

CEE

chemical engineering education

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NUMBER 1

WINTER 1983



CHEMICAL ENGINEERING DIVISION OF AMERICAN SOCIETY FOR ENGINEERING EDUCATION

• *Special Feature* •

*R. W. Wilhelm's Influence on the
Development of Chemical Reaction Engineering*
ARIS

J. M. SMITH
OF U. C. DAVIS

and...

INTEGRATING CHEMISTRY, ENGINEERING
Schrader, Pigford, Gates

PROCESS CONTROL UNDERGRAD OPTION
Hassler, Mumme'

SURVEY: COMPUTER USAGE IN DESIGN COURSES
Henley

SOLAR HOT WATER HEATING BY NATURAL CONVECTION
Noble

DIRECT DIGITAL CONTROL LIQUID LEVEL EXPERIMENT
Adb-El-Bary

TUTCHE - A PROGRAM PACKAGE FOR TUTORING CHEMICAL ENGINEERS
Stainthorp, Lomas, Alonso

also...

CHE AT CLEMSON



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Aerial photo of Clemson campus.

ChE department

CHE AT CLEMSON

J. M. HAILE AND D. D. EDIE
Clemson University
Clemson, SC 29631

CLEMSON UNIVERSITY, THE LAND-GRANT institution for the State of South Carolina, is the realization of a long-held dream of its founder—Thomas Green Clemson. Clemson was born in Philadelphia in 1807 and, although the events of his childhood are obscure, it is certain that during his mid-teens Clemson acquired a lifelong interest in science in general and chemistry in particular. By 1826 Clemson was in Paris where he audited lectures of Thénard, Gay-Lussac and DuLong at the Sorbonne, studied in the laboratory of Robiquet, and attended the Royal School of Mines. In 1831 Clemson received an assayer's certificate from the Royal Mint and during the years 1831-39 he developed a profitable business as a consulting and mining engineer in Paris, Philadelphia, and Washington.

While in Washington in 1838 Clemson met Anna Maria Calhoun, the daughter of the South Carolina statesman, John C. Calhoun. By this time

Clemson was a successful engineer and businessman, a world traveler, a linguist and conversationalist, a man interested in science and politics though himself neither scientist nor politician, and one whose hobbies included painting in oils and music-making on the violin. The Calhoun-Clemson marriage took place in November 1838 and subsequently Clemson assumed the management of the Calhoun plantation, Fort Hill, located in the northwest corner of South Carolina. Impressed by the value of proper training for those who farm, Clemson began to consider ways of applying scientific knowledge to agriculture. From 1844 until 1851 Clemson served as chargé d'affaires to Belgium and he took the opportunity of those years in Europe to broaden his study of agriculture.

In 1852 the Clemsons bought a small farm in Prince Georges County, Maryland, where Clemson began testing his ideas on scientific methods of agriculture. He wrote and published extensively on agricultural chemistry; he promoted the establishment of the Maryland Agricultural College (later a part of the University of Maryland); he actively supported passage of the Morrill Act for

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Land-Grant Colleges; he gave, at the Smithsonian Institution, a series of lectures entitled "Chemistry Applied to Agriculture." Following his appointment in 1860 as U.S. Superintendent of Agricultural Affairs, Clemson began developing plans to create a U.S. Department of Agriculture. Those plans and his position as Superintendent had to be abandoned when war broke out in 1861.

In 1866, with both John C. Calhoun and his wife dead, the Fort Hill plantation became the object of legal entanglements that were resolved by holding a public sale. Clemson bought the plantation at that time. Over the last decade of his life Clemson's principal interest was establishing an agricultural college on the Fort Hill plantation. Clemson died in 1888, leaving Fort Hill's 814 acres to the State under the provision that the land become the site of the Clemson Agricultural College of South Carolina. The South Carolina legislature ratified an Act of Acceptance of Clemson's will on December 24, 1888.

DEVELOPMENT OF CLEMSON UNIVERSITY

Construction of college buildings on the Fort Hill plantation was begun in 1890 and in July 1893 the college opened its doors to its first class—446 students. From its inception until 1954, the student body was all male and organized as a corps of cadets.

In the early 1930's the college benefited from the land resettlement policy of Roosevelt's New Deal: the government purchased some 27,469 acres within a ten mile radius of Fort Hill and assigned Clemson College the responsibility of overseeing its revitalization. The entire acreage was deeded to the college in 1954 and the land now serves as an extensive laboratory for the colleges of Agriculture and Forest Resources.

In 1964 the name of the college was formally changed to Clemson University. Today, the university is composed of a graduate school and nine colleges: Agriculture, Architecture, Education, Engineering, Forest and Recreation Resources, Liberal Arts, Nursing, Sciences, and Commerce and Industry. From circa 1970 the university administration has limited total enrollment to about 10,500 students. The university library is housed in an attractive modern building and its holdings number well over one million items, including bound volumes, microfilm, and microfiche. The university computer is an IBM 370/3033 supported by a complete selection of peripheral devices. In addition, the College of Engineering has purchased

two DEC VAX computers: one dedicated to computer graphics, the other to "number crunching" research problems.

No description of Clemson University would be complete without mention of intercollegiate sports. Because of fanatical alumni loyalty and a well-organized athletic fund-raising machine, Clemson has been able to sustain national prominence in several minor sports, especially soccer, baseball, and tennis. As our obligatory comment on football, we note that the legendary John Heisman coached at Clemson from 1900 to 1903 and during that period led the team to its first undefeated season.

DEVELOPMENT OF CHE AT CLEMSON

Chemical engineering was first introduced as a course of study at Clemson in 1917. There was no chemical engineering department or any faculty; the curriculum was drawn from courses in mathematics, physics, chemistry, mechanical engineering, etc. The university catalog for 1920 is the first to show any enrollment in this curriculum—seven students. In the spring of 1923 four of these were the first chemical engineering graduates from Clemson; the attrition rate has changed little since that first class.

The chemical engineering curriculum does not appear in the University Catalogs for the years 1923-1933 but was reintroduced in expanded form

Undergraduate chemical engineering students achieve a high degree of camaraderie and identify strongly with the department, both as students and later as alumni. Much of this is due to an extremely active student chapter of the AIChE.

in 1933 again with no department, courses, or faculty of its own. The catalog attempts to entice students into the curriculum with the following words:

Competition is compelling the industries to abandon rule-of-thumb methods. They are using more and more men trained in the principles of Chemical Engineering—to design their plants and to supervise the operations of various processes.

In 1934 there were 27 students in chemical engineering and the number grew steadily to 81 by 1939. In the 1939 catalog the curriculum no longer appears under the supervision of Engineering but pops up in the Chemistry Department under a

new name, "Chemistry-Engineering," which persevered until 1946.

The 1946 catalog lists the curriculum back under the supervision of Engineering and, for the first time, includes a separate Department of Chemical Engineering with its own courses. The catalog of 1947 indicates two faculty members in the fledgling department: C. E. Stoops, Jr., Professor and Head, and C. E. (Charlie) Littlejohn, Assistant Professor.

In the 1948 catalog Professor Stoops does not appear; rather, the Department Head is listed as Allan Berne-Allen, who remained as Head until 1955. The year 1955 marked something of a turning point in the development of the department: Charlie Littlejohn was the sole faculty member and, hence, Head of the department. The catalog lists sixteen chemical engineering courses, of which eleven were required, and the enrollment stood at 125. It is intriguing to try to imagine Charlie Littlejohn meeting all those courses



Earle Hall, home of the Chemical Engineering Department.

and grading all those papers. In fact, however, Dr. Littlejohn had teaching help from a professor in agriculture who had a Bachelor's degree in chemical engineering.

In January 1956 George Meenaghan joined the faculty and enrollment was 156. In 1958 Chris Alley and Bill Barlage brought the department's faculty complement to four and enrollment had climbed to 184. In 1958 Clemson received a grant of \$1.175 million from the Olin Foundation for construction of a building and purchase of equipment for chemical engineering. Construction was begun in September 1958 and Earle Hall was dedicated at the end of 1959. (Samuel B. Earle was Dean of Engineering from 1933 to 1950 and acting President of Clemson in 1918 and again in 1924-25.) Earle Hall is a 50,000 square-foot facility containing five classrooms, eleven faculty offices, a library, an auditorium, a student

lounge, a seminar room, shop, eight general purpose laboratories, thirteen two-man research laboratories, and a three-level 9,000 square-foot unit operations laboratory. The UO Lab was laid out and equipped under Charlie Littlejohn's direction and has served as a model for similar labs at several other universities. The undergraduate chemical engineering curriculum was first accredited by the Southern Association of the Engineer's Council for Professional Development (ECPD) in 1959.

In 1960 a Master of Science program in chemical engineering was started and in 1962 the PhD program was added. The first PhD in engineering in South Carolina was awarded in 1965 to Jerry A. Caskey, a student under Bill Barlage. Today Dr. Caskey is a member of the Faculty at Rose-Hulman Institute of Technology. Other PhD graduates who are now following academic careers include: Dick Stewart, 1966 (Northeastern); Dan Reneau, 1966 (Louisiana Tech); Dendy Sloan, 1974 (Colorado School of Mines); Gary Mock, 1976 (North Carolina State); Eric Snider, 1978 (Tulsa); David Cooper, 1980 (Central Florida).

In May 1975 Charlie Littlejohn died of cancer. He had taught chemical engineering at Clemson since the founding of the department and had served as Head since 1956. It was his strong personality that molded the attitudes and aspirations of the department—both faculty and students. His philosophy was simple: the department at Clemson exists to provide training in chemical engineering for undergraduates who will follow industrial careers. Charlie was an excellent teacher, that rare individual who inspires diligence, respect, professionalism, and affection in his students. On his death, alumni spontaneously created the C. E. Littlejohn Scholarship Fund to provide support for the education of highly qualified undergraduates in chemical engineering. Industrial gifts were also forthcoming to refurbish a room in Earle Hall as the C. E. Littlejohn Memorial Student Lounge. Since 1975 W. B. (Bill) Barlage, Jr. has served as Head of the department.

