURE 1. Process Dynamics and Control and Real-Time Computing Offerings.

tunity. Figure 1 indicates how the real-time sequence fits together with the undergraduate and graduate process control program, also how the three different groups of students—undergraduate and graduate chemical engineers and “out-of-department” (C.S., E.E., etc.)—can be accommodated.

The remaining two courses in the sequence (labeled “Real-Time Computing I and II” in Figure 1) cover the major areas of multitask and multiprocessor applications, respectively, with an emphasis on applications of computers, either singly or in networks, for control purposes. Tables 5 and 6 furnish a brief description of the course content for each of these courses; there necessarily must be a small degree of repetition to bring entering students up to operating speed.

Real-Time Computing Laboratory. The present real-time laboratory (shown in Figure 2 with one

of the undergraduate process dynamics and control experiments visible in the background) contains three minicomputers, two of which are configured for real-time operations. These facilities, built up over the past ten years, will be substantially replaced in early 1980 by the single-computer system shown schematically in Figure 3. This multiprogrammed system will accommodate up to six real-time user programs in main memory simultaneously and, potentially, can be expanded to handle many more if program swapping using the fast disk can be tolerated. Features of the new system will include a link with the main campus computer, full graphics capabilities, a dial-up facility for one remote user, and one or more terminals in remote study rooms and laboratories.

TABLE 5
Second Course in Real-Time Computing
(2 hr. lecture and 2 hr. lab per week)

- Overview of real-time computing
- Introduction to real-time FORTRAN
- Analog and digital input/output
- Operating systems and schedulers
- Introduction to multitask programming
- Multitask program design
- File handling and bulk storage
- Assembly language device driver routines
- Multitasking applications

As part of the instructional laboratory we have constructed several interesting auxiliary units:

- a set of input and display panels for experiments involving input, output and conversion of analog and digital quantities;
- an air pressure experiment with binary inputs (solenoid-operated valves) and outlays (pressure-operated) relays for instruction in digital I/O and simple on-off control;
- a metal bar heated at one end, with eight temperature



FIGURE 2.
The Real-Time Computing Laboratory (Foreground).

TABLE 6
Third Course in Real-Time Computing
 (2 hr. lecture and 2 hr. lab per week)

- Real-time computers in process control
- Controller and filtering algorithms
- Controller design and applications
- Overview of computer networks
- Network architectures
- Interprocessor communications
- Distributed processing
- Networks in process control

sensing elements located along the unheated section for multipoint data logging studies;

- a fully interfaced model railroad designed to demonstrate the control of multiple, largely-random processes.

A list of experiments which typically would be performed as part of the introductory real-time course is given in Table 7. The model railroad is used as the basis of a sequence of five experiments in the second course. In the third course, several of our present computers as well as the new system will form the basis for the networking portions of the course. The stirred-tank heating systems are used for the process control portions. Students completing the laboratory sequence will, as a final project, put together a two-computer real-time system (one computer for data acquisition and control, the other for process operator communications and report generation) with inter-processor communications carried out over an existing multiprocessor bus.

SUMMARY AND CONCLUSIONS

CHEMICAL ENGINEERS WHO plan to work closely with digital computer control systems need a much more fundamental exposure to real-time systems principles than can be obtained through a brief exposure as part of a senior-level control course. Even a single-quarter course in real-time computing cannot cover important advanced topics in the field such as real-time operating systems, multitasking, multiprogramming, and

TABLE 7
First Course in Real-Time Computing:
Laboratory Experiments

- Calibration of a resistance thermometer for a stirred tank heating system
- Estimation of dynamic measurement error in the stirred tank temperature transducer
- Automated number conversions
- Digital input/output: "super pong"
- Analog input/output: simulation of a staircase ADC
- Data logging of the heated bar temperature profile
- Data logging and control of the pressure tank

... in a rapidly changing field such as real-time computing, the presence of relatively advanced computer science students in our courses has kept the discussions lively and the lectures more nearly "state of the art."

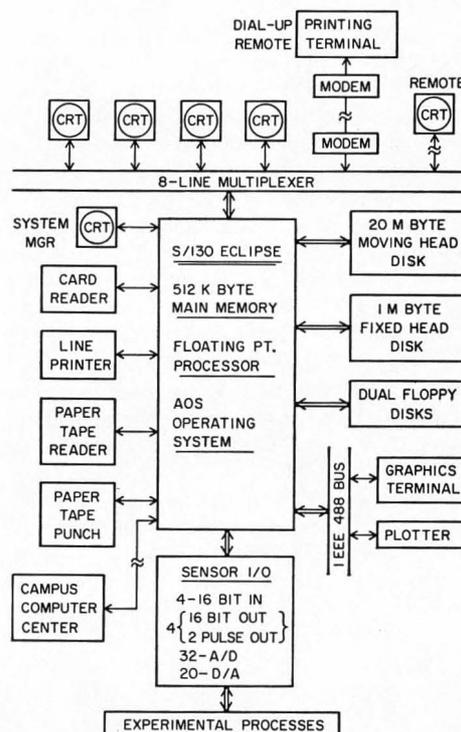


FIGURE 3. The UCSB Real-Time Computing System.

networking. At Santa Barbara we have expanded our offerings to a three-quarter sequence with heavy emphasis on laboratory exercises and experiments. As a service course, the sequence attracts enough outside students to warrant augmented teaching support staff from the college. Also, chemical engineering students appear to benefit from the experience of working with computer specialists; still it is clear that mixing them at too early a stage is not optimum. The move we have made to restrict enrollment to chemical engineers in the introductory class has eliminated most of the problems arising from mismatches in basic skills. This year, considerably more of our own students elected to take the first course than have in the past, and more of them are continuing in the sequence. Additionally, the teaching loads over the entire academic year have been considerably smoothed out by closing the first course to EE and CS students.

TEXT MATERIALS

Before 1977-78 there was available virtually no single source of information which could be used as a text in a course on real-time computing. In 1977 the first volumes of the CACHE Monograph Series in Real-Time Computing, edited by this author, appeared. The monograph series, an attempt to produce a definitive treatment of each major area in the field, will consist of eight volumes initially. All of them will be available in 1979. A listing of the titles in the present series:

- I. An Introduction to Real-Time Computing
- II. Processes, Measurements, and Signal Processing
- III. Introduction to Digital Arithmetic and Hardware
- IV. Real-Time Digital Systems Architecture
- V. Real-Time Systems Software
- VI. Real-Time Applications Software
- VII. Management of Real-Time Computing Facilities
- VIII. Process Analysis, Data Acquisition, and Control Algorithms

In 1978 a good book dealing with industrial applications of real-time computers was published: *Minicomputers in Industrial Control*, T. J. Harrison (Editor), Instrument Society of America, Pittsburgh (1978).

With respect to the laboratory facilities, the author earlier documented the three real-time laboratory experiments developed at Santa Barbara in reports, a few copies of which are still available:

D. A. Mellichamp and F. Kayihan, *The Tank Pressure Experiment*, UCSB Department of Chemical and Nuclear Engineering Report C-74-1, 79 pp, (August 1974).

D. A. Mellichamp and G. P. Engelberg, *The Digital Computer Controlled Model Railroad*, UCSB Department of Chemical and Nuclear Engineering Report C-74-3, 119 pp, (October 1974).

D. A. Mellichamp and T. W. Moore, *The Heated Bar Experiment*, UCSB Department of Chemical and Nuclear Engineering Report C-76-1, 96 pp, (March, 1976). □

ChE book reviews

CHEMICAL REACTOR DESIGN FOR PROCESS PLANTS; VOLUME I, PRINCIPLES AND TECHNIQUES; VOLUME II, CASE STUDIES AND DESIGN DATA

By Howard F. Rase

Wiley-Interscience, New York, 1977

Reviewed by Charles H. Ware, Jr.,

Commercialization Insights, Poughkeepsie, N.Y.

The author has written this book, as the preface states, "for the professional engineer who either daily or periodically must deal with design or operation of chemical reactors. But in addition to serving as a reference in the personal libraries of professionals, it should also be useful as a textbook for advanced design courses, including courses taught in continuing education." It will serve all of these purposes very well.

Volume I (772 pages) is divided into four parts: basic data and principles of design; general aspects of reactor design; single-phase reactors; and design of reactors for multiphase processes. Volume II (242) pages consists of 14 case studies including three oxidation reactions, two polymerizations, and two hydrogenations.

Part 1 is devoted to reaction rate theory and applications; chemical and physical aspects of catalysis and catalysts; idealized models of reaction rates and reactor performance; and experimental methods and equipment for developing design data. Two chapters devoted to catalysis and catalysts provide a good summary of them with attention to both theoretical foundations and practical considerations. Experimental methods and equipment to obtain chemical reaction data free of transport effects are emphasized.

Part 2 is concerned with selection of reactor type and mode of operation based upon yield and safety, as well as general design considerations such as mixing of reactants, flow distribution, residence-time distribution within reactors, and briefly, vessel design.

Part 3, which comprises almost half of the text in Volume I, covers the design of CFSTRs, tubular, batch, semi-batch, fixed-bed catalytic, fluid-bed catalytic, and many special reactors. In addition to the various design equations, there are numerous drawings of actual reactors and considerable attention is given to flow and heat effects, feed systems, pressure drop, scale-up, start-up and shutdown procedures.

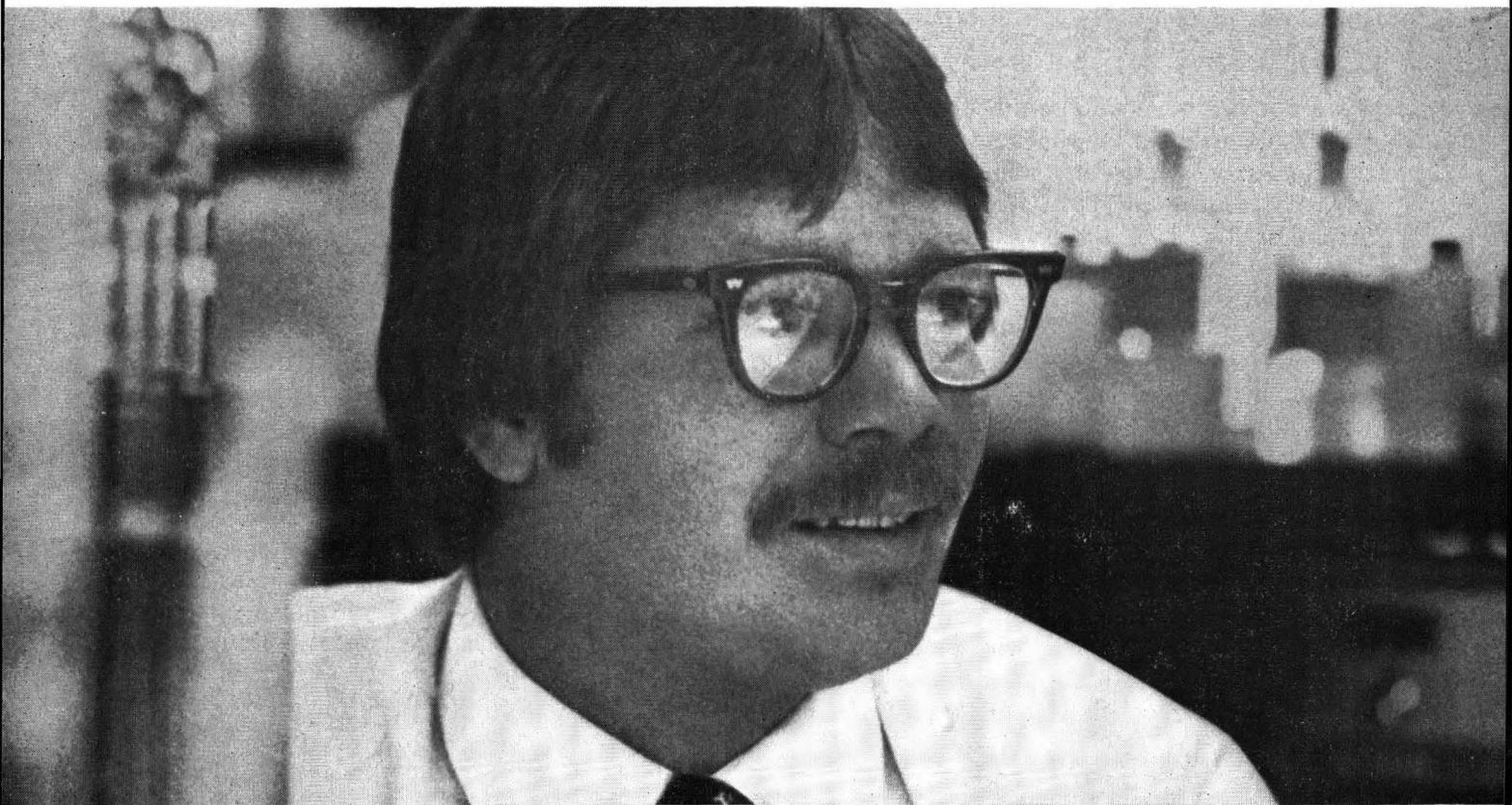
Part 4 consists of an excellent chapter on gas-liquid reactors plus a short account of liquid-liquid reactors. In the former, stirred tanks, sparged vessels, plate and packed columns, trickle beds, and pipeline contractors are considered. Many theoretical and practical aspects are discussed: scale-up, heat transfer, power consumption, pressure drop, design models and procedures, hold-up, mass transfer, dispersion, liquid distribution, and many others. Only the agitated reactor is treated in the last chapter.