CHE AT CLEMSON TODAY

In 1981 the department was composed of 168 freshmen, 89 sophomores, 78 juniors, 90 seniors, 22 graduate students, and a dozen faculty. Freshmen enrollment in the department has increased steadily from 32 in 1972. (The department does teach a course to second semester freshmen.)

Equally dramatic has been the increasing coed enrollment: in the fall of 1981, 30% of the incoming class was female.

The undergraduate curriculum is a strong traditional program requiring 144 semester hours for graduation. Thirty-eight of these are taught in the department. Required courses include stoichiometry, numerical methods, kinetics, process design, process control, transport phenomena, two semesters of thermodynamics, and three semesters of unit operations theory. Communication skills are emphasized in two semesters of unit operations laboratory, a FORTRAN programming course, senior seminar, and junior plant-inspection trips. Furthermore, selected juniors and seniors are invited to join in work on research problems in collaboration with graduate students and faculty.

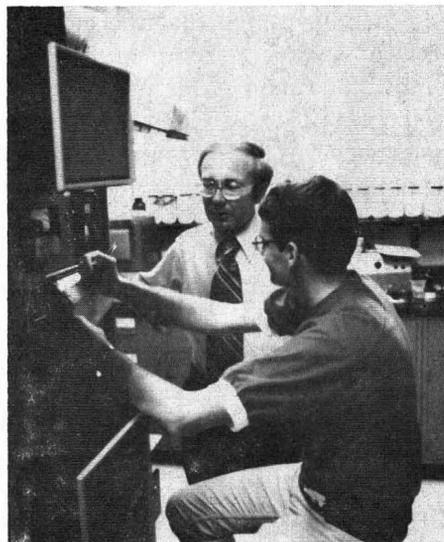
About six years ago an undergraduate cooperative education program was instituted. Under the nurture of Joe Mullins, the department's co-op program has been the most successful of any on campus and co-op students formed one-third of the chemical engineering class of 1981.

Undergraduate chemical engineering students achieve a high degree of camaraderie and identify strongly with the department, both as students and later as alumni. Much of this is due to an extremely active student chapter of the AIChE. Each fall the chapter sponsors a shrimp boil to welcome new and returning students; each spring a pig roast is held to send off the graduating class. During the academic year the chapter holds monthly meetings at which invited speakers present talks on a variety of technical, business, or popular topics. In addition, the chapter holds informal drop-ins throughout the year, organizes tutoring services, sponsors a float in the fall football parade, and makes sporadic trips into the mountains or down the Chatooga River. The chapter has received the Regional Outstanding Student Chapter Award in five of the previous seven years and has been recognized by the national AIChE as an Outstanding Student Chapter in each of the last eight consecutive years.

At the graduate level, the department offers MS and PhD programs to full-time students and a Master of Engineering (ME) program to part-time students. The MS degree requires 24 hours of graduate coursework plus a thesis written on a research project; the ME degree requires 30 hours of coursework plus satisfactory completion of an advanced engineering design problem. In recent years the graduate enrollment has averaged

about twenty students, of which about 20% have been tramontane.

In 1981 two new programs were started with the goal of bolstering graduate student enrollments. One of these is a type of graduate co-op program called the Industrial Residency Program. This program terminates with an MS and functions as follows: On graduation with a BS in chemical engineering in the spring, the new graduate resident selects the company and project upon which he intends to work. The selection is made from projects that participating companies have previously submitted to the department. The student is then assigned a faculty advisor from the department and a project advisor from the company. The student spends the first summer at the company becoming familiar with the project. In the fall the student returns to Clemson and takes two consecutive semesters of graduate courses, completing the 24 semester hour course requirement. The second summer the student returns to the company and works full-time for about seven months completing the research project and writing the thesis. The student is paid by the company at a BS-level rate for the months he is actually working at



Professor Dan Edie with student and INSTRON Rheometer.

the plant. Typically, the salary is prorated over the nominal nineteen months needed to complete the program.

The second new graduate program is an Industrial Fellowship Program in which exceptionally promising students are awarded generous,

Continued on page 48.

J. M. Smith *of U. C. Davis*

N. MCGUINNESS
University of California, Davis
Davis, CA 95616

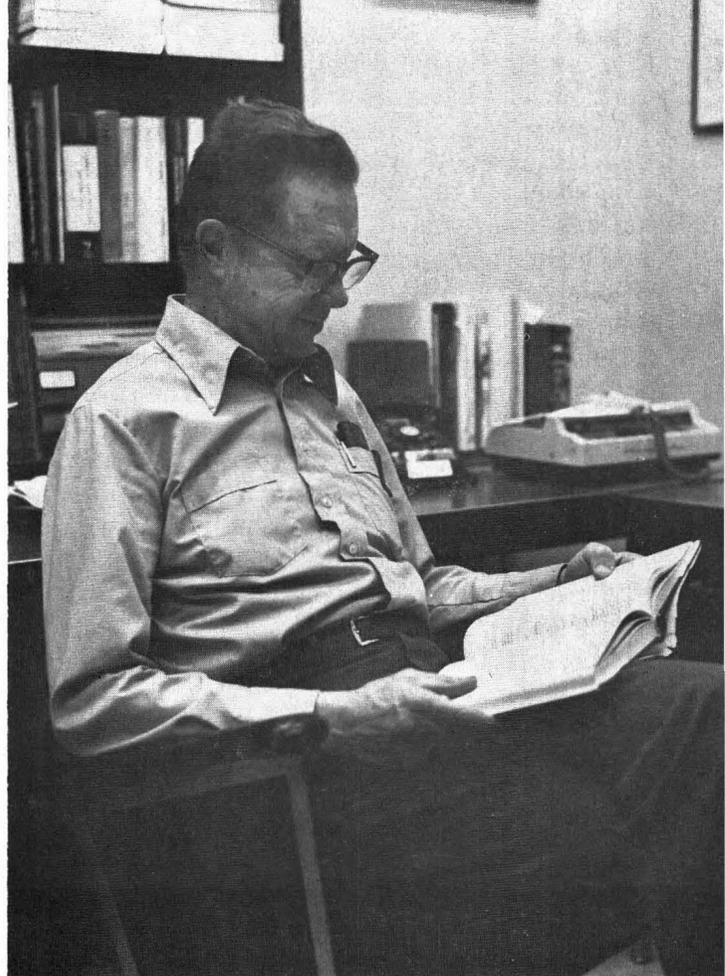
JOE MAUK SMITH is known at the University of California, Davis, as "Mr. Chemical Engineering". As founding Chair of the Chemical Engineering Department and its tireless protector in its fledgling years, he became so closely identified with his department in the minds of his Academic Senate colleagues across campus that they see him largely as its guardian. His colleagues within the profession give Joe the same appellation, but for a different reason: for his prominence in his field.

As a member of the National Academy of Engineering, J. M. Smith has been accepted by his peers as one of a very select group of engineers. As winner of the Richard H. Wilhelm Award of the American Institute of Chemical Engineers in 1977, he was recognized for "advancing the frontiers of chemical reaction engineering with emphasis on originality, creativity, and novelty of concept and application." He was named to the AIChE Wm. H. Walker Award in 1960. In addition to awards from the American Chemical Society, American Society for Engineering Education, and the Guggenheim Foundation, he has been recognized by the entire faculty of his campus, being named to the highest Academic Senate honor, Faculty Research Lecturer, in 1970.

The present Department Chair, Ben McCoy, describes J. M. Smith's contributions in this way:

"Dr. Smith makes it a point to get to know students by name. He attends student functions whenever possible and was a regular fan at the Senior class intramural softball games."

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"Joe has made substantial contributions to the areas of kinetics, reactor analysis, mass transfer, and thermodynamics with both experimental and analytical methods. His career work has resulted in over 260 publications. One most influential paper—N. Wakao and J. M. Smith, "Diffusion in Catalyst Pellets", *Chem. Eng. Sci.* 17, 825 (1962)—was recently identified and honored as one of the most cited in its field. Joe Smith has made major contributions in chromatographic systems. He has pioneered in applying moment methods to the analysis of dynamic response experiments. Adsorption, intraparticle diffusion, dispersion, channeling, chemical reaction, and regeneration are some of the phenomena examined, clarified, and quantified. Whereas in pulse response experiments his students once picked data points off recorder chart paper for subsequent numerical integrations, they now punch buttons on computers to get the temporal moments."

Recently Joe and his coworkers have been focusing their attention on trickle-bed reactors. These three-phase systems with gas and liquid flowing over catalytic particles pose interesting challenges with combined fluid mechanics, mass transfer, and chemical reaction phenomena. Current interests also include thermodynamics and

kinetics of supercritical extraction of oil shale and tar sands. As is much of his research, Joe's studies in these areas were motivated by practical questions arising in industrial processes.

Joe's work has gained recognition through his major textbooks, his journal publications, and the prominence of his former students, now dispersed throughout the international chemical engineering community. Professor McCoy reports: "Joe Smith publishes at least eight papers each year, in the most widely read research chemical engineering journals. Nearly all of these have as co-authors graduate students or post-doctoral scholars who go on to responsible positions in corporations and universities around the world. Most of these research associates come to U.C. Davis specifically to study with Joe." Not only have graduate students and postdoctoral students come to Davis to work with him, he has also gone on Fulbright appointments to the Netherlands (1953), Argentina (1963), Spain (1965), Ecuador (1970), and Chile (1970). His two textbooks have influenced a generation of chemical engineers around the world. *Introduction to Chemical Engineering Thermodynamics*, coauthored with Hank Van Ness of Rensselaer, was published in 1949. *Chemical Engineering Kinetics* first appeared in 1956. Both texts are in the McGraw-Hill Chemical Engineering Series, and both are now in their third editions. The texts are filled with problems of practical interest, reflecting Joe's wide-ranging experience in industrial consulting.

His former and current students bear eloquent witness to his teaching effectiveness. Bob Reid of M.I.T. says this of his former professor (CEE 9, 106 (1975)): "Joe really turned me on; he was the first teacher who gave me problems I couldn't solve. As a matter of fact, I'm still using some of them. I had never met a professor who wanted to know you as an individual. If I were working in the lab late at night, he'd stop in, put his feet up on the desk, and talk with me, not necessarily about my thesis, but about almost anything."