The case studies of Volume II have been selected to illustrate various types of design problems. They are indicated in each case, often accompanied by a comment on the principal weakness of the design. The data that are needed are presented, along with intermediate results, alternatives, and bases for decisions.

Continued on page 47.

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ADVANCED PROCESS CONTROL EXPERIMENTS

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IN A COURSE ON ADVANCED process control a substantial portion of the time is spent in discussing the fundamentals, design, and implementation of advanced control concepts. When the course was first offered several years ago, computer simulations were used to demonstrate the concepts. While simulation is certainly a very valuable tool in the analysis and design of control systems, the students felt that it would have been much more satisfying if they had a physical process to work with. In subsequent years, several laboratory experiments were developed to eliminate this deficiency.

The equipment for the process, around which the present experiments were developed, was constructed from data provided by Exxon Oil Company (then Humble Oil & Refining Co.) on an identical setup at their Bayway refinery. [1] The rig was used by Exxon to train their instrument and process personnel. It has four of the most

It has four of the most commonly encountered control loops in process industry, i.e., liquid-level, flow, pressure, and temperature.

commonly encountered control loops in process industry, i.e., liquid-level, flow, pressure and temperature. The equipment was used to demonstrate feedback control concepts for these loops. Additional instrumentation has been added to the apparatus at the University of Louisville in order to demonstrate advanced control concepts.

EQUIPMENT & INSTRUMENTATION

A schematic of the thermal process unit is shown in Figure 1. The process involves heating of a continuous stream of water by steam. A vertical cylindrical tank approximately one foot in diameter is located in the center of the unit. The tank contains a steam pipe in the form of a vertical U tube. Water flows continuously in and out of the tank where it is heated by steam.

As shown in Figure 1, the process is instrumented with conventional controllers as well as with computer control hardware. Three variables can be controlled in this process: the flow rate of water into the tank, the level of water in the tank, and the temperature of water in the tank.

FLOW CONTROL LOOP

This loop regulates the flow of cold water into the tank. Supply water passes through a 7/16-inch diameter orifice mounted in a 1/2-inch pipe, then through a 1/2-inch control valve made by Uniflow Valve Corporation, and into the top of the tank. The differential pressure across the orifice is transmitted to a mercury manometer (FI in Figure 1) and to a Honeywell flow indicating transmitter (FT). The pneumatic 3-15 psig output of the transmitter is fed to a flow recording controller (FRC). It is also fed to an AMTEK pneumatic to voltage (P/E) transducer. The electrical output of the P/E transducer is con-

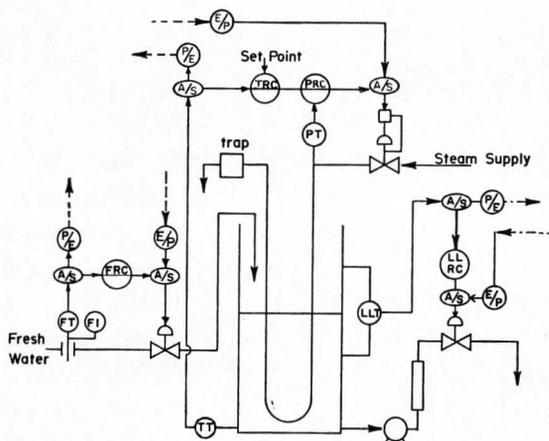


FIGURE 1. Schematic of Process Control System (Arrows indicate Signal transmission between the process and the computer).

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nected to one of the analog-to-digital (A/D) converter channels of the control computer. As indicated in Figure 1, the position of a Foxboro air-switch determines whether the transmitter output is fed to the conventional controller or to the control computer.

The conventional flow recording controller is a Honeywell, proportional + reset type, controller which sends a signal to an "air-to-open" control valve on the process unit. Alternately, the signal to the control valve may also come from one of the digital-to-analog converter channels on the control computer, via a Fisher E/P transducer. Again, the position of an air switch determines whether the signal to the valve comes from the conventional controller or from the control computer.

LIQUID-LEVEL CONTROL LOOP

Water level in the tank is controlled by manipulating the flow of water out of the tank. The level sensor infers the liquid level by measuring the pressure required to cause air bubbles to form slowly at the bottom of the tank. This pressure signal is fed into the high pressure side of a

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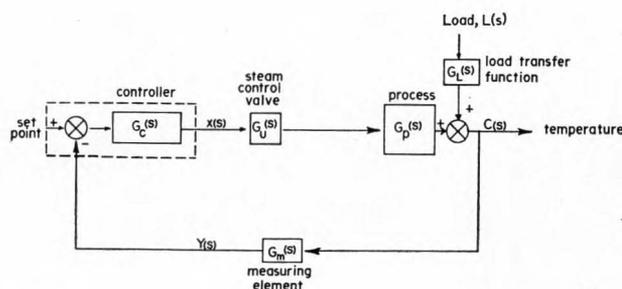


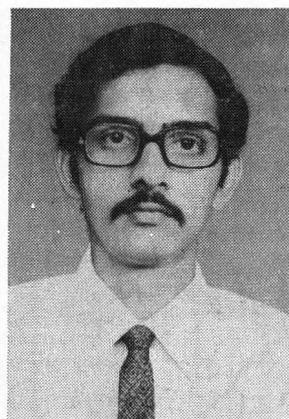
FIGURE 2. Block Diagram of the Temperature Control System

Foxboro differential pressure transmitter (LLT), set at a range of 40 inches of water. The low pressure side of the transmitter is vented to the atmosphere as is the surface of the liquid in the tank. Thus, the differential pressure transmitter output is proportional to the liquid level. The signal from the transmitter is fed to a Honeywell proportional + reset controller (LLRC) and to one of the A/D converter channels via an air switch which determines whether the loop will be on conventional control or on computer control.

The outputs of the controller and a D/A converter channel are fed to an air switch and then to a 3/4-inch, "air-to-close" control valve made by the Uniflow Valve Corporation, installed in the drain line from the tank. The air switch selects computer control or conventional control. A 1/4-hp, Barray pump in this line insures sufficient fluid pressure on the upstream side of the valve.

TEMPERATURE CONTROL LOOP

The temperature of water near the bottom of the tank is measured by an iron-constantan thermocouple immersed in an oil-filled well extending into the bottom portion of the tank. The voltage produced by the thermocouple is converted by a Honeywell electropneumatic transducer (TT)



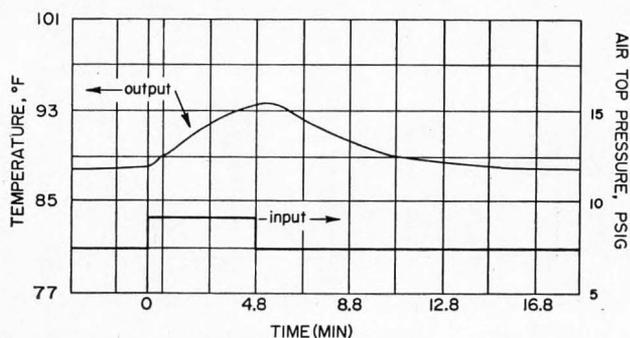


FIGURE 3. Input/Output Records From Pulse Test

into a pneumatic signal. This air signal is fed to a Foxboro three-mode controller (TRC). When conducting cascade control experiments, this controller serves as the master controller. The transmitter output is also fed to an A/D converter channel via an air switch. The output of the three-mode controller is fed to the set-point input of the Honeywell, proportional + reset, pressure recording controller (PRC). In cascade control experiments PRC serves as the slave controller.

The coil-side steam pressure is fed to a Honeywell transmitter. The output of the transmitter is fed to the pressure controller. The output of the controller operates a 1/2-in. Uniflow pressure control valve. The signal to the valve may alternately come from a D/A converter channel of the control computer.

In conventional control experiments, cascade control is achieved if both, master and slave controllers, are placed in automatic. If the pressure (slave) controller is switched to manual, the input to the control valve comes from the temperature controller. The temperature control loop is then a simple closed-loop rather than a cascade system.

The control computer used in some of the ex-

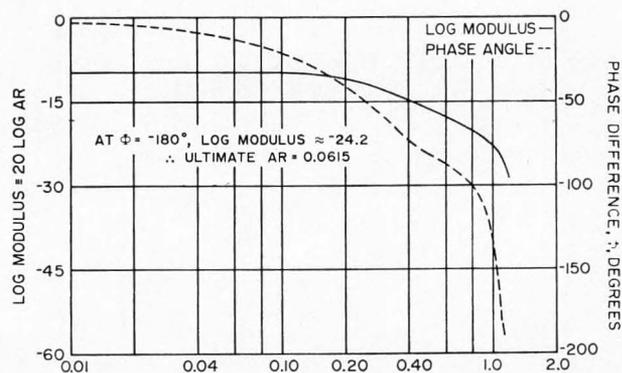


FIGURE 4. Frequency Response Diagram
Frequency ω , Radians/min.

periments is a PDP 1103 microcomputer system manufactured by the Digital Equipment Corporation. It has 24K words of memory and is equipped with an 8-channel D/A converter and a 16-channel A/D converter. The computer comes with a dual disk drive. A floppy disk, containing systems programs (e.g. Fortran support programs, real-time subroutines) resides in one of the drives while a second floppy disk, containing user-developed control programs, resides in the other drive. Communication with the computer is via a teletypewriter (LA 36 DECWRITER).

EXPERIMENT 1: Process Identification

This experiment is concerned with dynamic identification of an open-loop process by pulse testing. The resulting information is used to find (1) suitable tuning constants for a feedback controller or (2) to develop an approximate process model which is useful in designing advanced control strategies. The pulse testing technique [2, 3] has been applied to the temperature control loop whose block diagram is shown in Figure 2.

The input and output records from the pulse test are shown in Figure 3. Numerous data points from these records are entered into a computer program [3, 4] which generates frequency response data as shown in Figure 4.

From Figure 4, the ultimate AR, which refers to the amplitude ratio for which the phase lag equals 180 degrees, is 0.0615. Also, the crossover frequency, which is the frequency corresponding to the phase lag of 180 degrees, is 1.1 radians per minute. Therefore, the ultimate gain, K_u , and the ultimate period, P_u , are

$$K_u = \frac{1}{0.0615} = 16.23 \text{ psi/}^\circ\text{F} \quad (1)$$

$$P_u = \frac{2\pi}{1.1} = 5.71 \text{ min.}$$

Since the gain of the transmitter, K_T , is 0.06 psi/ $^\circ$ F, the Ziegler-Nichols tuning constants for a PI controller are

$$\begin{aligned} \text{Gain, } K_c &= 0.45 K_u / K_T = (0.45) (16.23) / 0.06 \\ &= 121 \text{ psi/psi} \\ \text{Integral Time, } \tau_I &= P_u / 1.2 = 5.71 / 1.2 \\ &= 4.75 \text{ min.} \end{aligned} \quad (2)$$

To assess the adequacy of the controller settings found in this section, a closed-loop control experiment was conducted. The response of the system to a step change in set point and load is shown in

Figure 5. This plot shows that the tuning constants found through pulse testing are adequate.

EXPERIMENT 2: Multivariable Control

Most large processes have many controlled variables and many manipulated variables. Ideally, a change in a given manipulated variable should affect only its own controlled variables and no others. Unfortunately, in many cases, this is not the case. The interaction among different loops can lead to poor control and even instability.

Since interaction can be a problem in multivariable control systems, it is important to know the extent of interaction and to be able to develop criteria for proper pairing of manipulated and controlled variables.

A measure of the extent of interaction in multivariable control is obtained by Bristol's method [5]. The method is based on steady-state input-output relationships for the process. It yields a measure of steady-state gain between a given input-output pairing. By using the most sensitive input-output connections, interaction is minimized.

Since Bristol's method does not take systems

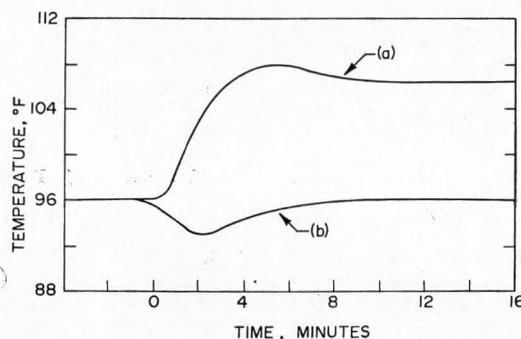


FIGURE 5. Transient Closed-Loop Response to (a) Set Point Change (b) Load Change

dynamics into account, it would be very useful to evolve an experiment which assesses the beneficial effects of proper pairing upon the dynamic response of the multivariable system. The present experiment [6] is designed to accomplish this objective.