Former student Ray Fahien of the University of Florida says, "It is apparent from his numerous papers and several widely adopted books that Joe Smith is a scholar of international stature. But what is not apparent is that he is also a warm, sensitive person who thoroughly enjoys the company of others—as well as a charismatic leader who knows how to motivate people. He does this by imparting a sense of purpose or mission to

every activity in which he is engaged. For example, in his lectures Joe would begin by asking the question: 'Why are we, as chemical engineers, interested in this topic?' In his discussions with beginning graduate students, he would always emphasize the project's importance in science or engineering. His books also first make clear the relevance of each chapter or section before going into the theory.

"Joe also motivates his students by being profuse in his praise for work well done, but sparing in his negative criticism. Even before Skinner became a popular name in engineering education, Joe recognized the motivating effects of positive reinforcement."

Joe's work has gained recognition through his major textbooks, his journal publications, and the prominence of his former students, now dispersed throughout the international chemical engineering community.

Each year Joe Smith has taught an average of five courses, both graduate and undergraduate, at U.C. Davis. The custom at Davis is to divide the sections of senior chemical engineering laboratory among the faculty. Exercising his usual initiative, curiosity, and innovation, Joe recently devised a new chemical reaction kinetics experiment for the course. In addition to supervising a number of research graduate students and post-doctoral scholars, Joe advises his share of chemical engineering undergraduates.

Students applaud Professor Smith's teaching style, which they characterize as organized and thorough, with lectures clearly and enthusiastically presented. Joe frequently applies the Socratic method in the classroom; all agree the method encourages preparation.

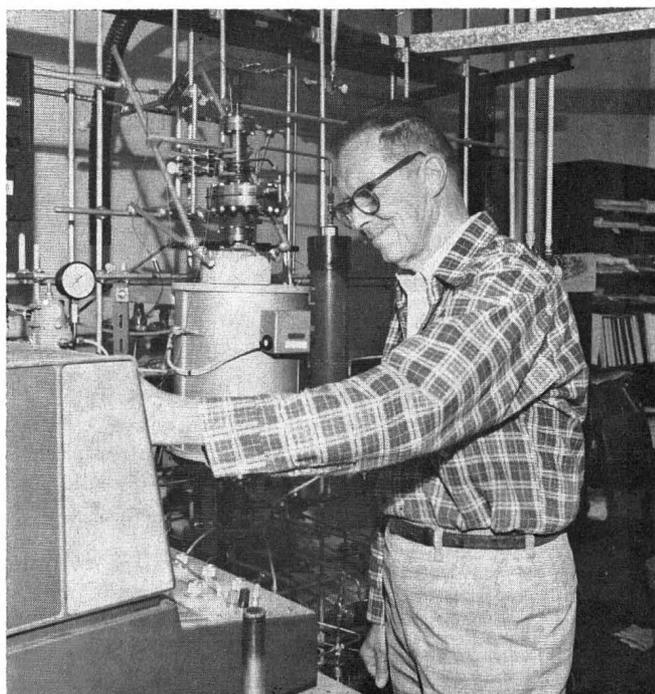
One of Smith's recent undergraduate students, Anne McGuinness of the Class of '82, gave this view of Joe as a lecturer, lab instructor, and mentor: "Any overview of his accomplishments cannot neglect his ability as a teacher. Dr. Smith received the AIChE Outstanding Teacher Award from the Davis chapter in 1982, his 21st year of teaching here. Dr. Smith begins his lectures with a short review of homework, emphasizing the important aspects of the problems. When introducing new material he calls on students in class to answer questions, insuring that the class is following the development of his presentation. He

is always willing to stop his lecture to answer questions and uses them to clarify his points.

"In laboratory courses, Dr. Smith has students review their proposed experiments with him prior to lab sessions. He uses these sessions to ask questions and stimulate the students to look at other possible aspects of the experiment.

"Dr. Smith makes it a point to get to know students by name. He attends student functions whenever possible and was a regular fan at the Senior class intramural softball games."

Speaking of his methods of guiding students in research Joe recently said: "As the years go



Joe examines output data from reactor for super critical extraction of oil shale.

by it becomes ever more clear to me that there are many effective ways to collaborate with students in chemical engineering research. The most effective approach for one professor may not be suitable for another. Hence, the following comments represent simply a single procedure which has been useful for me. For research which is at least in part experimental it is helpful to visit students in the laboratory each day. Perhaps there seems little to discuss, but, from a general conversation about the problem and apparatus, new ideas and new approaches usually emerge. During these discussions it may be helpful to present unanswered technical questions to the student. Also it is stimulating to offer challenges in the direction and extent of the research that are per-

haps a bit beyond reasonable expectations in the time available. On the other hand, students seem to be discouraged if a thesis problem is not clearly defined beforehand, but is left open-ended. Of course research cannot be described in detail in advance, but the impression can be given to the student that diligent application to a particular phase of a research project should result in a thesis in a reasonable amount of time.

"Formal, weekly meetings, for which the student must summarize prior work and plan for future studies, have merit. When there are data to analyze, such weekly meetings might last several hours. During routine aspects of the project, the meetings may last but a few minutes. Nevertheless, the idea of having a weekly meeting where the students will have time to talk to the faculty member at length, and must summarize their thoughts, seems to be helpful. Also, in working with graduate students it is often valuable to have the students write down in a clear fashion their progress during a previous period and their plans for future work. The act of putting thoughts and results on paper requires clear thinking about the project."

The care for and attention to students, the constant "offering of challenges", and the insistence on clarity in expression of these remarks characterizes Joe Smith's teaching methods. He claims to have learned some of these from his own teachers and colleagues.

"I was first introduced to chemical engineering in a most fortunate way with William N. Lacey teaching a course to two students using the classical book authored by Walker, Lewis, and McAdams. During that period at the California Institute of Technology with the small number of chemical engineering students, all chemical engineering courses were taught by William Lacey and Bruce Sage. These men were specialists in thermodynamics and I was fortunate enough to be able to take, while employed by Chevron Research, a graduate course in thermodynamics with Bruce Sage. These professors taught me some of the elegance and precision involved in thermodynamic thinking and also introduced me to the fascinating area of the interaction of chemical and physical processes which constitutes the essence of chemical engineering."

Of Dr. Lacey's continuing influence Smith goes on to say: "Dr. Lacey, along with Walter Dayhuff of Chevron Research, was instrumental in teaching me how to write clearly. Dr. Lacey

was kind enough to review a chapter in my first attempts to write a text on chemical engineering thermodynamics. He found 37 split infinitives which he brought to my attention in a gracious way. Ever since a split infinitive has, figuratively, jumped off the page at me."

He was equally "fortunate" in his professors at MIT where, he says, "my interest in thermodynamics was further enlarged by the experience of taking graduate-level courses with Harold Weber. The contrast in approach to the laws and applications of thermodynamics from these two institutions was, at first, perplexing and confusing. With the passage of time, the strong points of the methodical, careful approach at Cal Tech and the thought-provoking, more applied methods at MIT provided a more complete and satisfying understanding of the subject.

"Thesis work with W.K. Lewis was an inspiration. One of the most lasting benefits of this association was learning the importance of being able to generate new ideas about chemical engineering problems. Dr. Lewis was an inspiring innovator and his students could not help but see the beauty and advantages of innovative approaches to difficult problems. Dr. Lewis had no patience with inferior work and transferred this characteristic to his co-workers." The same might be said by the students of Dr. Smith.

Joe Smith's influence on students is not limited, however, to those he individually reached in lecture rooms or labs. Not only is he "the man who wrote the book", he is also one of "the men who built the College at UC Davis".

Roy Bainer, Dean Emeritus of the College of Engineering at UC Davis, describes Joe's herculean efforts in these early years. "Hired as a chemical engineer in the Department of Food Science and Technology, Smith was a member of the UC Davis faculty when the possibility of the College was being considered. Local committees were appointed to develop curricula in the main disciplines, utilizing the engineering talent at Davis. For example, Dr. Smith of Food Science and Technology was asked to chair a Committee for Chemical Engineering." When the local committee's report was accepted, chemical engineering was approved as part of the College of Engineering, not, as at Berkeley, as part of the School of Chemistry. To continue with Dr. Bainer's account: "This meant that Dr. Smith could serve as first chairman of chemical engineering at Davis and could become involved in hiring new faculty



Essie and Joe Smith enjoying a departmental social function.

and the planning of the new building. . . The current enrollment in engineering at Davis reached 1900 students twenty years after the Regents' establishment of the College. Much of the credit for success must go to the many contributions of Dr. Smith".

Not only the College benefited from Joe Smith's talents as an administrator. The chemical engineering department owes its existence to his persuasive advocacy. After discussing the struggle to establish a separate department ("It became clear that if chemical engineering were to develop as a recognized discipline at Davis a separate department was necessary"), Joe describes the continuing struggle, familiar to chemical engineering educators everywhere, the need for which he attributes "to a lack of understanding of the essence of chemical engineering": "After the establishment of the department our worries about developing a strong program were not completely eliminated. It seemed a continual struggle during the late sixties to justify inclusion of sufficient credits in chemistry and separate courses in thermodynamics and fluid mechanics, distinct from the existing courses in these subjects taken by all other students in the College of Engineering."

Professor Smith worked equally hard on campus recruiting for his department. Contributing to the struggles on behalf of the department in those early days were Steve Whitaker and Dick Bell, who joined it in 1964 and 1965, respectively; Ben McCoy and Alan Jackman, both alumni of Minnesota, arrived in 1967 and 1970; Ruben Carbonell and Dave Ollis, both with backgrounds at Princeton University, joined the department

Continued on page 47.

R. H. WILHELM'S INFLUENCE ON THE DEVELOPMENT

RUTHERFORD ARIS

*University of Minnesota
Minneapolis, MN 55455*

WE ARE TOLD ON THE highest authority that "no prophet is accepted in his own country". That may well be, for the charge of the prophet is usually an uncomfortable message aimed at the conscience rather than the intellect. Scholars fare rather better. Their message is to the mind with its rational and aesthetic sensibilities and very happy it is when a man's work receives that quiet, but coveted, comment that it is "true scholarship". It is therefore a pleasure to recall that Princeton did not fail to recognize one of its most distinguished professors,* and that the profession at large will forever keep his name in verdant memory through the Wilhelm Award, designed to recognize significant and new contributions in the field to which Wilhelm contributed so much.