The hardware for this experiment is essentially that shown in Figure 1 with the exception that the steam line is replaced by a pipe which introduces hot water into the tank. The air switches must be in the computer control position for this experiment.

Since interaction can be a problem in multivariable control systems, it is important to know the extent of interaction and to be able to develop criteria for proper pairing of manipulated and controlled variables.

The process objective is to control the level (in effect, total flow) and temperature of water in the tank. There are two inputs to the process, namely, the flow of cold water and the flow of hot water into the tank. So, the controlled variables are temperature and total flow and the manipulated variables are cold water flow rate and hot water flow rate. The question is, should the temperature be controlled by manipulating hot water flow and level (i.e. total flow) by cold water flow or vice versa? Bristol's method provides the answer.

Bristol's Relative Gains Analysis

The functional steady-state relationship between temperature, total flow and the flow streams is

$$T = f(m_c, m_h) = (m_c T_c + m_h T_h) / m_t \quad (3)$$

$$m_t = f(m_c, m_h) = m_c + m_h$$

Around some steady-state operating point, these relationships can be expressed as

$$\begin{aligned} \Delta T &= \frac{\partial T}{\partial m_c} \Delta m_c + \frac{\partial T}{\partial m_h} \Delta m_h \\ &= K_{11} \Delta m_c + K_{12} \Delta m_h \end{aligned} \quad (4)$$

and

$$\begin{aligned} \Delta m_t &= \frac{\partial m_t}{\partial m_c} \Delta m_c + \frac{\partial m_t}{\partial m_h} \Delta m_h \\ &= K_{21} \Delta m_c + K_{22} \Delta m_h \end{aligned}$$

The K's are the open-loop steady-state gains which quantitatively describe how the m's affect T and m_t . They can be determined from a mathematical model of the process or by experimental step or pulse-testing on the plant. To evaluate K_{11} and K_{21} for example, a small change in the flow of cold water is made, while the process is operating under steady state conditions (under manual control with the flow of hot water maintained constant). When the temperature and level reach their new steady-state values, K_{11} and K_{21} can be evaluated by

$$K_{11} = \left(\frac{\Delta T}{\Delta m_c} \right)_{m_h = \text{constant}} \quad (5)$$

and

$$K_{21} = \left(\frac{\Delta m_T}{\Delta m_c} \right)_{m_h = \text{constant}} \quad (6)$$

The gain K_{11} , then, determines the change in temperature, T , due to a change in m_c when m_h is held constant. Now, suppose instead of holding m_h constant, while a small change in m_c is being made, m_h is manipulated so as to bring m_t back to the original value it had before the change in m_c was made. Then, another gain A_{11} can be defined as

$$A_{11} = \left(\frac{\Delta T}{\Delta m_c} \right)_{m_t = \text{constant}} \quad (7)$$

A_{11} is a measure of how m_c affects temperature T , if level were under closed-loop control (i.e. held constant). The ratio of K_{11} to A_{11} is called the relative gain λ_{11} . Thus,

$$\lambda_{11} = \frac{K_{11}}{A_{11}} = \frac{(\Delta T / \Delta m_c)_{m_h = \text{constant}}}{(\Delta T / \Delta m_c)_{m_t = \text{constant}}} \quad (8)$$

By comparing the relative gains for each manipulated variable, it is possible to assess which m has the most effect on a given controlled variable

The equipment for the process, around which the present experiments were developed, was constructed from data provided by Exxon Oil Company . . . on an identical setup at their Bayway refinery.

and therefore how to pair the manipulated and the controlled variables.

While K 's can be determined easily, the experimental determination of A 's is not so easy. However, they can be evaluated from the K 's as follows:

By definition

$$A_{11} = \left(\frac{\Delta T}{\Delta m_c} \right)_{m_t = \text{constant}}$$

The open-loop relationships (Equation (4)) become

$$\Delta m_t = 0 = K_{21}\Delta m_c + K_{22}\Delta m_h \quad (9)$$

Thus,

$$\Delta m_h = -\frac{K_{21}}{K_{22}}\Delta m_c$$

Also in view of Equation (4)

$$\Delta T = K_{11}\Delta m_c - \frac{K_{12}K_{21}}{K_{22}}\Delta m_c \quad (10)$$

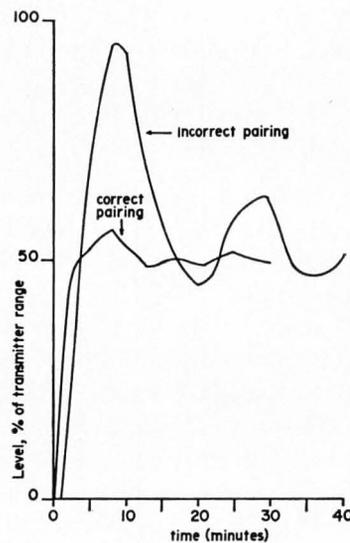


FIGURE 6. Transient Response of Level

Therefore,

$$\Delta T = \frac{K_{11}K_{22} - K_{12}K_{21}}{K_{22}}\Delta m_c \quad (11)$$

and,

$$A_{11} = \left(\frac{\Delta T}{\Delta m_c} \right)_{m_t = \text{constant}} = \frac{K_{11}K_{22} - K_{12}K_{21}}{K_{22}} \quad (12)$$

The relative gain λ_{11} is then

$$\lambda_{11} = \frac{K_{11}}{A_{11}} = \frac{K_{11}K_{22}}{K_{11}K_{22} - K_{12}K_{21}} \quad (13)$$

Similar analysis yields the remaining relative gains. Thus,

$$\lambda_{12} = \frac{K_{12}K_{21}}{K_{12}K_{21} - K_{11}K_{22}} \quad (14)$$

$$\lambda_{21} = \frac{K_{12}K_{21}}{K_{12}K_{21} - K_{11}K_{22}} \quad (15)$$

$$\lambda_{22} = \frac{K_{11}K_{22}}{K_{11}K_{22} - K_{12}K_{21}} \quad (16)$$

To facilitate the pairing of manipulated and controlled variables, it is convenient to present the relative gains in a matrix form as shown in Equation (17).

$$\begin{array}{c|cc} & m_c & m_h \\ \hline T & \lambda_{11} & \lambda_{12} \\ m_t & \lambda_{21} & \lambda_{22} \end{array} \quad (17)$$

For each controlled variable, the manipulated variable selected is the one which has the largest positive relative gain. Since a property of this

matrix is that each row and column sums to one, only one λ need be explicitly computed in a 2×2 system.

Results

The relative gains matrix for the current process is shown in Equation (18).

$$\begin{array}{c|cc} & m_c & m_h \\ \hline T & \frac{m_c}{m_t} & \frac{m_h}{m_t} \\ \hline m_t & \frac{m_h}{m_t} & \frac{m_c}{m_t} \end{array} = \begin{array}{c|cc} & m_c & m_h \\ \hline T & 0.172 & 0.828 \\ \hline m_t & 0.828 & 0.172 \end{array} \quad (18)$$

This equation shows that: T should be controlled by manipulating m_h and m_t by manipulating m_c . Both loops use a proportional + integral control algorithm on the digital computer as the control element. The algorithm was tuned by trial and

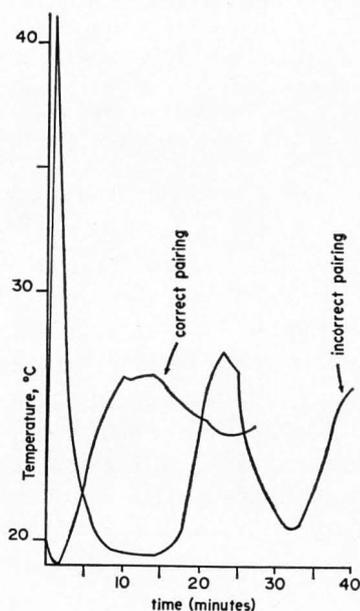


FIGURE 7. Transient Response of Temperature

error. The steady-state operating conditions were: level set point, 50% (which corresponded to total outlet flow of 11.6 lit/min); temperature set point, 24.4°C; cold water flow, 9.61 lit/min; hot water flow, 1.99 lit/min. The process was operated with correct pairing as well as with incorrect pairing. The benefits of proper pairing are clearly evident in the set-point responses shown in Figures 6 and 7. These results show that Bristol's approach is a simple and powerful tool in the control systems design of multivariable processes.

If the relative gains in Equation (18) had turned out to be numerically close to each other,

interaction ("fighting loops") would have been a problem, particularly if the response times of the two loops were comparable. Severe cross-coupling can drive the multivariable system to instability. In such cases decoupling will be required. Interested readers may consult reference 7 to obtain further information on the various techniques currently available for decoupling a multivariable control system. □

NOMENCLATURE

AR	=	amplitude ratio
A's	=	closed-loop gains
$G_p(s)$	=	process transfer function
K_T	=	temperature transmitter gain, psi/°F
K_c	=	proportional gain on temperature controller, psi/psi
K_P	=	steady-state gain of process, °F/psi
K's	=	open-loop gains
K_u	=	ultimate gain, psi/°F
m_c	=	cold water flow, lb/hr
m_h	=	hot water flow, lb/hr
m_t	=	total flow $m_c + m_h$, lb/hr
Pu	=	ultimate period, min.
T	=	temperature of the mixture, °F
T_c	=	temperature of cold water, °F
T_h	=	temperature of hot water, °F

Greek

ϕ	=	phase angle
θ_d	=	process dead-time, minutes
τ_P	=	time constant, minutes
τ_I	=	integral time, minutes
$\lambda_{i,j}$	=	relative gain
ω	=	frequency, radians/minute

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THE INTEGRATION OF REAL-TIME COMPUTING INTO PROCESS CONTROL TEACHING

PART II: THE UNDERGRADUATE COURSE*

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PROCESS CONTROL FOR undergraduates is offered each semester and has enrollments of 30 to 50 students. The course has two lecture periods, one recitation period, and one 3 hour laboratory period each week. The curriculum (shown in Tables 1 and 2) has been selected to give the student a balanced mixture of useful theory and hands-on practical experience in process dynamics, measurement, and control.

COURSE DESCRIPTION

THE INSTALLATION OF A PDP11/55 minicomputer system described in Part I of this article has allowed a complete restructuring of the course material. A large library of computer programs for the design of control systems is available and is still growing. The use of these programs makes it possible to design control systems for meaningful practical processes without the drudgery of laborious hand calculations. Thus, course time is freed and it becomes possible to cover topics generally neglected in undergraduate courses,

TABLE 1

Undergraduate Process Control Lecture Topics

1. Review of Laplace transforms and matrix algebra
2. Principles of real-time computation and data acquisition
3. Transient and frequency response of linear systems
4. Feedback control of linear systems
5. Stability of linear systems
6. Control system design for linear systems
7. Nonlinear systems
8. Case studies

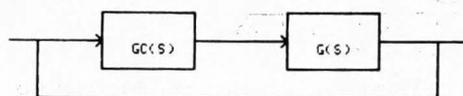
*Part I dealing with graduate education in process control appeared in the Fall 1979 issue of *CEE*.

TABLE 2

Undergraduate Process Control Laboratory Experiments

1. Techniques of analog simulation
2. Techniques of digital simulation
3. Dynamics of interconnected water tanks
4. Computer aided data acquisition
5. Frequency response and process identification through pulse testing
6. Calibration and dynamic response of PID controllers
7. Feed forward, feedback, and cascade control
8. Multivariable control of a gas distribution system
9. Multivariable control of a multi-sidestream distillation column
10. Tuning of a level controller with strong system nonlinearities

e.g. multivariable control. The lecture material is listed in Table 1 and includes considerations of how to choose loop pairings, how to minimize interactions between control loops and how to tune multivariable systems. In the latter part of the semester a number of graphical interactive computer aided design programs are used for detailed case studies. The present library includes routines for the generation of Bode plots, root loci and



DESIGN MODEL

```

1) G(S)=C*(P1*S+1)*(P2*S+1)/(T3*S+1)*(T4*S+1)*(T5*S+1)
OR
2) G(S)=[A(1)+A(2)*S+...A(N)*S**(N-1)]/[B(1)+B(2)*S+...B(M)*S**(M-1)]
G(S) = K*(1 + TD*S + 1/TI*S)
WHICH WOULD YOU LIKE:1 OR 2?1
INPUT C = 1
INPUT P1 = 0
INPUT P2 = 1
INPUT T3 = 2
INPUT T4 = 8
INPUT T5 = 5
INPUT TIME DELAY = 0
UP TO WHAT VALUES OF K WOULD YOU LIKE?10
WOULD YOU LIKE THE ROOTS LISTED ON THE LINE PRINTER?Y/NJN
CONTROLLER
1) P 2) PD 3) PI 4) PID
TYPE1 TO 4?1
    
```

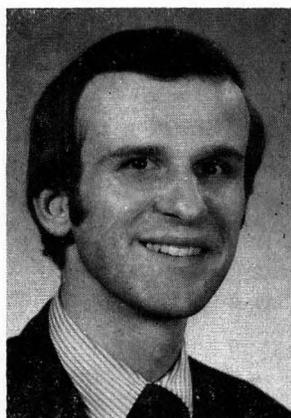
FIGURE 1. Input Data for Root Locus Program: Process

$$G(s) = \frac{(s + 1)}{(2s + 1)(8s + 1)(5s + 1)} \text{ is under Proportional Feedback Control.}$$

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Nyquist diagrams for open loop, closed loop and cascade control systems. In addition, a number of programs for the design of multivariable systems are presently available. Output from these programs usually appears as plots drawn on the screens of graphic terminals, and paper copies (to be included in student reports) are obtained by the student at the push of a button. Example: if a root locus diagram is to be drawn the user would be asked to specify the transfer function parameters and other variables as shown in Fig. 1. Upon completion of the questions a diagram (as in Fig. 2) will appear which can be subsequently enlarged or otherwise modified.

The laboratory, which is designed to complement the lecture material, is comprised of some



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W. Harmon Ray was born in Washington, D.C., on April 4, 1940. He received the B.A. and B.S. Ch.E. degrees from Rice University, Houston, Texas, in 1962 and 1963 respectively, and the Ph.D. degree in ChE from the University of Minnesota in 1966. He has been on the faculty of the University of Waterloo in Canada (1966-70), the State University of New York at Buffalo (1970-76), and the University of Wisconsin, Madison, where he is presently Professor of ChE. During the 1973-74 academic year, he was on sabbatical leave as a Guggenheim Fellow in Belgium and Germany. His research interests include chemical reactor engineering and process modelling, optimization, and control. His publications include an edited volume "Distributed Parameter Systems" (Dekker, 1977), and two monographs "Process Optimization" (Wiley, 1973) and "Advanced Process Control" to be published by McGraw-Hill in 1980. (R)

The use of these programs makes it possible to design control systems for meaningful practical processes without the drudgery of laborious hand calculations. Thus, course time is freed and it becomes possible to cover topics generally neglected in undergraduate courses

ten experiments (cf Table 2). Most of these experiments are carried out by each laboratory group in the course of the semester. Many experiments involve real time computation and are selected to familiarize the students with the modern methods of implementing control algorithms. These presently include:

- Data acquisition (noise suppression, signal amplification, A/D conversion, sensor calibration, etc.)
- Pulse testing (data acquisition, input pulse selection, Fourier transformation of data, frequency spectrum analysis, frequency response parameter determination, etc.)
- Multivariable feedback control of interconnected gas storage tanks (process modelling, data acquisition, single loop PI control, supervisory computer control, direct digital control, etc.)
- Multivariable feedback control of a multi-side-stream distillation column (process modelling, data acquisition, single loop control, supervisory computer control, and direct digital control)

Let us discuss two of these experiments in more detail.

Pulse Testing

THIS EXPERIMENT CONSISTS of putting a measured pulse of hot water into a stirred mixing tank having continuous inflow and outflow. Input and output temperatures are measured under computer control and the resulting data analyzed to provide frequency response informa-

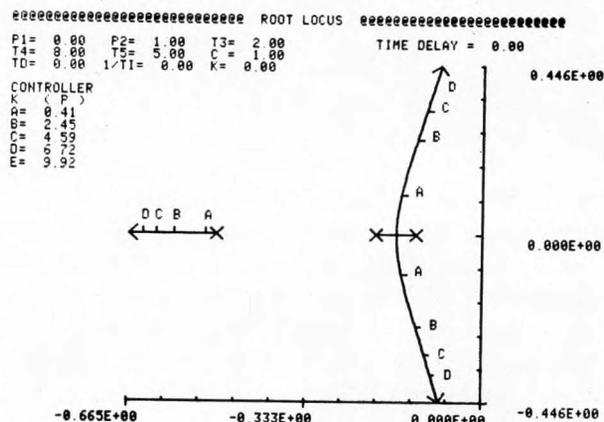


FIGURE 2. Root Locus Diagram for the Feedback Control Loop in Figure 1.

tion and parameters for a process model (i.e., a gain and time constant for this simple first order process). Typical results, taken from a student lab report, are shown in Figures 3 and 4. The measured input and output temperatures are shown in Figures 3 while the resulting Bode plot showing the frequency response may be seen in Figure 4. The process gain of 1.0 is readily found from the low frequency asymptote of the amplitude ratio (AR). By using both amplitude ratio (AR) and phase angle (ϕ) to estimate the corner frequency, ω_c , two separate estimates of the tank time constant are found. Usually these are in reasonable agreement with the "theoretical" value determined from the mean residence time of the tank.

Multivariable Control of Interacting Gas Storage Tanks

One of the most sophisticated experiments carried out by the students is the modelling and multivariable feedback control of a pair of inter-

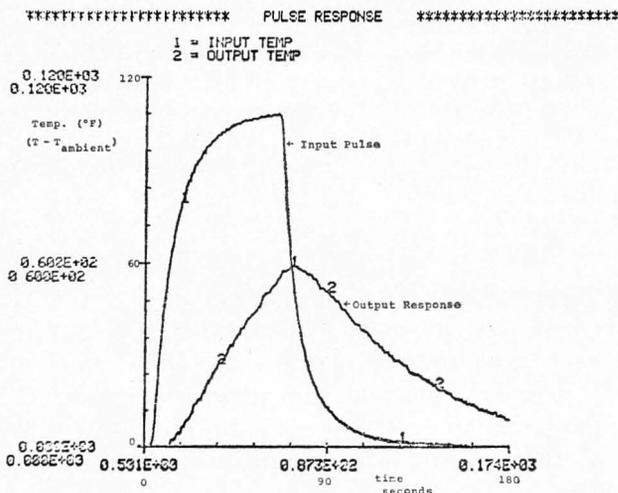


FIGURE 3. Pulse Test Data for Mixing Tank.

acting gas storage tanks. This experiment requires three laboratory periods plus some lecture preparation. The purpose of this experiment is to demonstrate to the student the effects of interactions in multivariable systems and to give him or her the possibility of testing different multivariable control schemes on a real system.

A simplified version of the system flow sheet is given in Figure 5. Air enters the system at a constant pressure of 60 psig, flows through a control valve into the first tank and from there through another control valve into the second tank. Finally, the air passes through a fixed ori-

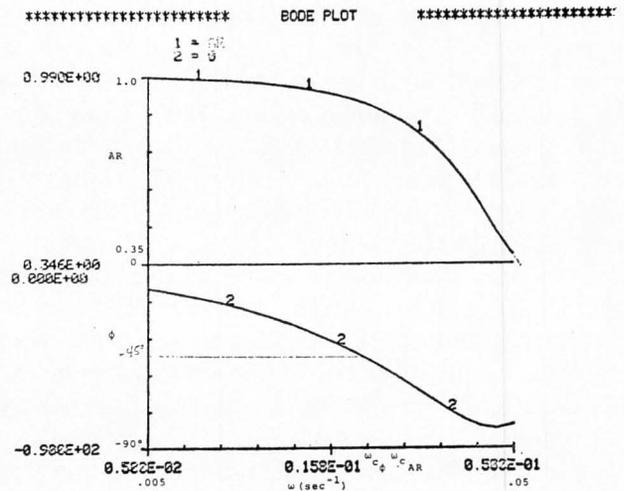


FIGURE 4. Frequency Response Bode Plot for Mixing Tank.

fice, a rotameter, and is vented. The equipment is fully instrumented with two pressure gauges, pressure transducers, PI analog controllers and is also interfaced with the minicomputer allowing data acquisition, supervisory and direct digital control.

The first task given the students is to develop a mathematical model for the tank system. An unsteady state mass balance for each of the two tanks yields

$$\frac{dp_1}{dt} = \frac{RT}{V_1 M} [C_{d1} A_1 \phi(p_0, p_1) - C_{d2} A_2 \phi(p_1, p_2)] \quad (1)$$

$$\frac{dp_2}{dt} = \frac{RT}{V_2 M} [C_{d2} A_2 \phi(p_1, p_2) - C_{d3} A_3 \phi(p_2, p_3)] \quad (2)$$

where

- R = universal gas constant
- T = absolute temperature
- V_i = volume of tank i
- M = mean molecular mass of air stream
- C_{di} = discharge coefficient for orifice i
- A_i = area of orifice i

$$\phi(p_i, p_{i+1}) = \begin{cases} K_1 (p_i (p_i - p_{i+1}))^{1/2} & p_{i+1}/p_i > .5 \\ K_2 p_i & p_{i+1}/p_i < .5 \end{cases} \quad (3)$$

K_1, K_2 = material constants

All parameters of the model are available to

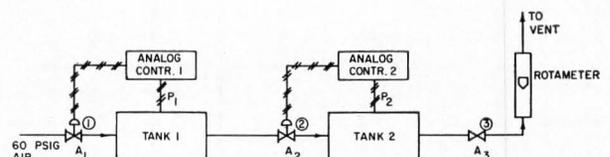


FIGURE 5. An Interacting Gas Storage System.

the student in tabulated form except the discharge coefficients which have to be determined through steady state experiments.

Computer control experiments are carried out with the goal of achieving a given gas production rate while meeting certain pressure constraints in the two gas storage tanks. Both Supervisory Control and Direct Digital Control algorithms are tested by the student. Different control objectives can be selected by the student but they all result in the regulation of the two pressures through changes in the two control valves. Let us briefly indicate some of the choices available to the student.

A. Supervisory control:

Possible control objectives:

- 1) specified gas flow rate from tank 2 and
- 2) p_1/p_2 fixed or p_1 minimized or p_1 maximized

In supervisory mode, the valves are under local analog control. After a control option is

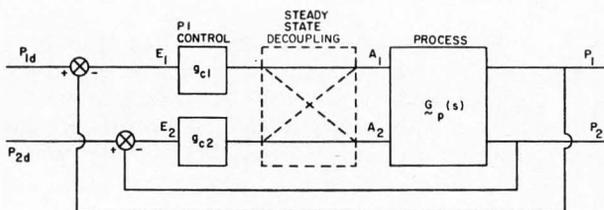


FIGURE 6. Control Structure for DDC Control with Single Loop PI Controllers and with Added Steady State Decoupling (dashed lines).

entered by the student via the computer terminal, the set points are computed and transmitted by the computer to the local controllers. The response to changes in objectives is observed for different flow regimes. (Critical or subcritical flow through the valves.) Set point compensation is attempted to yield a smoother servo behavior.

B. Direct digital control (DDC):

The possible control objectives are identical to those listed in part A. Different multivariable control algorithms are developed by the students and supplied to the main control program in the form of Fortran subroutines. As an example, steady state decoupling is implemented and compared with the usual single loop PI control. The controller structure is seen in Figure 6. The results of one laboratory group are shown in Figures

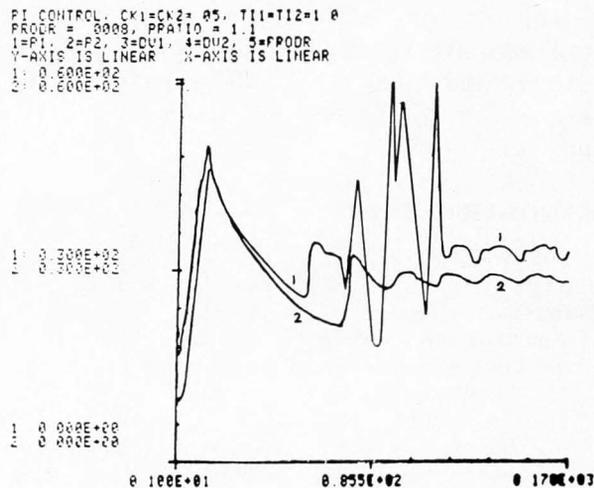


FIGURE 7. Process Response Under DDC With Single Input-Single Output PI Control.

7, 8. With simple PI control, significant oscillations in the pressure response were found (cf. Figure 7). However, with the addition of steady state decoupling, the response was much improved (Figure 8).