Twelve years and more have passed since his death and it seems not inappropriate to take this opportunity to consider the nature of his contri-

*He was appointed the Henry Putnam University Professor in 1968.



After a few years in chemical industry and a brief spell teaching mathematics at the University of Edinburgh, Aris came to the University of Minnesota in 1958 and has been in its Department of ChE ever since. He particularly appreciates the lively intellectual atmosphere of the department and the excellent quality of students that it serves and has endeavored to make some contribution to its good repute. His research has centered on the mathematical models of chemical engineering, particularly those of chemical reactors. He is currently Regents' Professor of ChE at the University of Minnesota.

bution to the subject of chemical reaction engineering. It would be impertinent for me to add many personal reflections, for I knew him far less well than many. But if I may be permitted to be personal for a moment, I can illustrate how his papers influenced at least one of the lesser mortals who have climbed on his shoulders. I was in the employ of Imperial Chemical Industries in a Physical Chemistry Research Department when I was taken off work on the theory of chromatography, in which I was just beginning to find some interest, and was ordered to "get up" reactor design. In those days basic design of their converters was in the hands of mathematicians (mathematicians were called mathematical physicists and lumped with physical chemists) and stalwarts like F. F. Snowdon in a so called Technical Department. My predecessor, Dorothy Annable, had had notable success in using Temkin's expression for ammonia synthesis. In trying to learn what reactors were, it was Wilhelm's papers to which I turned and that I found the most enlightening. These included his 1943 paper on "Conduction, Convection and Heat Release in Catalytic Converters" and his review of "Rate Processes and their Application to Reactor Design" (1949c). His paper on the measurement of diffusion in beds of solids by a frequency response technique (1953a) linked with one of the approaches that I had used in connection with the theory of chromatography. It is therefore to Wilhelm in large measure and after him to Hougen and Watson, that I own an introduction to chemical reactor design. To analytic understanding of reactors it was the work of Amundson that later provided the great illumination. (I cannot leave this personal intrusion without acknowledging my further indebtedness to Wilhelm. In 1955 I was fortunate enough to catch his attention with some early work on optimal design and it was his good offices that obtained for me my first research grant—from the Research Corporation, to whom he was an advisor. I am sure that I am far from being alone among those whose

OF CHEMICAL REACTION ENGINEERING

from the Wilhelm Lectures at Princeton

early efforts have been encouraged in this typically self-effacing way by a truly great scholar.)

THE RANGE OF WILHELM'S WORK

In trying to discern the current of Wilhelm's thoughts on the great questions of chemical engineering, it will be useful first to discover the main lines of his work. I will consider only those publications that have to do with reaction, leaving aside some very interesting but marginally relevant matters that he took up in other papers. Thus, I will not refer to his work on fluid flow and viscometry in 1939 or on the rate of solution in 1941, some questions of textile drying in the late 40's or of parametric pumping in his last years. Of these miscellaneous topics his discussion of flames is really the only one close to our subject.

In a certain sense all Wilhelm's work served the general problem of the design of reactors on an *a priori* or scientific basis. Specifically there is a series of general, or review, papers* (1949c, 1950, 1951a, 1953b,c, 1954) that lead up to the general survey of 1962. On more specialist topics, we note two papers on the tubular reactor, the first (1950e) a kinetic determination, and the second (1956d) a discussion of the effect of a viscous profile on the conversion. In dealing with packed beds he quickly recognized the importance of the interaction of physical and chemical factors and there is a whole series of papers concerned with questions of longitudinal dispersion (1953a, 1956a, 1957c), of heat and mass transfer (1943, 1950d, 1959, 1963b) and of the measurements of fluctuations of concentration (1957a, 1960, 1963a). He took an early and continued interest in fluidized beds (1948c, 1949a, 1950f, 1951b, 1952, 1956b, 1958b), and a somewhat lesser interest in stirred vessels, though he discussed the fluctuations in the stirred vessel (1963a) and was concerned with the mass transfer of oxygen in a

*All references to Wilhelm's papers are by year and letter in keeping with arrangement of his bibliography in the Appendix. Other references are to be found in the list just before the appendices.

In his discussion of packed-bed reactors, the question of lateral and longitudinal dispersion by the circuitous paths that fluid elements take in passing around the particles was a constantly recurring theme.

fermentation reaction, (1950a, b). Though the diffusion within the catalyst particle received only one paper in its own right (1961), questions of mass transfer are the continual burden of his interest in the reactor design problem as a whole. Without attempting to be comprehensive I will sketch the lines he followed in some of these papers.

Let us take a particular component of Wilhelm's work and examine it in more detail. In his discussion of packed-bed reactors, the question of lateral and longitudinal dispersion by the circuitous paths that fluid elements take in passing around the particles was a constantly recurring theme. His first paper on this was one with Bernard (1950a). In it they solved the steady-state equations for diffusion with plug-flow for the boundary condition corresponding to a finite tube. By injecting methylene blue from a point source on the axis and comparing concentration profiles they estimated a radial Peclet number ranging from 8 to 15. The equations contain no hint of the anisotropy that Wilhelm commented on in his 1962 review (see quote below), but this he was to measure later with McHenry (1957c). Using a sinusoidal wave input produced by an ingenious mechanism which varied the individual flows of a binary mixture without varying the total flow, they found an axial Peclet number of 1.88 ± 0.15 over the Reynolds number range of 100-400. It was an extension to higher frequencies of earlier work with Deisler (1953a), who had measured both the axial and the internal diffusivity when the pellets of the packing were porous. It complemented and was complemented by some of Prausnitz' work (1956c) on fluctuations of concentration in a packed bed.

It is instructive to see how Wilhelm brought this all together in his plenary lecture in 1962. Because it shows the mode of his thought and his manner of expression so well, I will take the liberty of quoting five paragraphs *in extenso*.

We now come to an interesting question: Why do the magnitudes of the dispersive Peclet numbers, although constant, have different values in the fully developed mixing regimes? Why is the system anisotropic? The radial Peclet number is noted to have a numerical value of about twelve and that of the axial group, of about two. These values would appear to arise naturally from the properties of the cell mixing model and the ideas involved merit brief discussion.

The lateral dispersion effect is consistent with a random walk, a Galton quincunx description. As tracer material flows from one mixing cell level to the next in the tube, a succession of lateral displacements must occur because of the physical presence of the particles. The thorough mixing at each stage assures that the direction of travel of a tracer element shall be sta-

In contrast . . . the modern scientific design method tries to make as much progress with a model of the system in projecting forward the behavior at each stage.

tistically independent of the direction of lateral motion in the previous cell. Through a straightforward elementary statistical development of the mean square displacement of tracer substance after passage through n layers of mixing cells, it may be shown that the lateral Peclet group should be constant (this was verified experimentally). It was also shown to depend in its absolute value on (a) the average scale or side-step distance in walking around a particle and on (b) the number of layers of mixing cells between source and measuring point. If we take the number of mixing cells in the axial direction to be of the order of the number of particles in that direction and the average scale of individual lateral displacements to be a fraction of the particle diameter, an estimate of the value of the lateral Peclet number is made which closely approximates the experimental value. Prausnitz* in a detailed study of concentration fluctuations in a tracer plume, rather than of the time-average values of which we have been speaking, was able to determine directly that the scale of lateral displacement mixing was one-quarter of a particle diameter. In short, an elementary random walk analysis serves to describe the observed lateral dispersion effects. Such description has been made by a number of investigators including Baron¹, Boreskov², Latinen³ and Singer⁴.

As we turn to the axial dispersion process, a key point, as suggested by Beek⁵ is whether, in a sequence of interconnecting and thoroughly mixed stages, there is a significant amount of fluid backflow against the main stream. The state of the reactor in a local region

will depend greatly on the presence or absence of such flows. For these to be effective it is necessary for the distance that should be traversed by backflow elements of fluid to be larger than the average size of the particle-associated mixing stages or permanent eddies. Such backflow streamers would of course mix with the fluid in stages directly upstream and thus would be the means for conveying a signal against the main stream. Such random backflow motions would provide the physical basis for a purely diffusive transport. If backflow is a predominant effect the form of the system may be closely approximated by a normal differential diffusion equation and characterized by a meaningful diffusion constant.

However, in the absence of backflow, and when the predominant dispersion effect is due to mixing in stages, reactor design should be accomplished by the solution of the difference equations which represent the discrete nature of the physical situation. Under the latter circumstances a diffusion constant in the local region of a well-stirred eddy must approach a value of zero and the designation of the diffusion equation to describe the state becomes meaningless. Although there have been no direct experiments devised, to date, to measure the extent of backmixing, the value of the axial Peclet number of two as determined by measurements in the limits of deep beds gives strong evidence that stage-wise mixing rather than backmixing is the predominant dispersion action. It will be recalled that the Peclet number is an inverse proportionality constant in the Einstein equation; it represents the spreading rate of a tracer pulse after a large number of mixing cells have been traversed if each cell is one particle diameter in depth. Aris and Amundson⁶ analysed the axial dispersion property by tracing the changes in the probability density function with distance into the bed. This function, it will be recalled, is the probability that a molecule, introduced into the first mixer at the bed entrance at time, $T = 0$, will be located in the n th layer at time, T . As expected, a Poisson distribution represents conditions in the initial discrete stages at the bed entrance; with increasing bed depth and number of mixing stages a normal distribution is approached for which the diffusion equation becomes an appropriate description. A substantial approach toward this limit occurs in a depth of about twenty particles. The first authors to propose the cell mixing model, Kramers and Alberda⁷, analysed the same problem by making theoretical comparisons of the frequency response properties of the solutions of difference and of differential equations at various bed depths for a forcing sinusoidal tracer concentration input.

In order to summarize this point, we can state that within the specified high-velocity fluid mechanical regime a single model now exists which describes satisfactorily both lateral and axial dispersion effects in packed bed reactors. However, if the only advantage in the prescription of a difference equation formulation were to describe properly reaction behaviour in the regions of the bed entrance the accomplishments would be small at best. The significant gain is derived from a mathematical simplification which has a de-

*See 1957a.

Another paper that illustrates his paene-Taylorian combination of theory and experiment is his discussion (coauthored with Cleland) of a viscous flow profile on the yield of a tubular reactor.

cisive advantage as we look forward to the detailed design of reactors for realistic chemical kinetics. As stated previously, if backmixing were important in contributing to axial dispersion, coupled non-linear differential equation heat and mass balances would be the appropriate system descriptions and the state within the reactor would depend on both the upstream and downstream boundary conditions. This state would lead to a mathematical situation that for a complete model is analytically intractable and numerically beyond present digital solution capacities in a practical sense. On the other hand, in the difference equation stirred-tank model, only conditions at the bed inlet need be satisfied and calculation may proceed down the bed in a so-called step by step marching technique.

Of course he was standing at the brink of some important numerical developments that would have changed some of his last sentences. Of this he was not unaware, though he does not emphasize it, preferring to describe the cell model of the packed bed that Lapidus and Deans [37] had recently devised.

Another paper that illustrates his paene-Taylorian combination of theory and experiment is his discussion (coauthored with Cleland) of the effect of a viscous flow profile on the yield of a tubular reactor (1956d). In it, an analysis of the equations and computational solution were combined with some simple and direct experiments which were not only confirmed by the theory but also served to show its limitations.

THE CURRICULUM OF CHEMICAL REACTION ENGINEERING

Let us try and locate Wilhelm's contribution within the general course of the development of chemical reaction engineering as a self-reflective subdiscipline of chemical engineering in general (see Table 1). Chemical reactors, of course, have been built, and have often performed excellently, from the earliest times. Their analysis and their design, by other than *ad hoc* or trial and error methods, however, is a fairly late phenomenon. In the growth of chemical industry the standard technique was to rely on scale-up by stages in which a potentially useful chemical reaction found in the laboratory would first of all be tried in one or more intermediate sizes of apparatus (often known as semi-technical stages) before being incorporated in a main-line plant. It was hoped that

some of the problems which might arise in the larger scale would be discovered in the semi-technical stage or stages and any difficulties overcome in this way. In contrast to this the modern scientific design method tries to make as much progress with a model of the system in projecting forward the behavior at each stage.

The interaction of physical and chemical effects and their just disposition was recognized as one of the keys to the understanding of reactors. Though hinted at in a half-formed notion of Lomonosov, the first definite applications of this was the work of Nernst and Brunner [8] which recognized that the rate of reaction at a heterogeneous surface might be limited by the transfer through a stagnant film of liquid. By 1908 Bodenstein and Wolgast [10] had used a flow reactor for the homogeneous hydrogen-iodine reaction, but they were only able to analyze certain limiting cases. Langmuir [9], in the same year, treated the problem of simultaneous diffusion and reaction and obtained the correct boundary conditions for this system. This last was a point which Wilhelm was later to investigate with Wehner in 1956.

In 1913 a physicist by the name of Ferencz Jüttner [11] solved the equations for diffusion and reaction in a porous catalyst but, so far as is known, no notice was taken of his paper. Meanwhile, in connection with combustion limits, Tafanel and LeFloch [12] had recognized that multiple steady-state could arise though they were more interested in the close approach of the heat generation and rejection curves than in their intersection. However, it was Liljenroth [13] who, in 1918, first made this explicit in his discussion of ammonia burners. Little seems to have been published of an analytical nature about chemical reactors until the late 30's when the whole question of design and performance was opened up by Damköhler [15] in his papers on "the influence of flow, diffusion and heat conduction on the yield of reactors." Almost simultaneously Thiele [16] and Zeldovich [17] obtained the same essential result on the question of diffusion and reaction in catalysts. Namely, that there was a dimensionless parameter, of the nature of a $(\text{length})^2 \times (\text{the first order rate constant}) / (\text{the diffusivity})$, which governed the seriousness of any diffusion limita-

TABLE 1

Year	Notable Papers (O)	Transient Behavior Stability	Fluid Beds	Diffusion and Reaction	Transport	General Design	Wilhelm's coauthor & interest (W)	Books and Monographs (B)
1904	Nernst/Brunner ⁸				O		(*denotes paper with RHW as sole author).	
1908	Langmuir ⁹				O			
	Bodenstein/Wohlgast ¹⁰				O			
1909	Jüttner ¹¹			O				
1913	Taffanel/LeFloch ¹²	O						
1918	Liljenroth ¹³	O						
1934	Hottel/Tu/Davis ¹⁴						RHW joined Princeton faculty	
1938	Damköhler ¹⁵			O	O	O		
1939	Thiele ¹⁶ /Zeldowitch ¹⁷			O				
	Wicke ¹⁸			O	O			
1941	Zeldowitch/Zysin ¹⁹	O						
1943						W	Johnson/Acton	
1945	Wagner ²⁰			O		O		
1944-8	Denbigh ²¹	O		B		W	Johnson/Wynkoop Collier	Hougen/Watson
						B		
1949	Wicke & Brotz ²²		W*	O	W	W*	*:McCune	
1950					W	W	Toner:Singer:Wynkoop	
							Bernardi: Bartholomew et al	
1951	Hougen ²³	W				W	Valentine	
1952		W*					*	
1953	van Heerden ²⁴	O			W	W*	*: Deisler	
1954						W*	*	
1955	Amundson/Bilous ²⁵	O			W		Deisler/McHenry	
	Wheeler ²⁶			O				
1956		W			W	WB	Wehner: Prausnitz: Hanratty: Latinen: Cleland	J. M. Smith
1957	Amundson/Aris ²⁷	WO			W		McHenry: Prausnitz	
1958			W			B	Rice	W. Brötz, Birdfoot
1959					B,W		Hill	
1960		W					Lamb/Manning	
1961	Carberry ²⁸ Weiss/ Hicks: ²⁹					B	Villet	Aris (Opt. Design)
	Amundson/Schilson: ³⁰			O				
	Tinkler/Metzner: ³¹			W				
1962						*	* IUPAC Lecture	
1963	Amundson/Schmitz ³²	WO	B	B	W	B	Lamb: Manning	{ Davidson/Harrison Kramers/Westerterp Satterfield/Sherwood
1964				B				
1965	Bischoff ³³ :Petersen ³⁴ : Aris ³⁵			O		BW	Blum	Aris Denbigh: Petersen
1966								
1967	Amundson/Luss ³⁶				B			Astarita
1968							RHW's death	Gavalas:Boudart

tion. It was left to Thiele however to see that this modulus, which is now called after him, could be incorporated in a scientific fudge-factor called the effectiveness of the catalyst particle. This is the ratio of the actual rate of reaction to that which

would obtain if there were no diffusion limitation and it is, I think, a mark of true engineering insight that Thiele should have seen the opportunity to wrap-up a lot of difficult calculations in so simple a factor. This betrays an essential dif-

ference in outlook between the engineer and the physicist, the latter portrayed in Jüttner's work. By this time Wicke [16] was also beginning his studies in adsorption, desorption, diffusion, and their influence on chemical reaction, studies which have continued until the present day. The question of multiplicity of steady-states and, indeed, of isolas was also investigated in Russia by Zeldowitch and Zysin [19] in a paper which has largely been overlooked. (D. Luss drew it to my attention and reference is made to it in Gray's valuable chronology [39].

It was in the mid-forties that Denbigh [21] built on his experience in industry and produced a general analysis of the well-stirred reactor. His was the first mathematical analysis of transient behavior and later he was a leader in some aspects of optimal design. To the late forties belongs the confirmation of the diffusion limitation of a reaction by Wicke and Brötz [22] through the observation that the apparent activation energy was reduced by a factor of 2 at high temperatures. An earlier result belongs to the 1930's when the external film diffusion limitation was shown to give an even greater reduction in the apparent activation energy for the combustion of carbon spheres [14].

Of course the need for various synthetic chemicals during the war had greatly spurred interest in the general design of reaction and the book of Hougen and Watson published in 1945 represents the outcome of much practical experience. Watson had gained a great reputation for the start-up of the butadiene plants so necessary to the synthetic rubber program. Hougen [23] was later to summarize his experience in the 1951 Institute lecture published as the first of the Chemical Engineering Progress Monographs. The 50's saw the publication of van Heerden's [24] paper on autothermic reactors which, done in ignorance of Liljenroth [13] and Zeldowitch [19], was very influential in bringing questions of uniqueness and stability to the attention of a much wider public than ever before. In particular, the nature of the multiplicity of steady states and the associated transient behavior was taken up by Amundson who recognized it immediately as cognate with the work on nonlinear differential equations that had prospered so notably in the previous decade. Amundson in the mid 50's was also concerned with the sensitivity of such features as the hot-spot in the exothermic tubular reactor and his papers with Bilous [25] mark the founding of the

mathematical study of stability and sensitivity in chemical reactors. Indeed, Amundson [32, 36] continued this work in the late 50's showing that under the influence of control there could arise limit cycles. He went further in the early 60's to discuss two-phase reactors, polymerization and was approaching the more difficult question in the

Wilhem stands out for his marriage of the concept of a priori design, as he called it . . . and the laboratory-scale experiments that would be needed to understand the physical effects.

distributed system, the tubular reactor, at about the time of Wilhelm's death.

The internal economy of the catalyst particle, a question which Wilhelm was always aware of and frequently refers to, though he did not contribute much to the direct literature on this topic, was also the subject of much research during this period. In 1951 Wheeler had given a valuable review of work on diffusion and reaction which helped greatly in drawing attention to Thiele's work (*Advances in Catalysis* 3, 249, Academic Press, New York). He further discussed some questions of selectivity in 1955 [26]. Just as there had been a flurry of independent work in the late 30's which resulted in the basic notion of the effectiveness factor, so in the early 60's there were almost simultaneous solutions to the nonisothermal problem. Of these Amundson and Schilson's [30] went back to Schilson's PhD work in the mid fifties and of which Wilhelm had probably learned directly from Amundson. But almost simultaneously Carberry [28], Weisz and Hicks [29] and Tinkler and Metzner [31] obtained essentially the same result. It was the curves of Weisz and Hicks which became so well known and served to remind people that multiplicity of steady state could occur within the catalyst particle itself. Another curious independent simultaneity occurred in 1965 when Bischoff [33], Petersen [34] and Aris [35] found that the effectiveness factors for all shapes and all kinetics could be brought together in an asymptotic sense.