CONCLUSIONS

THE NEW MINICOMPUTER has become an integral part of the undergraduate control course at Wisconsin. Aspects of digital computer control are demonstrated to the students and they have the opportunity to gain some practical experience with the implementation and application of modern control algorithms. Computer aided control

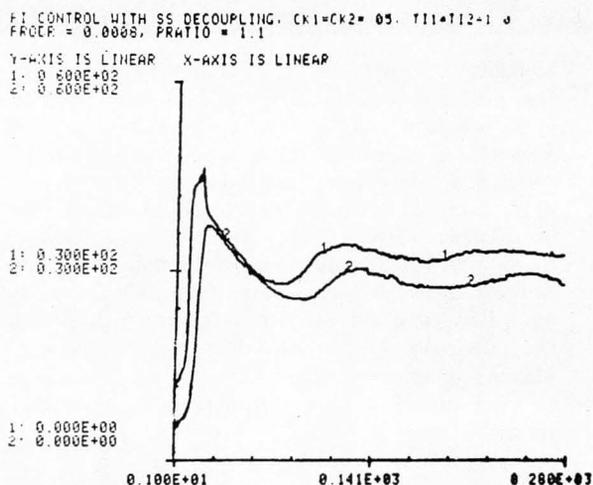


FIGURE 8. Process Response Under DDC With Steady State Decoupling and PI Control.

system design methods utilizing interactive graphics have replaced classic pencil and paper methods and have thus made time available to include new theoretical material in the curriculum. □

ACKNOWLEDGMENTS

Our progress in bringing real time computing into the process control curriculum at Wisconsin is due to the cooperative efforts of many individuals:

1. Emeritus Professor R. J. Altpeter, who originally established process control as a discipline at Wisconsin. He laid the foundation upon which the present curriculum is built.
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5. The more than 200 undergraduate and graduate students who have "consumer tested" the changes in curriculum and provided useful feedback.

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PROCESS CONTROL EXPERIMENT: THE TOILET TANK

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THE LEVEL CONTROL mechanism in the home toilet tank is a nonlinear, proportional control system that illustrates various process control concepts. It can also serve as an introduction to data acquisition, process analysis, and model development. This simple experiment can be developed as an example problem, a classroom demonstration, or a laboratory exercise.

DESCRIPTION

A TYPICAL TOILET TANK is shown in Figure 1. The level control system regulates the tank water level C at the desired steady state C_s by manipulating the inlet water rate M to compensate for the disturbance (the flushing rate U). The control logic is given in the flow diagram of Figure 2A.

An actual toilet tank can be used for the laboratory exercise if a flowmeter is installed in the feed line and a measuring scale is fastened to the inside of the tank wall. For classroom demonstrations, the level mechanism can be installed in a clear plastic tank (0.5 by 0.15 by 0.4 meters high). A quick-opening valve can provide the necessary flush for the plastic tank.



Tom Ward has been on the chemical engineering faculty at Clarkson College of Technology for many years. He received his M.S. from the University of Texas and his Ph.D. from RPI. His research interests are principally in the area of process control.

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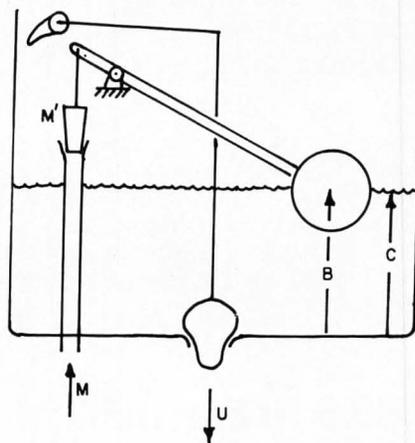


FIGURE 1. A typical tank.

Typical exercises involve the development of analytical models, determination of model parameters, and measurement of the closed-loop response to a flushing disturbance. Two suitable process models are presented in the following sections.

NONLINEAR MODEL

THE EQUATIONS FOR EACH of the elements of Figure 2A can be obtained as follows:

Tank: A mass balance on the tank gives

$$A \frac{dC}{dt} = M - U \quad (1)$$

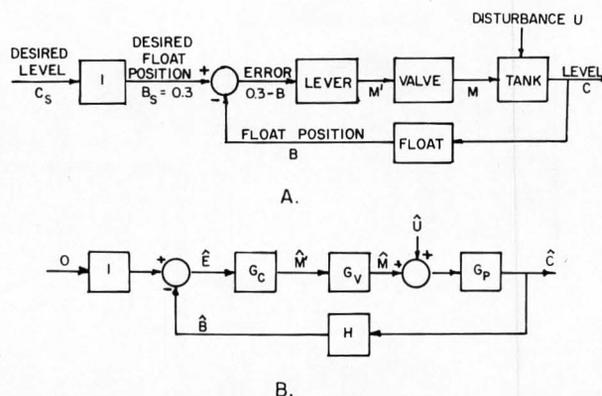


FIGURE 2. Information flow diagrams: A. Nonlinear logic, B. Linear block diagram.

where A is the tank cross-sectional area. A typical value for A is suggested by the plastic tank dimensions given above so that

Tank: A mass balance on the tank gives

$$A = (0.5)(0.15) = 0.075 \langle m \rangle^2 \quad (2)$$

Float: The float center height B is assumed to correspond to the water level so that the equation for the measuring element is simply

$$B = C \quad (3)$$

Alternately, it could be assumed that the float is characterized by a first or second order model. While this would lead to an interesting higher-order process model, it might be difficult for students to estimate the parameters in a higher-order model.

Valve: It is assumed that the valve flow rate M can be related to the valve position M' by the equation

$$M = \alpha (M')^{0.5} \quad (4)$$

Many toilet valves have an adjustable ring so that the valve coefficient can be changed. A typical value for the coefficient α is $0.0021 \langle m \rangle^{2.5}/s$. The experimental determination of a suitable valve equation and coefficient can provide an interesting short study.

Lever: A reasonable controller equation relating the valve position M' to the error ($C_s - B$) can be written as

$$M' = K (C_s - B) \quad (5)$$

where the controller gain K is given by the lever ratio. A typical value for the desired steady-state level C_s is assumed to be 0.3 meters. If the lever is assumed to be 0.40 meters long (to the float center) and the pivot is 0.04 meters from the valve end, then the controller gain is given as

$$K = 0.04/0.40 = 0.1 \quad (6)$$

These can be combined to give the nonlinear model as

$$A \frac{dC}{dt} = \alpha [K(C_s - C)]^{0.5} - U \quad (7)$$

LINEARIZED MODEL

AS NOTED ABOVE, the steady state is selected as the filled tank (a nonflow condition). For any variable X, the perturbation from the steady state is defined as $\hat{X} = X - X_s$. In terms of such perturbation variables, the equations for three of the elements are

$$\text{Tank: } A \frac{d\hat{C}}{dt} = \hat{M} - \hat{U} \quad (8)$$

$$\text{Float: } \hat{E} = -\hat{B} = -\hat{C} \quad (9)$$

$$\text{Lever: } \hat{M}' = K\hat{E} \quad (10)$$

The nonlinear valve equation can be linearized around the steady state by the truncated Taylor series approach to give

$$\hat{M} \cong \left(\frac{dM}{dM'} \right)_s \hat{M}' = \beta \hat{M}' \quad (11)$$

where β should be the slope of the valve curve at the origin. As can be seen in Figure 3, this would

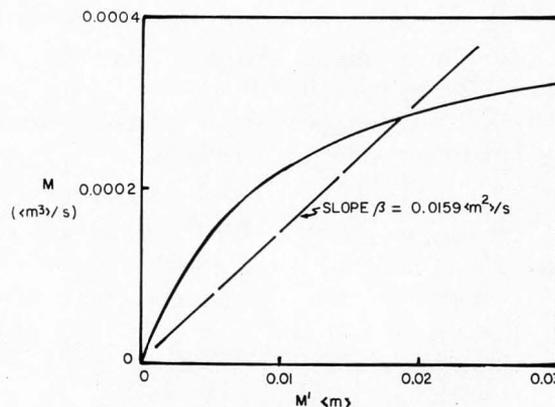


FIGURE 3. Linearization of valve response.

give a value of β that would be much too high away from the origin. A line with slope $\beta = 0.0159 \langle m^2/s \rangle$ is arbitrarily selected to approximate the value behavior over the region of interest. This illustrates how experimental data can be used to improve on the classical steady-state linearization.

The linear model corresponds to the block diagram of Figure 2B, where $G_c = K$, $G_v = \beta$, $H = 1$, $G_p = 1/AD$, and $D = d/dt$. These can be combined to give the linear model as

$$(TD + 1)\hat{C} = -\alpha\hat{U} \quad (12)$$

where $T = A/\beta K$ and $\gamma = 1/\beta K$.

DISTURBANCE INPUT

IT IS ASSUMED THAT the flush, given by $\int U dt$, empties the tank. Then $\int U dt = (0.5)(0.15)(0.3) = 0.0225 \langle m \rangle^3$. Various approximations can be suggested for the disturbance U. A suitable function might be the displaced cosinusoid with a period of 10 seconds

$$U = \begin{cases} -0.00225 \cos 0.2\pi t + 0.00225 \\ 0 \end{cases} \quad \begin{cases} 0 \leq t \leq 10 \text{ sec} \\ t > 10 \text{ sec} \end{cases} \quad (13)$$

Since the flush occurs quickly compared to the filling time, it might be reasonable to approximate the disturbance as an impulse of $0.0225 \langle \text{m}^3 \rangle$ occurring at $t = 0$.

MODEL RESPONSES

THE RESPONSE FOR VARIOUS model and disturbance forms can be compared with experimental responses to show the significance of the approximations made. Three model responses will be given here:

a. **Nonlinear Model With Cosinusoid Disturbance.** The response for this case was obtained numerically for the parameter values assumed above. This is given by the curves NL-C in Figure 4.

b. **Nonlinear Model With Impulse Disturbance.** If the flush is an impulse at $t = 0$, then the solution for $t > 0$ can be obtained by assuming that $U = 0$ and $C = 0$ at the instant $t = 0^+$. Equation 7 can then be solved by the separation of variables technique to give

$$(C_s - C)^{0.5} / 2A)t + C_1 \quad (14)$$

For the assumed parameter values, the integration constant $C_1 = (0.3)^{0.5}$. The response curves for this case are given as NL-I in Figure 4.

c. **Linear Model With Impulse Disturbance.**

If it is assumed that $\hat{U}(0^+) = 0$ and $\hat{C}(0^+) = -0.3$, then the solution to Equation 12 is

$$\hat{C} = -0.3 e^{-t/T} \quad (15)$$

The responses for this case are shown in Figure 4 as the curves LI.

OTHER FEATURES

THE TOILET TANK CAN be used to illustrate other process control concepts. Some of these are:

a. **Offset.** The leaking toilet provides one of the simplest demonstrations of offset. If the outflow at steady-state is not zero, then the inflow at steady state is not zero. Since the flow into the tank is a fixed function of C , then the steady-state level must decrease if the toilet tank is leaking.

b. **Measurement Error.** The water-logged float implies that the float center-line does not

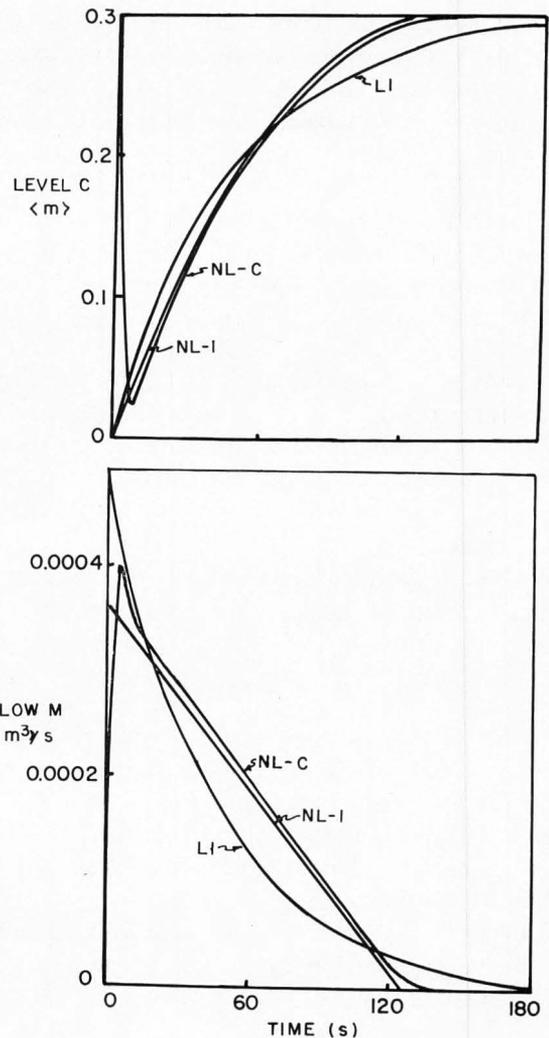


FIGURE 4. Level and flow responses (LI = linear model with impulse disturbance, NL-I = nonlinear model with impulse disturbance, NL-C = nonlinear model with cosinusoid disturbance).

correspond to the level. At steady state, the level must increase in order to close the feed valve.

c. **Setpoint Changes.** The float end of the level can be bent to represent setpoint changes.

d. **Controller Gain.** Most toilet tank controls have some provision for changing the loop gain. In some cases, this is accomplished by changing the effective lever ratio. In others, an adjustable ring is used to change the valve gain.

CONCLUSION

The toilet tank, as either a classroom problem or experiment, provides a simple introduction to process control. □

rec·og·ni·tion \ , rek-ig-'nish-ən,
-əg-\ n **1** : the action of recognizing; the state of being
recognized; as **a** : ACKNOWLEDGMENT **2** : special notice
or attention.

rec·og·ni·tion \ as we see it \

1 : the primary motivation to do creative work for an out-
standing company **2** : ACKNOWLEDGMENT of the quality of
that work; as **a** : self-satisfaction and pride **b** : respect
from peers and associates **c** : opportunity for advancement
3 : to recognize the challenge of the world today **4** : to be
recognized for doing something to meet those challenges
tomorrow.