WILHELM'S PLACE IN THE DEVELOPMENT OF CHEMICAL REACTION ENGINEERING

The plenary address to the International Union of Pure and Applied Chemistry which Wilhelm

Continued on page 38.

INTEGRATING CHEMISTRY AND ENGINEERING

A Course in Industrial and Engineering Chemistry

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CHEMISTRY IS AT THE heart of chemical engineering practice. And chemistry—as the lifeblood of innovation and design—is intimately involved in the creation of new technology. The ability to integrate chemistry and engineering is a hallmark of the chemical engineer. A course taught to seniors and graduate students at the University of Delaware and at Iowa State University is based on such a confluence of chemistry and engineering. The theme of the course is process conceptualization: the creation of chemical processing routes. There are no new subjects in the course; rather, information and ideas are synthesized from organic and inorganic chemistry, stoichiometry, thermodynamics, kinetics, reactor design, physical chemistry, heat and mass transfer, and fluid mechanics. This emphasis on synthesis is the key both to creating processing routes and to demonstrating the interplay between chemistry and engineering.

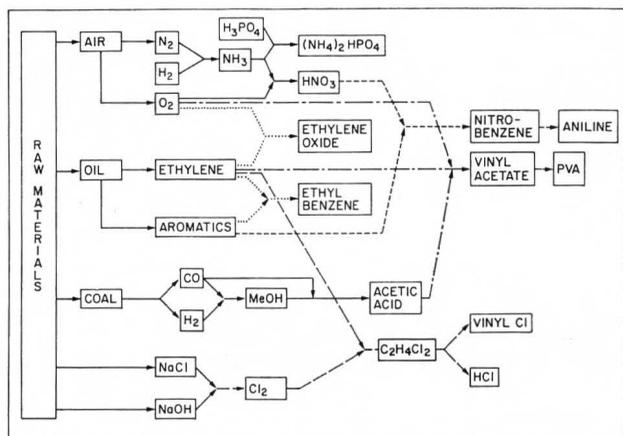


FIGURE 1

This emphasis on new routes rather than old, and synthesis rather than analysis, provides a course with an orientation toward innovation and creativity. Many aspects of the discussion of the processing routes are . . . qualitative, but an exclusively descriptive orientation is avoided.

The course is organized around a sequence of chemical processes. The processing chemistry and engineering are covered in detail but not to the extent which occurs in a typical senior-level design course. Since all processes depend on both chemical and engineering insights, it is the combination of these insights which is prime. Some processes rely on well-understood routes; however, the discovery of new routes is emphasized.

This emphasis on new routes rather than old—and synthesis rather than analysis—provides a course with an orientation toward innovation and creativity. Many aspects of the discussion of the processing routes are necessarily qualitative, but an exclusively descriptive orientation is avoided. Quantitative evaluation and reasoning are essential to understanding industrial chemistry.

The format for teaching the course is unconventional. But we have discovered that students can be led to view chemistry and engineering as being interdependent—and often inseparable. Here we present the content of the course and the teaching method which has been developed during the past four years.

CASE STUDY ORGANIZATION

The course in industrial and engineering chemistry is organized on a case-study approach, and the processes are shown in Fig. 1. This master flowchart presents a large portion of the structure of the chemical and petroleum industries as an interrelated whole. This approach increases the students' recognition of specific chemicals as raw materials, intermediates, end-use products, by-products, or wastes. Students particularly need

information about existing industrial paths and respond eagerly to the real-world orientation. A sequential presentation reinforces the strong interdependence of industrial processes.

The case studies were also chosen on the basis that they illustrate many important aspects of industrial chemistry. Ammonia and ammonium phosphate production and chlorine production are representative of inorganic syntheses. Classic organic reactions are involved in the production of nitrobenzene and aniline. Some reactions rely on relatively unspecific homogeneous free radical chemistry, such as ethane cracking to ethylene; reactor design is relatively simple. In contrast, the conversion of ethylene to ethylene oxide relies on the complexities of catalytic selective oxidation. Most industrial processes involve catalysts, and the integration of chemistry and engineering can be vividly demonstrated for these processes. In addition, a discussion of materials of construction and catalyst properties (surface area, porosity, dispersion) permits aspects of solid state chemistry to be introduced. The production of poly(vinyl acetate) is an excellent example of the combination of polymer chemistry and engineering. Environmental chemistry is encountered in the synthesis of chlorinated hydrocarbons and in the production of synthesis gas from coal. Thus, from the beginning, the overall flowchart provides a basis

for identifying the broad range of concepts which are integrated in industrial practice.

However, the goal of the instructor is to stress the impermanence of this overall scheme. Evolution and modifications in the flowchart are emphasized throughout the course. The student is encouraged to consider drastic changes—typically leading to the disruption of an entire train of processes. The motivation is frequently the need for alternate sources of raw materials. Several specific examples can be chosen:

- vinyl acetate production without the availability of ethylene from refinery gas or natural gas
- aniline production without the availability of benzene derived from petroleum refining
- methanol production without the availability of coal or natural gas

The development of alternative industry-wide routes requires basic information concerning sources of elementary chemical constituents. It is useful to preface the coverage of the overall flowchart by a discussion of sources of carbon, nitrogen, hydrogen, phosphorus, and chlorine. The discussion is much more than a listing of raw materials and their relative abundance. Students are directed to critically evaluate the sources—primarily from a chemical viewpoint. This exercise provides a good opportunity to review elementary chemical concepts such as oxidation state and stability. As an example, although

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R. L. Pigford was born in Meridian, Mississippi, and got his B.S. at Mississippi State College in 1938. M.S. and Ph.D. followed from the University of Illinois in 1940 and 1942. He worked for E. I. duPont de Nemours and Company at the Experimental Station in Wilmington, Delaware, until 1947 under T. H. Chilton. Then he replaced A. P. Colburn as Chairman of the Chemical Engineering Department at the University of Delaware, later becoming the first Colburn Professor.



Between 1966 and 1975 he was Professor of Chemical Engineering at the University of California in Berkeley. (C)

Bruce C. Gates is Director of the Center for Catalytic Science and Technology and Professor of Chemical Engineering at the University of Delaware. His research group includes graduate students in chemical engineering and postdoctoral fellows with backgrounds in physical, organometallic, and surface chemistry. They are studying catalysis by supported metal complexes and clusters, zeolite-entrapped metal clusters, supported superacids, and metal sulfides. The research is directed toward fundamental characterization of industrial catalysts and reactions, and conception and design of new catalysts. (R)



Most industrial processes involve catalysts, and the integration of chemistry and engineering can be vividly demonstrated for these processes. In addition, a discussion of materials of construction and catalyst properties . . . permits aspects of solid state chemistry to be introduced.

students may be surprised to discover the overwhelming abundance of carbon in precipitate or solid form, they quickly distinguish the utility of carbonates versus carbohydrates; a similar comparison can be made between gaseous nitrogen and nitrides. Frequently, a change in raw material may mean the introduction of new impurities into a processing route. Thus, lignite might be considered as a replacement for coal or natural gas, as a source of carbon monoxide. Lignite, however, contains considerable amounts of water, with many consequences in the downstream processing. In proposing oil shale as an alternative source of benzene, the relative amounts of sulfur, nitrogen, and heavy metals change, all with enormous consequences in the catalytic chemistry of reforming.

FLOWCHARTING

Flowcharting is the primary mode used to demonstrate process conceptualization. The ability to think in terms of flowcharts (including their creation, modification, and evaluation) is emphasized throughout the course.

Flowcharts are introduced at various levels of detail. The detail is determined by the utility of the flowchart, i.e., to quickly express a new chemical route and possible alternatives or to describe a key scheme of separation processes. In other cases, crucial aspects of processing may not appear until recycle streams are drawn or heat transfer operations are introduced.

The most elementary form of a flowchart expresses the stoichiometry of the process: raw materials transformed into products. The essence of the chemical innovation is frequently contained within this simplest stoichiometry. We have found that students are adept at suggesting alternatives. But, sometimes, these "inventions" must be presented to the student with development of the remainder of the flowchart being an assignment. In writing a simplified stoichiometry, we stress that industrial processes rarely involve only the nominal reaction. During the initial portion of the course, the production of side products, wastes, and pollutants is emphasized. Students are reminded of the limitations in the purity of their

raw materials, since the fate of impurities frequently is not expressed in the simplest stoichiometry. The dire consequences of ignoring impurities can be illustrated by "well-developed" processes which are fatally flawed by catalyst poisons or sources of water or oxygen.

Consideration of specific unit operations adds the next level of detail to the flowcharts. The most frequently expressed initial combination of unit operations involves reactors and separation units. Even the most elementary flowchart is influenced by the chemistry of the process. Generally, the selection of specific unit operations proceeds from the restrictions dictated by the chemistry. To illustrate these ideas, the instructor can lead the student to think of fluidized bed reactors for highly exothermic oxidations and fixed bed reactors for reforming petroleum distillates. Reactor systems for synthesis gas reactions using homogeneous catalysis provide a vivid contrast to those using heterogeneous catalysis. Separation processes can be dominated by the chemical route chosen initially. Methanol carbonylation requires separation of a heavy catalyst, a light promoter, and an intermediate product.

Conversely, engineering requirements often strongly restrict the chemistry which can be employed. This interplay between chemistry and engineering is presented by the modification of flowcharts. Typical alterations include the addition of recycle streams and by-product purges. Heat and mass transfer requirements may specifically limit the chemistry which can be attempted. The students can also be confronted with reactions such as the production of methanol, for which equilibrium limitations require low temperatures, but for which the kinetics demands higher temperatures. The selection of specific unit operations may also be affected by safety or environmental restrictions. For example, the conceptualization of a process for nitrating benzene is dominated by the recognition of the high exothermicity of the reaction. Safety precautions, which are necessary to prevent reaction runaway and explosion, strongly influence reactor design. Ethylene chloride production is dominated in some respects by environmental concerns.