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A SURVEY OF PROCESS CONTROL EDUCATION IN THE UNITED STATES AND CANADA*

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IN FEBRUARY, 1978 a questionnaire on process control education was distributed to the 158 chemical engineering departments in the United States and Canada. Completed questionnaires were returned by 143 schools, or 90% of the 158 departments. This response compares quite favorably with the 59-101 replies that were received in recent AIChE surveys of undergraduate curricula [1, 2]. The large number of replies is probably due to two factors: 1) the questionnaire was kept very brief, and 2) copies of the final report were promised to those departments which submitted completed questionnaires.

SURVEY RESULTS

THE SURVEY RESULTS indicate that process control is firmly established in the undergraduate curriculum since only 7 of the 143 respondents (5%) do not offer undergraduate courses. By contrast, 108 schools (75%) have required courses and an additional 28 schools (20%) offer elective courses. Interestingly enough, 4 of the 7 schools which do not offer undergraduate courses in process control do offer graduate courses. Thus only 3 schools of the 143 respondents do not offer any process control courses.

Process control courses are also firmly established at the graduate level. Seventy-two schools (50%) offer graduate courses while an

The survey results indicate that process control is firmly established in the undergraduate curriculum since only 7 of the 143 respondents (5%) do not offer undergraduate courses.

*A preliminary version of this paper was presented at the Miami Beach AIChE Meeting.

TABLE 1

Textbook Selection for Undergraduate and Undergraduate/Graduate Courses

TEXT	NUMBER OF DEPTS.
Coughanowr and Koppel	69
Luyben	21
Weber	9
Harriott	6
Douglas	6
Perlmutter	3
Smith, Cecil	2
Ogata	2
Others (one each)	17
Total	135

additional 15 schools (10%) offer courses which are open to both graduate students and advanced undergraduate students. Tables 1 and 2 list the process control textbooks which have been adopted for undergraduate and graduate courses, respectively.

The most striking result here is the continuing popularity of the book by Coughanowr and Koppel which has been selected as an undergraduate text by 69 departments and as a graduate text by 7 departments. The dominant position of this 15 year old text is quite remarkable in view of the significant developments which have occurred since 1965 in both computer control hardware and

TABLE 2

Textbook Selection for Graduate Courses

TEXT	NUMBER OF DEPTS.
Smith, Cecil	10
Coughanowr and Koppel	7
Luyben	4
Douglas	2
CACHE Monographs	2
Lapidus and Luus	2
Other (one or two each)	17
Total	44

TABLE 3
Laboratory Control Experiments in Undergraduate Courses

NUMBER OF EXPERIMENTS/COURSE	NUMBER OF DEPTS.
0	43
1-2	30
3-4	26
5+	37
Some experiments (number not available)	7
Total	143

in control theory. The results in Table 1 agree quite well with a 1975 survey on undergraduate process control courses [1]. It should be noted that the numbers in Tables 1 and 2 are reported on the basis of individual departments rather than on the basis of courses offered. For example, if a particular department offers two undergraduate process control courses which use the same textbook, this was counted only once in Table 1 rather than twice. By contrast, if two textbooks were required for a particular course, they both were included. Many of the 17 textbooks included in the "Other" category in Tables 1 and 2 were written for mechanical or electrical engineers and are used in classes taken by both chemical engineering students and other engineering students.

One hundred departments (70% of the respondents) indicated that their curriculum in-



Dale E. Seborg received a B.S. degree from the University of Wisconsin in 1964 and a Ph.D. degree from Princeton University in 1969. Both degrees were awarded in chemical engineering. He taught at the University of Alberta for nine years before joining the University of California, Santa Barbara in 1977. He is presently Professor and Chairman of the Department of Chemical and Nuclear Engineering at UCSB. Dr. Seborg is co-author of the book, *Multi-variable Computer Control: A Case Study*. He is also the past chairman of Area 15B (Systems and Process Control) of the AIChE National Program Committee.

The most striking result here is the continuing popularity of the book by Coughanowr and Koppel which has been selected as an undergraduate text by 69 departments and a graduate text by 7 departments.

cludes one or more laboratory experiments in process control. Table 3 shows that 63 departments offer courses that contain at least three control experiments and 30 departments have one or two experiments, usually as part of a unit operations laboratory.

In compiling these statistics, each department was included in only a single category. Thus if a particular department offers two process control

TABLE 4
Use of Real-Time Computers or Micro-Processors in Control Experiments

	NUMBER OF DEPTS.
Currently have a real-time system	48
Equipment on order or being installed	19
No equipment (but have tentative plans to add equipment)	22
No equipment (and no plans for future equipment)	53
Total	143

courses which include three and five experiments, respectively, this department was included in the tally for the "5+" category in Table 3.

During the past decade there has been considerable interest in "real-time computing," that is, in digital computers which are used for data acquisition and control. Both industrial and academic personnel in the process control field have maintained an active interest in the field of real-time computing for the following reasons:

- The widespread availability of inexpensive minicomputers and microprocessors;
- Changing process control objectives in industrial plants due to energy and environmental considerations;
- The realization that the application of most advanced control strategies will inevitably require an on-line digital computer.

The results in Table 4 indicate that 48 departments (34%) currently have control experiments which involve a real-time computer while an additional 19 departments (13%) have computer systems on order or being installed.

Table 4 includes only those departments which use real-time computers in conjunction with undergraduate control experiments. It does not include

TABLE 5
Real-Time Computers or Microprocessors
Currently Installed (53) or On Order (19)

EQUIPMENT AND VENDOR	NUMBER OF DEPTS.
Minicomputers	
Digital Equipment Corp.	24
Data General Corp.	8
Hewlett Packard	5
IBM	5
Texas Instruments	3
Foxboro	2
Interdata	2
Miscellaneous (one each)	6
Not specified	7
Microprocessors	10
Total	72

other departments which use minicomputers or microprocessors exclusively in research laboratories. The 22 departments in the third category in Table 4 typically are in a preliminary planning stage or are seeking funds to purchase a real-time system. Thus the results of this survey indicate a continuing trend for incorporating a real-time computer system in the undergraduate curriculum.

Table 5 presents a summary of the 62 minicomputers and 10 microprocessors which are currently operating in chemical engineering departments or on order. The numbers in Table 5 do not correspond directly to those in Table 4 since several chemical engineering departments use more than one real-time computer in the undergraduate curriculum.

CONCLUSIONS

THE RESULTS OF THIS survey indicate that the topic of process control has become firmly established in the chemical engineering curriculum. Only 3 of the 143 departments surveyed do not teach any courses in process control. One hundred and eight schools (75% of the respondents) have required undergraduate courses while 87 schools (61%) teach graduate level courses in process control. Laboratory experiments in process control are now available at 100 schools (70%). There is a continuing trend toward providing students with exposure to real-time computer systems in conjunction with process control experiments; 67 departments currently have such a system operating or on order while an additional 22 departments have tentative plans for such a system.

Fifteen years ago, process control was generally regarded as a new, specialized topic

which was not part of mainstream chemical engineering. The present survey demonstrates that this situation no longer exists. Process control has joined the more traditional topics such as transport phenomena, thermodynamics and reactor analysis in playing a central role in the chemical engineering curriculum. □

REFERENCES

1. Eisen, E. O., "Teaching of Undergraduate Process Dynamics and Control," paper presented in a mini-session at the 68th Annual AIChE Meeting, Los Angeles (November, 1975).
2. Barker, D. H., "Undergraduate Curriculum 1976," *Chem. Eng. Educ.*, Vol. XI, No. 2, (Spring, 1977).

BOOK REVIEW: Contact Catalysis

Continued from page 12.

hope of being able to reproduce catalysts of a given type in different laboratories is rapidly becoming a reality.

As one might infer from the variety of topics and extent of treatment, these volumes are not exactly for the beginner. One might have wished some discussion of homogeneous catalysis, at least in terms of analogs to heterogeneous systems, and a more general inclusion of the concepts of coordination chemistry as they relate to catalysis. In all, however, some balance must be struck between coverage and length and the editor has done an admirable job. The English translation of the original Hungarian edition of 1966 is excellent and the text has been updated. The dust jacket states that "the book will be useful to workers studying catalysis in industrial and university laboratories." The present reviewer feels this is a correct statement and commendable for its modesty. □

ChE news

ART HUMPHREY HONORED

Arthur E. Humphrey, dean of Penn's School of Engineering and Applied Science, became the eighth honoree to receive the James M. Van Lanen Distinguished Service Award for his "life long dedication and service to fermentation science and the fermentation industry.

The award is named for a pioneer in fermentation technology and was established in 1976 as the foremost award and citation of the ACS Division of Microbial and Biochemical Technology.

ChE class and home problems

The object of this column is to enhance our readers' collection of interesting and novel problems in Chemical Engineering. Problems of the type than can be used to motivate the student by presenting a particular principle in class or in a new light or that can be assigned as a novel home problem are requested as well as those that are more traditional in nature that elucidate difficult concepts. Please submit them to Professor H. Scott Fogler, ChE Department, University of Michigan, Ann Arbor, MI 48109.

SOLUTION: MIRROR FOG PROBLEM

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Editor's Note: Professor Kabel presented the "Mirror Fog Problem" in the Fall 1979 issue of CEE. We extended an invitation for student solutions to this problem at the time of publication and would like to congratulate Mauricio Fuentes of Ecole Polytechnique, Montreal, Canada, who submitted the winning entry and by so doing has won a year's subscription to CEE. Professor Kabel graded the responses and, in his words, Mr. Fuentes' entry was both "correct and excellently done." The following is Professor Kabel's solution to the problem.

Derivation of equations:

Use a microscopic model because momentum and energy equations are not required due to isothermality and no bulk flow.

Mass balance equation:

$$\frac{\partial C_A}{\partial t} + v_x \frac{\partial C_A}{\partial x} + v_y \frac{\partial C_A}{\partial y} + v_z \frac{\partial C_A}{\partial z} = D_{AB} \left[\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2} \right] + R_A$$

Since $v_x = v_y = v_z = 0$, $C_A \neq f(x, z)$ and there is no generation in the vapor space this equation becomes.

$$\frac{\partial C_A}{\partial t} = D_{AB} \frac{\partial^2 C_A}{\partial y^2}$$

which shows that the concentration at any point changes with time because of diffusion in the y-direction.

Initial condition: At $t = 0$, $C_A = C_{A, \text{sat}}$ at all y

Boundary conditions: At $y = 0$, $C_A = C_{A, \text{room}}$ at all time

At $y = Y$, $C_A = C_{A, \text{sat}}$ at all time

where Y is the location of front edge of the remaining fog on the mirror. Note however that Y varies with time going from 0 when $t = 0$ to 0.3 m when $t = t_f$.

If an analytical solution of the equation is to be sought this second boundary condition should be respecified. If the

solution is to be numerical, then one merely needs to keep track of $Y(t)$. The end of the calculation is $t = t_f$ when $Y = Y_{\text{max}} = 0.3$ m. $Y(t)$ can be obtained by equating the total amount evaporated to the integrated mass flux into the room neglecting the slight accumulation of water vapor in the enlarging vapor space.

Let M_{A0} be the initial total mass of water condensed, then

$$\text{Amount evaporated} = M_{A0} \frac{Y}{0.3} = M_{A0} \frac{Y}{Y_{\text{max}}}$$

$$\text{Amount transferred to room} = \int_0^t D_{AB} \frac{\partial C_A}{\partial y} \Big|_{y=0} S \, dt$$

where $S = ZX$

$$Y = \frac{Y_{\text{max}}}{M_{A0}} \int_0^t ZX D_{AB} \frac{\partial C_A}{\partial y} \Big|_{y=0} dt$$

$$Y = \frac{XZY_{\text{max}}D_{AB}}{M_{A0}} \int_0^t \frac{\partial C_A}{\partial y} \Big|_{y=0} dt$$

The above is an adequate answer to the exam question. A very simple analytical solution can be obtained as follows. We can say that the flux at $y = Y$ is equal to the amount of moisture evaporated there per unit time. Then the amount of moisture can be related to the rate at which the boundary moves. Thus, if $R =$ thickness of liquid film,

$$D_{AB} \frac{dC_A}{dy} \Big|_{y=Y} = \frac{\text{g H}_2\text{O evap.}}{\text{area} \cdot \text{time}} =$$

$$\frac{\rho_{\text{H}_2\text{O}} ZR}{ZX} \frac{dY}{dt} = \frac{\text{g H}_2\text{O evap/time}}{\text{area of transfer}}$$

$$D_{AB} \frac{dC_A}{dy} \Big|_{y=Y} = \frac{\rho_{\text{H}_2\text{O}} R}{X} \frac{dY}{dt}$$

If we assume that a steady state concentration profile is established rapidly and maintained (shown by dynamic analysis to be an excellent assumption) we get

$$\frac{dC_A}{dy} \Big|_{y=Y} = \frac{C_{A, \text{sat}} - C_{A, \text{room}}}{Y}$$

A further simplification is obtained by taking $C_{A, \text{room}} = 0$.
Let $C_{A, \text{sat}} = C_{AS}$.

$$D_{AB} \frac{C_{AS}}{Y} = \frac{\rho_{H_2O} R}{X} \frac{dY}{dt}$$

$$\int_0^{t_f} \frac{D_{AB} C_{SA} X}{\rho_{H_2O} R} dt = \int_0^{t_f} B dt = \int_0^{Y_{\max}} Y dY$$

$$B t_f = 0.5 Y^2 \Big|_0^{Y_{\max}} = 0.5 Y_{\max}^2$$

and $t_f = 0.5 Y_{\max}^2 / B$

for the mirror fog problem

$$\rho_{H_2O} = 10^6 \text{ g} \cdot \text{m}^{-3}$$

$$R = 1.3 \times 10^{-5} \text{ m (obtained from experiment)}$$

$$D_{AB} = 2.47 \times 10^{-5} \text{ m}^2 \cdot \text{s}^{-1}$$

$$C_{AS} = 17.3 \text{ g} \cdot \text{m}^{-3}$$

$$Y_{\max} = 0.3 \text{ m}$$

$$X = 4 \times 10^{-3} \text{ m}$$

$$t_f = 3.5 \times 10^5 \text{ s} = 96 \text{ m} = 4 \text{ days}$$

This result appears high by about a factor of 4. There are several explanations and we have calculated for different assumptions. Probably the experimental circumstances (e.g. leakage around edges, etc.) do not meet the idealizations of the model. □

IN THE "HEAT" OF THE NIGHT

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YOU ARE SPENDING the evening in a small town on your way home for the holidays. At about 11:00 p.m. the local sheriff calls you and asks for your help. He knows from the desk clerk that you are a chemical engineer, and naturally assumes you have some knowledge of forensic chemistry.

It seems that the body of John Lurie, a local car dealer, had been found somewhat earlier in a wooded area just outside of town. The local coroner had gone fishing and there was no one else to estimate the time of death. John Lurie had been known to deal in "hot" cars and was thought to be going to the police to confess and name his four accomplices, Gus Nusselt, Bill Gurney, Ed Reynolds, and Bob Prandtl. Nusselt had been known to be out of town until 11:00 A.M. that morning, Gurney had a solid alibi from 1:00 p.m. on, Reynolds was with his girlfriend until about

6:00 A.M., when he left to go fishing, and Prandtl was in jail the night before for drunkenness, and was not released until about 8:00 A.M.

When you finally get to the body it is about 12:00 p.m. (midnight). You measure a rectal temperature of 80°F, and an air temperature of 70°F. The air temperature has been about 70°F all day.

Luckily, you brought your Perry's along. Recognizing that the human body is mostly water, 1) calculate the latest possible time the murder could have occurred and 2) state the possible suspect.

NOTE: For practical purposes, John Lurie can be assumed to be shaped like a rectangular slab. He is 10 inches thick from his back to his breastbone. Body temperature is 98.6°F. Rectal temperature is equivalent to core or centerline temperature.

For comparison, a pathology formula sometimes used to estimate the time of death is*

$$\text{No. of hrs. since death} = \frac{98.6 - \text{rectal temperature}}{1.5}$$

ONE-DIMENSIONAL SOLUTION

We will use the Gurney-Lurie charts, Perry's 4th Ed., p. 10-6, 10-7. To calculate the latest time the murder could have occurred, assume maximum rate of cooling, or in other words that the surface of the body is at 70°F (same as saying $h = \infty$ or $m = 0$). We also neglect radiative losses since the body was found in a "heavily wooded" area.

Then, if we assume infinite width and depth,

$$Y = \frac{T_s - T}{T_s - T_o} = \frac{70 - 80}{70 - 98.6} = 0.35$$

From graph, for $n = 0$

$$X = \frac{\alpha t}{(x_1)^2} \cong 0.54$$

$$\alpha = \frac{k}{\rho C_p} = \frac{0.36}{62.4 \times 1.0} = 0.0058 \text{ ft}^2/\text{hr}$$

$$x_1 = \frac{5 \text{ inches}}{12} = 0.42 \text{ ft.}$$

$$t \cong \frac{0.54 \times (0.42)^2}{0.0058} = 16.4 \text{ hours or } 16 \text{ hours, 24 minutes}$$

1) Murder had to occur before 7:40 A.M.

*"Medical Jurisprudence and Toxicology," Glaister and Rentoul, 12th Ed., Livingston Ltd., Edinburgh, 1966, p. 110.

2) Possible Suspects: Gurney, Reynolds

From the pathology formula:

$$\frac{98.6 - 80}{1.5} = 12.4 \text{ hours}$$

(or murder occurred at 12 noon)

This formula, however, takes no account of changes in room temperature, or body thickness, and in fact is known to underpredict the time of death except for the first few hours. From our superior knowledge of heat transfer, we have eliminated Prandtl and Nusselt as suspects. □

ACKNOWLEDGMENT:

Helpful comments were provided by Professor J. H. Hand, University of Michigan.

Editor's Note: Professor Gordon's purpose in his solution to the foregoing problem, "In The Heat of the Night," was to illustrate the use of the Gurney-Lurie charts assuming a simple one-dimensional model. Professor Fogler, CEE Problem Section Editor, asked his student, Alan Basio, to comment on this simplified solution. Mr. Basio's reply follows.

TWO-DIMENSIONAL HEAT TRANSPORT

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It was previously assumed that Lurie, the dead man, is an infinite slab. From this assumption, the time is 16.4 hours since Lurie was killed.

I used Newman's Rule and assumed Lurie is an infinitely long slab with a finite width and depth. Newman's Rule in this situation is the following:

$$Y = Y_x Y_y = \frac{T_s - T}{T_s - T_0} = 0.350 \quad (1)$$

Let Lurie be 10" deep, as previously specified, and 1.3 feet wide. Use the same values as before for Y and α . There are now two values of X to be found on the Gurney-Lurie Charts:

$X_x = \alpha t / (5/12)^2$ and $X_y = \alpha t / (1.35/2)^2$. The time must be the same in both X_x and Y_y , and the product $Y_x Y_y = 0.350$.

Criteria for solution: (1) $Y_x Y_y = 0.35$

$$(2) \frac{X_x(x)}{\alpha} = \frac{X_y(y)}{\alpha} = t$$

Results: By trial and error the times are found

to be within 2.7% of each other.

$$\begin{aligned} Y_x &= 0.420 & Y_y &= 0.833 \\ X_x &= 0.45 & X_y &= 0.18 \\ Y_x Y_y &= (0.42)(0.833) = 0.350 \end{aligned}$$

$$t = \frac{(0.45)(5/12)^2}{0.0058} = 13.47 \text{ hrs.}$$

$$t = \frac{0.18(0.65)^2}{0.0058} = 13.10 \text{ hrs.}$$

$$\frac{13.47 - 13.10}{13.47} \times 100 = 2.7\% \text{ difference}$$

If the width of Lurie is 1.3 ft., he died 13.3 hrs. ago, not 16.4 hrs.

The width of Lurie is important. If Lurie is 2.6 ft. wide, for example, he dies 16.3 hours earlier. In other words, the infinite slab assumption improves when Lurie is assumed over 2.0 feet wide, approaching an answer of $t = 16.4$ hrs. □

BOOK REVIEW: Reactor Design Continued from page 24.

The book is an excellent work. The author has covered a very large area of relatively difficult material in a highly readable fashion and has provided enough detail so that the reader is able to come to grips with the realities of chemical reactor design. It is accurate and relatively complete. There is a considerable amount of specialized knowledge, based upon over 1000 references, augmented by the author's own considerable experience. In many areas, it stands at the edge of chemical reactor design knowledge that is in the public domain. As such it will continue to be a valuable reference work for many years to come.

Its only major shortcoming is insufficient illustrations and a lack of exercises or problems for the student. The fourteen case studies of Volume II serve to illustrate design principles but only cover a fraction of the material in Volume I. In order to serve as a text for a graduate course in chemical reactor design, it would have to be supplemented by problems developed to reinforce specific points and others which would require the student to integrate these ideas into a chemical reactor design. The latter would be an undertaking of the order of a term paper.

These two volumes are a major contribution to the chemical engineering literature. They belong in the library of every chemical engineer who is concerned with research, development, design, or, in many cases, operation of chemical reactors or conversion processes. □

RATE OF REACTION

Continued from page 16.

The evaluate $\nabla \cdot \mathbf{v}$ the continuity equation is used (see ref. 19):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (10)$$

But for this system $\nabla \rho = 0$. Besides $\rho = m/V$ and $\partial m / \partial t = 0$ because the total mass of the system is constant in time. Substituting these relationships into equation (10) and operating:

$$\nabla \cdot \mathbf{v} = \frac{1}{V} \frac{\partial V}{\partial t} \quad (11)$$

Substituting C_i by N_i ($C_i = N_i/V$) and performing the differentiation, the equation for r , in the case of an isothermal variable volume batch reactor, results:

$$r = \frac{dN_i}{a_i V(t) dt} \quad (12)$$

The partial differential is now a total differential insofar as N_i is a function of time only. It must be noticed, however, that we should know the relationship existing between the change of volume and the reaction extent, i.e., if the extent of the reaction is expressed in terms of conversion, there should be at hand a relationship of the following type: $V(t) = V(V_o, x)$. In most gaseous systems a linear variation of volume with conversion is often assumed (9).

STEADY STATE ISOTHERMAL CONTINUOUS PLUG FLOW REACTOR

UNDER STEADY CONDITIONS, general equation (7) is reduced to:

$$\nabla \cdot \mathbf{N}_i = a_i r$$

If, according to the model it is supposed that there are no diffusion or dispersion effects, the mass flux is only due to the global convective flow. Hence:

$$\mathbf{N}_i = C_i \mathbf{v}$$

from where we finally have:

$$r = \frac{d(C_i v_z)}{a_i dz} \quad (13)$$

since in this reactor the flow is uni-directional. (Direction z has been chosen as representative of the model).

If the total number of moles is not preserved and, furthermore, if the reaction takes place in a

gaseous phase, equation (13) is not so useful for v_z will become a function of z and it will not be possible to take it out of the differential. If the number of moles stays constant, equation (13) is reduced to:

$$r = \frac{v_z dC_i}{a_i dz} \quad (14)$$

which, obviously, also includes the assumption that pressure changes along the reactor are small (due to losses by friction, for example) because otherwise v_z would not be independent of z , either.

Equation (13) can be adequately modified to become useful even in those cases in which the number of moles is not constant.

To do so, we simply transform the equation and work in terms of mass fractions (w). Recalling that:

$$C_i = \frac{\rho w_i}{M_i}$$

In this equation w_i is the mass fraction of component i and M_i its molecular weight. Substituting in equation (13):

$$\frac{d}{dz} \left[\frac{\rho w_i}{M_i} v_z \right] = a_i r \quad (15)$$

and since the mass flow rate G_o is constant: $\rho v_z = G_o = \text{constant}$; hence, the rate of reaction can be written as:

$$r = \frac{G_o dw_i}{a_i M_i dz} \quad (16)$$

STEADY STATE, ISOTHERMAL CONTINUOUS FLOW STIRRED TANK REACTOR

The SSICFSTR is an ideal type of system, in which concentration of reactants does not depend upon time or position within the reactor. The mathematical description of the flow within the reactor is exceedingly difficult, as we are dealing with a highly idealized case which, consequently, cannot be fully achieved in practice. Nevertheless, in many cases the deviations are almost negligible and the system has been successfully modelled. The exact mathematical description cannot be accomplished because the model implies a transport of mass, instantaneously, over finite distances.

But the difficulty may be overcome if we do away with the necessity of describing the internal pattern of the flow inside the reactor. To do so, the general equation (7) is integrated over the

**This statement sums up the whole problem:
The rate of reaction expression is the "sink" or "source" term in the
continuity equation for multicomponent systems which will take into account the creation
or destruction of the said species by chemical reaction.**

volume of the reactor so as to obtain a macroscopic balance.

$$\int_V \frac{\partial C_i}{\partial t} dV = - \int_V (\nabla \cdot \mathbf{N}_i) dV + \int_V a_i r dV \quad (17)$$

Under steady state conditions the left-hand side is zero and, as the assumptions of the model grant that all properties within the reactor are constant, r is not a function of the space coordinates and it may be taken out of the integral. With this, the previous equation is reduced to:

$$a_i r V_R = \int_V (\nabla \cdot \mathbf{N}_i) dV \quad (18)$$

Applying the divergence theorem to the right-hand side of equation (18), we obtain:

$$a_i r V_R = \int_A (\mathbf{N}_i \cdot \mathbf{n}) dA \quad (19)$$

The integration performed over the whole surface of the reactor may be evaluated because the flux is non-zero only at the inlets and outlets.

$$\int_A (\mathbf{N}_i \cdot \mathbf{n}) dA = \int_{\text{In.}} (\mathbf{N}_i \cdot \mathbf{n}) dA + \int_{\text{Out.}} (\mathbf{N}_i \cdot \mathbf{n}) dA \quad (20)$$

On the right-hand side, the first term represents the inlet flow of component i and the second one, the outlet flow. Taking into account the directions of unit normal vectors \mathbf{n} , the final equation is:

$$r = \frac{1}{a_i V_R} (F_{i, \text{outlet}} - F_{i, \text{inlet}}) \quad (21)$$

which is the expression usually written for the reaction rate in a continuous stirred tank reactor. The integration of the differential equation (7), so accomplished, brings about a macroscopic balance for species i , which is usually the starting point of the derivations in the books on applied kinetics. In this work we have followed this approach in order to demonstrate the absolute generality of equation (7).