This approach emphasizes the creative develop-

ment of chemical processing routes rather than a descriptive presentation—and invention rather than memorization of the details of the process. The challenge to the instructor is to create a classroom atmosphere conducive to such an orientation. In the early portion of the course, the development of process flowcharts is fostered by having the students pose questions concerning the basic chemistry and engineering. Students are encouraged to ask a wide range of questions, including those that they or the instructor may be unable to answer fully. At this point the students' curiosity is undisciplined; this approach appears to be essential for providing an open "free-wheeling" orientation towards creativity. A typical set of questions posed by a class during the early portion of the course is shown in Table 1.

Flowcharts are constructed as these questions are considered. Initially, the students have difficulty in posing the "right" questions. However, skill in asking a sequence of questions can be developed by the instructor. Initially, a large set of questions is accepted, but an ordering and ranking is essential. Students are confronted with the need for a sequence in their consideration of the processing routes. Thus, consideration of the thermodynamic effects of temperature and pressure must be preceded by stoichiometry. Questions concerning kinetics of specific reactions should not arise until thermodynamic feasibility is examined. Some questions can be shown to lead naturally to others: knowledge of the heat of reaction raises the question of heat transfer in reactors. The instructor can guide this thought process through examples and illustrations offered by the case studies. The complexity of the questions generally parallels the detail of the flow chart, and therefore more explicit questions can be asked as the conception of the process develops. From our ex-

TABLE 1
Student Questions on Developing a Flowchart for Production of Methanol from CO and H₂

1. Is a catalyst needed? What is the catalyst?
2. Does the reaction require heat?
3. How can heat transfer be performed?
4. What temperature and pressure should be used?
5. Are there important side reactions?
6. What yields can be obtained?
7. Can a fluidized or a fixed bed reactor be used?
8. Are reaction rates available?
9. What is the purity of the feed?
10. What product separations must be performed?
11. What materials of construction can be used?

perience, a specific sequence of questions often evolves, dealing with the following subjects:

- stoichiometry of proposed reactions and potential side reactions
- thermodynamics
- kinetics
- reactor design
- mass transfer and heat transfer
- fluid flow
- safety
- environmental restrictions

The students recognize many of these as subjects of chemical engineering. A more mature set of questions posed by a class later in the course is shown in Table 2.

TABLE 2
Student Questions on Developing a Flowchart for Petroleum Reforming

1. What reactions are involved in reforming?
2. What is the chemical composition of the feed stream?
3. What concentration of impurities can be accepted?
4. What is the heat of reaction?
5. How do temperature & pressure affect the equilibrium yield?
6. What are the rates of the reactions?
7. Can a catalyst be used to improve the rates of reaction or selectivity?
8. Can the catalyst be poisoned or deactivated?
9. What is the role of hydrogen in the process?
10. Should a fixed bed or fluidized bed reactor be used?

However, the students are not encouraged to view any one sequence as a pattern for innovation or even for the duplication of existing processes. Examples are encountered which apparently involve complete reversals of the sequence, such as benzene nitration or hydrocarbon chlorination.

QUANTITATIVE ASPECTS OF INDUSTRIAL CHEMISTRY

The discussion of the basic chemistry of industrial processes requires a qualitative knowledge and understanding of chemical composition, relative stability, solubility, catalytic activity, and other intuitive concepts related to structure and reactivity. Although students have previously studied many of these ideas, their general usefulness is usually not appreciated and their integration into chemical engineering calculations is normally missing. We have deliberately attempted to incorporate these concepts into the course in a quantitative manner.

The complexity of industrial processes fre-

Continued on page 42.

SOLAR HOT WATER HEATING BY NATURAL CONVECTION

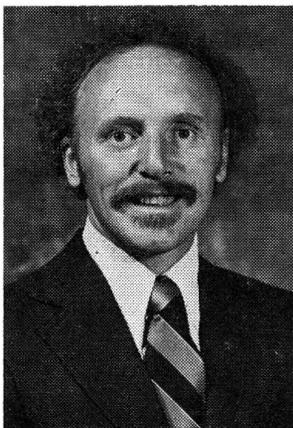
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THE PROBLEMS ASSOCIATED with fossil fuel supplies and the associated escalation in price has sparked renewed interest in solar energy as an alternate fuel source. One application of solar energy which has received considerable interest is domestic hot water.

This paper presents an undergraduate laboratory experiment which uses a solar collector to heat water for domestic usage. The water is circulated by natural convection so no pumping is required.

The experimental apparatus is relatively inexpensive to acquire. The solar collector can be built on site to reduce costs. This can be accomplished by students with supervision for which they can receive credit for construction and start-up of the system.

The quality of the data produced is very good. This enhances the educational experience since the students are more enthusiastic about an experiment which "works." The students can also sample the hot water produced to "experience" the results.



Rich Noble received his B.E. degree in 1968 and M.E. degree in 1969 from Stevens Institute of Technology. In 1976, he received his Ph.D. degree from the University of California, Davis. His current research interests include facilitated transport in liquid membranes, transient heat transfer, and problem solving skills.

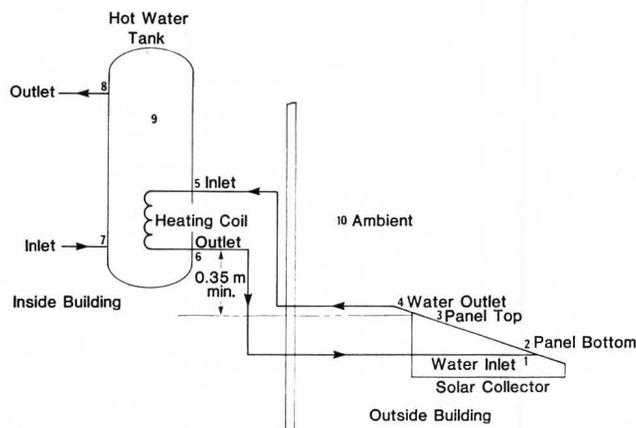


FIGURE 1. Schematic diagram of solar water heater with thermocouple locations.

The educational objectives of this experiment are the following. 1) to expose the students to the principles of solar energy collection, 2) to demonstrate the use of solar energy to heat water, 3) to demonstrate the use of natural convection to move fluid, and 4) to use experimental data obtained to do a preliminary design for a feasible household system.

EXPERIMENTAL

The experimental apparatus is shown schematically in Fig. 1. The students take temperature readings at least hourly for the 10 locations shown and also the short-wave solar radiation flux normal to the collector surface. A short-wave radiometer is attached to the collector with a millivolt read-out. This is done for the period 8 am to 5 pm and can usually be accomplished quite easily by the students in the group performing the experiments. They can take turns for each hour and obtain the data between classes if necessary. One set of data can be obtained in 2 or 3 minutes with the aid of a digital thermometer with a multiple dial so the student simply dials each thermocouple reading and writes down the temperature.

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The students are asked to determine:

- Overall system efficiency.
- Overall heat-transfer coefficient for the collector.
- Overall heat-transfer coefficient for the heating coil.
- Collector and heating coil surface area needed to provide 0.189m³ (50 gal) of water daily at 50°C which is initially at 15°C.

SYSTEM CONSTRUCTION

A diagram showing the construction of the solar collector is shown in Fig. 2. The solar panel is an aluminum plate (2.11m x 1.14m) which is painted black. Attached to the collector are 9 copper tubes (1.59cm O.D.) spaced 12.7cm apart ("a" in Fig. 2) and also painted black. The copper tubes are connected to a copper manifold (3.81cm O.D.) at the top and bottom. To avoid relative heat expansion effects, it is recommended that the plate and all tubing be made of the same material.

Below the collector is 0.15m of insulation. The collector and insulation are housed in a wooden frame (3.81cm thick) which is 1.22m x 2.43m x 0.24m. A piece of plate glass sits above the collector to prevent long-wave radiation from escaping.

The angle of the collector relative to the ground surface can be adjusted using a support frame with adjustable support arms on the top and a hinge on the bottom of the collector.

The return pipe from the heating coil should

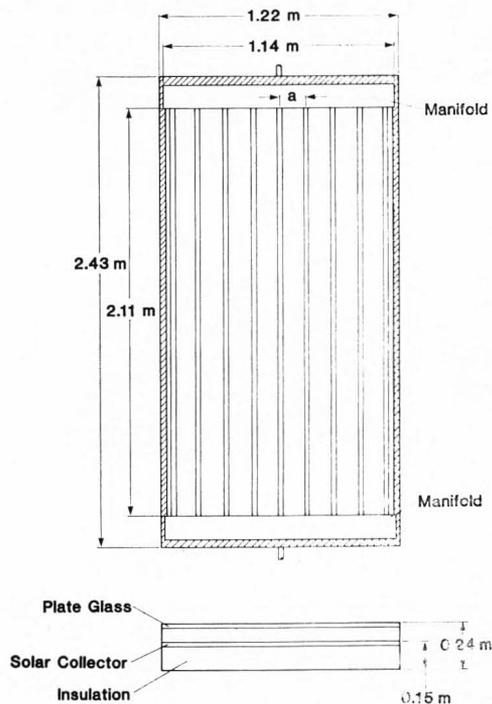


FIGURE 2. Solar collector

This paper presents an . . . experiment which used a solar collector to heat water for domestic usage. The water is circulated by natural convection so no pumping is required.

be downward sloping to the collector to aid the natural convective fluid motion. It is initially recommended that the angle of the collector be set at latitude + 10° [1].

Depending on climate, it is desirable to insulate all piping and the hot water storage tank to minimize losses. Also, in cold climates, an anti-freeze solution can be used as the working fluid since the heat transfer is through a closed loop.

DATA ANALYSIS

The data are analyzed using the following procedure: First, the heat transferred from the heating coil to the water in the tank is calculated.

$$q_t = mC_p \left(\frac{\Delta T}{\Delta t} \right)_t \quad (1)$$

where: q_t = heat transferred to the water in tank (W)

m = mass of stored water (kg)

C_p = isobaric heat capacity of water ($\frac{J}{kg \cdot K}$)

$\left(\frac{\Delta T}{\Delta t} \right)_t$ = change in water temperature in tank over time interval Δt ($\frac{K}{s}$)

Measurement of the short-wave solar radiation incident on the solar collector q_i determines the heat input to the system.