In the following section, this analysis will be extended to two more complex experimental systems, the recycle reactors. These are often

useful for obtaining kinetic data.

APPLICATION TO ISOTHERMAL RECYCLE REACTORS

RECYCLE REACTORS HAVE been widely used since the publication of the original papers by Hougen [20], Perkins and Race [21], Biskis and Smith [22], Korbach and Stewart [23], and Cassano, Matsuura and Smith [24] as a means of retaining the differential operation of the reactor and, at the same time, eliminating the restrictions of inaccuracy in the analysis of the small composition changes.

Moreover, control of the flow rates in the recycle allows the reduction of diffusional resistances and the elimination of temperature gradients. Difficulties may be centered around the effects of reaction by-products, the considerably longer time usually needed to obtain the steady state condition in the recycling section of the apparatus and the difficulty in operating under pre-fixed concentration conditions. (The last two are especially important for the continuous type).

Once more, "general definitions" will be useless and we shall have to resort to the general mass inventory. In order to simplify the matter, let us consider the case when the total number of moles is constant.

ISOTHERMAL CONTINUOUS RECYCLE REACTOR

FIGURE 1 (A) SHOWS the system under consideration. Operating conditions must be adjusted in order to fulfill the following assumptions:

- 1) The operation in V_R is differential, i.e., the outlet concentration $C_{i,f}$ is very close to the inlet concentration of the reactor $C_{i,i}$.
- 2) Differences in concentration between $C_{i,o}$ and $C_{i,f}$ are accurately measured.
- 3) High recycling flow rate (Q).

When $Q \rightarrow \infty$ the whole reactor, analyzed in the control volume (2), is an excellent approximation to a continuous flow stirred tank reactor, working at differential conversions as the reacting mixture goes through the control volume (1). The General equation (7) will be applied to each of these systems.

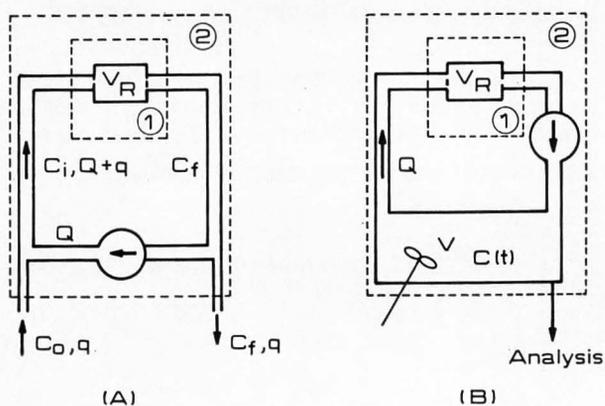


FIGURE 1

Under steady state conditions, the concentration in the reactor is independent of time. The differential equation is reduced to:

$$\nabla \cdot \mathbf{N}_i = r_i a_i \quad (22)$$

On the other hand, the operational characteristics allow us to neglect any form of dispersion or diffusion effects. Consequently:

$$\mathbf{N}_i = C_i \mathbf{v} \quad (23)$$

If the differential equation (22) is integrated over the control volume, the result is:

$$\int_V (\nabla \cdot \mathbf{N}_i) dV = \int_V r_i a_i dV$$

On the left-hand side we shall apply the divergence theorem and on the other side we shall take into account the fact that the reactor is differential. Substituting expression (23) yields:

$$\int_A (\mathbf{n} \cdot C_i \mathbf{v}) dA = r_i a_i \int_V dV$$

and finally:

$$(q + Q) (C_{i,f} - C_{i,i}) = a_i r_i V_R \quad (24)$$

On the other hand, if the whole system (2) is treated as a CFSTR the application of equation (21) will yield:

$$q (C_{i,f} - C_{i,0}) = r_2 a_i V_R \quad (25)$$

In equation (25) we have V_R only on the right-hand side, because it is the only part of the total volume where r is different from zero. But the global velocity r_2 has to be equal to that produced in the reactor itself, that is to say r_1 . If it is shown that r_1 accurately represents a differential rate of

reaction, then the values which may be obtained through the application of equation (25) will portray the exact rate of reaction and not an average value. This will be true if $C_{i,i}$ is very close to $C_{i,f}$ as has been initially assumed. The only remaining doubt would be to know how these conditions could be accomplished. As $r_1 = r_2$, we have:

$$(q + Q) (C_{i,f} - C_{i,i}) = q (C_{i,f} - C_{i,0})$$

$$C_{i,i} = \frac{Q C_{i,f} - q C_{i,0}}{q + Q}$$

If, as was first assumed, Q is sufficiently high, $Q \gg q$ and therefore $C_{i,i} \cong C_{i,f}$.

For isothermal continuous recycle reactors, working under the conditions stated above, an adequate expression for the rate of reaction results:

$$r = \frac{q (C_{i,f} - C_{i,0})}{a_i V_R} \quad (26)$$

Notice that the condition of a high recycling flow, necessary for the differential operation in V_R , coincides with the requirements for the operation of the global system as a continuous stirred tank reactor. The extension to a system with variable number of moles only complicates the algebra.

ISOTHERMAL BATCH RECYCLE REACTOR

FIGURE 1 (B) illustrates the system under consideration. For extremely slow reactions and for cases where one wishes to avoid serious limitations in the size of the samples for analysis, this is an adequate experimental device. Within this system there are no disadvantages such as those pointed out for a continuous recycle reactor, but an experimental problem may arise: the existence of a recycling device (with movable parts in most cases) could introduce contamination of the reacting mixture from the outside. For a batch system, the impurity level will grow with time. This is not so severe in continuous systems.

The operating conditions are as follows:

- 1) The operation in V_R is differential.
- 2) For reasonable intervals of time, concentration differences are accurately measured in V .
- 3) High recirculating flow, and adequate mixing in V .

We treat the whole system as a batch reactor: if the recirculating flow is high, the concentration will be uniform. Hence, $\nabla \cdot \mathbf{N}_i = 0$ and results:

$$\int_V \frac{dC_i}{dt} dV = \int_V a_i r dV$$

Since according to previous assumptions, concentration is not a function of position, the total derivative has been employed and it may be taken out of the volume integral. On the right-hand side, the integral will be different from zero only in those portions of the volume where r is different from zero. Due to the differential performance of V_R , one then obtains:

$$\frac{dC_i}{dt} (V + V_R) = a_i r V_R$$

and the rate of reaction, when there is no variation in the number of moles, is finally:

$$r = \frac{(V + V_R) dC_i}{V_R dt} \quad (27)$$

This equation must be corrected for additional changes of concentration, in case the sample volumes for analysis were significant. A great relationship of V/V_R reduces this problem, but may largely prolong the necessary reaction time to attain accurately measured conversions.

Abalance in the reactor itself shows the conditions for the differential operation of V_R . At each cycle the reactor behaves as a steady state isothermal continuous plug flow reactor.

$$\nabla \cdot \mathbf{N}_i = a_i r$$

$$\int_V (\nabla \cdot \mathbf{N}_i) dV = \int_V a_i r dV$$

Assuming, for the time being, an average value of r , the result will be:

$$Q (C_{i,f} - C_{i,i}) = a_i r_{\text{avg}} V_R$$

where $C_{i,f}$ and $C_{i,i}$ are the outlet and inlet concentrations of reactor V_R at each cycle. If the rate of reaction has a finite value and, as previously assumed, Q is high, the difference between inlet and outlet concentrations will be small. By increasing Q the difference could be made small enough to turn r_{avg} into a differential rate of reaction. Notice that this condition was also assumed as necessary to propose a uniform composition model. It must also be noticed that an adequate experimental device should minimize the volumes of the connecting lines between the reactor V_R and the tank V .

HETEROGENEOUS SYSTEMS OF REACTION

IN THIS WORK WE have emphasized the analysis of the different isothermal homogeneous react-

ing systems. The adequate treatment for heterogeneous reactions (catalyzed and non-catalyzed) is outside its scope.

It is not far-fetched, however, to notice that, in most cases, the flaws of the so-called definitions are even more evident within these systems. The problem may be summarized as follows:

- 1) At the microscopic level all heterogeneous reactions take place at interphases.
- 2) Even at the macroscopic level, many heterogeneous reactions take place at interphases.
- 3) In many cases the rate of reaction takes place not only inside the control volume but on its boundaries as well.
- 4) Hence, accurately speaking, the rate of reaction will, in many cases, be a boundary condition of the general mass conservation equation.
- 5) When this happens at the microscopic level (in the case of a catalyst, for example), an "effective" rate has been used due to the difficulty in solving the conservation equations with complicated geometries for the boundary conditions.
- 6) At the macroscopic level (for example, the case of free radical termination reactions on the walls of a reactor) when the rates of reaction are boundary conditions, the conservation equations are complicated, since diffusional terms cannot be neglected. See for example reference [25].
- 7) Even ontologically, the rates of reaction in heterogeneous systems undergo a change, insofar as their intensive character is attained by means of an expression referring to the area of this boundary (real or ideal).

All this makes even more evident the futility of trying to establish a general "definition" of a reaction rate.

CONCLUSIONS

IN THE PREVIOUS sections, six different expressions have been attained for the rate of reaction: equations (8), (12), (21), (26) and (27). Many others could be found for other physical systems using equation (7) as a starting point. Quoting Petersen [16]: "to argue that any of these (rate of reaction expressions) is more correct than all of the others as its defining equation, is to confuse a conservation equation with a definition." This statement sums up the whole problem. *The rate of reaction expression is the "sink" or "source" term in the continuity equation for multicomponent systems which will take into account the creation or destruction of the said species by chemical reaction.*

The rates of reaction thus attained will be independent of the system used to measure them (provided it is a homogeneous reaction). This means that the kinetic expression of the rate of

reaction $r = \phi(T, C_i, P, \text{etc.} \dots)$, if determined using equation (7) as a starting point, will be independent of the physical device employed to obtain the kinetic data.

There may exist a sound definition of an extensive rate of reaction based on the concept of the "extent of reaction," both introduced by De Donder [26], which may be useful for thermodynamic calculations but the idea becomes devoid of general validity when one needs an intensive property. For the purposes of reaction engineering this is legitimate but it is of little help.

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NOMENCLATURE

A	: Area (cm^2)
a	: Stoichiometric coefficient
C	: Concentration ($\text{mole}\cdot\text{cm}^{-3}$)
F	: Molar flow rate ($\text{mole}\cdot\text{s}^{-1}$)
G_o	: Mass flow rate per unit area ($\text{gr}\cdot\text{s}^{-1}\cdot\text{cm}^{-2}$)
M	: Molecular weight ($\text{gr}\cdot\text{mole}^{-1}$)
m	: Mass (gr)
N	: Number of moles
\bar{N}	: Molar flux ($\text{mole}\cdot\text{cm}^{-2}\cdot\text{s}^{-1}$)
\mathbf{n}	: Outwardly directed unit normal vector
P	: Pressure ($\text{Kgf}\cdot\text{cm}^{-2}$)
Q	: Volumetric recycle flow rate ($\text{cm}^3\cdot\text{s}^{-1}$)
q	: Volumetric input flow rate ($\text{cm}^3\cdot\text{s}^{-1}$)
r	: Rate of reaction (intensive) ($\text{mole}\cdot\text{cm}^{-3}\cdot\text{s}^{-1}$)
T	: Temperature ($^{\circ}\text{K}$)
t	: Time (s)
V	: Volume (cm^3)
v	: Linear velocity ($\text{cm}\cdot\text{s}^{-1}$)
V_R	: Volume of reactor (cm^3)
w	: Mass fraction
x	: Conversion
ρ	: Density ($\text{gr}\cdot\text{cm}^{-3}$)
ϕ	: Kinetic expression for rate of reaction ($\text{mole}\cdot\text{cm}^{-3}\cdot\text{s}^{-1}$)
∇	: Vector operator

Subindices and Supraindexes

avg	: Average value
i	: Indicates species or initial condition, according to context
f	: Final condition
o	: Inlet condition
R	: Indicates reactor
z	: Indicates direction
-	: Indicates vector
*	: Indicates molar average velocity

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