Therefore, the thermal efficiency of the system (η) can be determined.

$$\eta = \frac{q_t}{q_i} \quad (2)$$

This assumes that the system has no other heat gains or losses. If the storage tank and piping are well-insulated, this is a good assumption.

An overall heat-transfer coefficient for the solar collection (U_c) can be calculated as follows

$$U_c = \frac{q_i}{A_c (\Delta T)_{LM}} \quad (3)$$

where: A_c = surface area of the collector (m²)

TABLE 1. Experimental Data

TIME	Temperature (°C)										Radiometer Reading (mV)
	T ₁	T ₂	T ₃	T ₄	T ₅	T ₆	T ₇	T ₈	T ₉	T ₁₀	
8:00	3	5	7	8	23	17	21	19	24	8	3
9:00	13	35	41	29	16	22	21	18	24	12	8.5
10:00	23	63	71	57	54	24	22	19	24	15	13.6
11:00	25	79	88	68	66	25	24	19	24	16	16.5
12:00	26	74	83	67	66	26	24	20	25	16	19.5
1:00	25	36	44	46	46	26	24	20	26	15	4.5
2:00	27	59	68	60	60	27	26	20	26	19	19
3:00	29	83	92	70	69	29	29	21	27	23	17.5
4:00	29	72	78	61	59	29	27	22	28	23	12.5
5:00	30	59	68	61	61	30	27	23	28	23	9.0

Tank Capacity: 0.454m³ (120 gal): Area of Tank Coil 1.86 m²: Radiometer Calibration constant: 1(mW/cm²) = 0.272mV
Area of Solar Panel: 2.38m²

$$\begin{aligned}
 (\Delta T)_{LM} &= \text{log-mean temperature difference (K)} \\
 &= \frac{(T_3 - T_4) - (T_2 - T_1)}{\ln \frac{(T_3 - T_4)}{(T_2 - T_1)}}
 \end{aligned}$$

The subscripts on the temperatures refer to the locations shown in Fig. 1.

Similarly the overall heat-transfer coefficient for the heating coil (U_t) can be determined.

$$U_t = \frac{q_t}{A_t(\Delta T)_{LM}} \quad (4)$$

where: A_t = surface area of coil (m²)

$$(\Delta T)_{LM} = \frac{(T_6 - T_9) - (T_5 - T_9)}{\ln \frac{(T_6 - T_9)}{(T_5 - T_9)}}$$

SAMPLE CALCULATIONS

By scanning the data in Table 1, it becomes apparent that the collector does not start supplying any appreciable heat to the storage tank until

approximately 10 am. This is the time that the storage tank outlet temperature (T₆) equals the storage tank temperature (T₉). Before this time T₉ is greater than T₆ and the storage tank is heating the fluid in the coil. Therefore, using 10 am as a starting point for heating, the hourly data was sub-divided into periods where there was a rise in T₉. The average values of the data during these periods is shown in Table 2.

Sample calculations for the 10 am to 12 noon time period are shown below.

$$\begin{aligned}
 q_i &= (\text{radiation flux}) (\text{collector surface area}) \\
 &= 16.5\text{mV} \times \frac{1(\text{mW}/\text{cm}^2)}{0.272\text{mV}} \times \frac{1\text{W}}{10^3\text{mW}} \\
 &\quad \times 2.38 \times 10^4\text{cm}^2 = 1.45 \times 10^3 \text{ W} \\
 q_t &= mC_p \left(\frac{\Delta T}{\Delta t} \right)_t = 0.454\text{m}^3 \times 996.4 \frac{\text{kg}}{\text{m}^3} \times 4.183 \\
 &\quad \times 10^3 \frac{\text{J}}{\text{kg}\cdot\text{K}} \times \frac{1\text{K}}{2 \text{ hrs}} \times \frac{1 \text{ hr}}{3600\text{s}} = 2.63 \times 10^2\text{W} \\
 \eta &= \frac{q_t}{q_i} = \frac{2.63 \times 10^2\text{W}}{1.45 \times 10^3\text{W}} = 0.18
 \end{aligned}$$

TABLE 2. Averaged Data

TIME PERIOD	Avg Temperatures (°C)										Avg Radiation Rate (kW)	
	1	2	3	4	5	6	7	8	9	10		Avg mV Reading
10:00 12:00	24.7	72	80.7	64	62	25	23.3	19.3	24.3	15.7	16.5	1.45
12:00 1:00	25.5	55	63.5	56.5	56	26	24	20	25.5	15.5	12.0	1.05
1:00 3:00	27	59.3	68	58.7	58.3	27.3	26.3	20.3	26.3	19	13.7	1.20
3:00 5:00	29.3	71.3	79.3	64	63	29.3	27.7	22	27.7	23	13.0	1.14

TABLE 3
Calculated Results

TIME PERIOD	q_i (kW)	q_t (kW)	η (%)	U_c (W/m ² ·K)	U_i (W/m ² ·K)
10:00 12:00	1.45	0.263	18	20.6	15.2
12:00 1:00	1.05	0.524	50	28.1	38.6
1:00 3:00	1.20	0.262	22	33.8	15.7
3:00 5:00	1.14	0.262	23	18.0	12.9

$$U_c = \frac{q_i}{A_c(\Delta T)_{LM}} = \frac{1.45 \times 10^3 W}{2.38 m^2} \times \frac{\ln \frac{16.7}{47.3}}{(16.7 - 47.3) K} = 20.6 \frac{W}{m^2 \cdot K}$$

$$U_t = \frac{q_t}{A_t(\Delta T)_{LM}} = \frac{2.63 \times 10^2 W}{1.86 m^2} \times \frac{\ln \frac{0.7}{37.7}}{(0.7 - 37.7) K} = 9.8 \frac{W}{m^2 \cdot K}$$

Results for all time periods are shown in Table 3.

Sizing requirements for obtaining 0.189m³ (50 gal) of water at 50° which is initially at 15°C are shown below.

It is assumed that the actual time period for heat transfer is 8 hours. This assumption is due to the fact that the sun did not set until 7 pm and the collector surface was still quite hot at 5 pm.

$$q_t = mC_p \left(\frac{\Delta T}{\Delta t} \right)_t = 0.189 m^3 \times 99.64 \frac{kg}{m^3} \times 4.183 \times 10^3 \frac{J}{kg \cdot K} \times \frac{35 K}{8 hrs} \times \frac{1 hr}{3600 s} = 9.57 \times 10^2 W$$

$$q_i = \frac{q_t}{\eta} = \frac{9.57 \times 10^2 W}{0.251} = 3.81 \times 10^3 W$$

Assuming that the heat transfer rate is directly proportional to surface area

$$q \propto A$$

$$A_t = \frac{957 W}{300 W} (1.86 m^2) = 5.93 m^2$$

$$A_c = \frac{3.81 \times 10^3 W}{1.23 \times 10^3 W} (2.38 m^2) = 7.37 m^2$$

The average value of q_t is 300W and the average value of q_i is 1230W for the calculated results.

CONCLUSIONS

A laboratory experiment to demonstrate the feasibility of using solar energy to heat has been

discussed. The working fluid is moved by natural convection so no pumps are required. The experiment exposed students to the principles of solar energy and natural convection. The experiment also demonstrated the use of solar energy to heat water. Students used data obtained in the experiment to do preliminary design calculations to size equipment for a domestic hot water installation.

The experimental apparatus is simple in design and operation. The students can take data quickly and easily. The experiment also performed as desired (it works) so students can see the performance. □

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In Memoriam

Ralph E. Peck

Ralph E. Peck, professor emeritus of chemical engineering at the Illinois Institute of Technology, died November 6, 1982, at the age of 71.

Dr. Peck began at the institute in 1939 and was chairman of the chemical engineering department from 1953 to 1967. He was internationally recognized as an expert in drying, and was active as a consultant for industry and government. He taught in Israel, Brazil, Algeria and Korea, and established a department of chemical engineering at India's University of Punjab.

Dr. Peck was involved in peace and nuclear arms freeze organizations and was sometimes called on by the U.S. government to disarm chemical gas weapons.

He was a member of the Ethical Humanist Society of Chicago. He was honored for teaching excellence from the institute and from ASEE and was a fellow of the AIChE. An annual Ralph Peck lectureship was established in 1973 at Illinois Institute of Technology.

His work after his retirement in 1977 led to his invention of a process for removing sulfur oxide gases from burning coal and converting them to high-grade fertilization. □

A PROCESS CONTROL UNDERGRADUATE OPTION

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THE PRACTICE OF PROCESS control in the chemical processing industries is undergoing rapid technological change. The availability of powerful and inexpensive computers and micro-processor based controllers has made the use of sophisticated control algorithms routinely possible and economically necessary. Unfortunately, the supply of competent process control engineers lags far behind the demand produced by the available technology and potential applications. The typical B. S. chemical engineering graduate has been exposed to no process control beyond a first course in process dynamics. These graduates are completely unfamiliar with the concepts of "modern" or multi-variable control. Graduate work does not meet this need either, since there are few graduate students in chemical engineering and fewer still who are interested in studying advanced process control. The relationship between processes and their control systems is becoming increasingly sophisticated. Hence, there is an obvious need for control expertise in the chemical engineering profession which is not being met by the conventional chemical engineering curriculum [1,2].

Two factors have made it possible to initiate a course sequence in process control in the chemical engineering department at the University of Maine. The first was a bold change in the curriculum in the department. A program was instituted in which a student must choose an area of special concentration. Current options are process control, pulp and paper, polymers, honors, or, in exceptional cases, an individualized program. Each option consists of at least four courses at the junior and senior levels. The second is that there are two of us who are interested and competent in computers and process control. This allows us to overcome the very real barrier imposed by the "critical mass effect" as described by Waller [2].

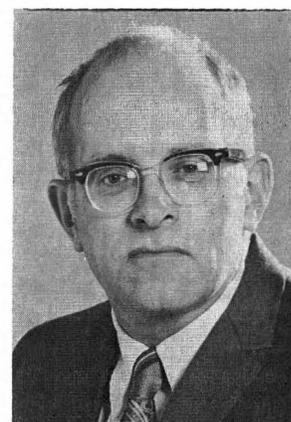
The Process Control Option is a dramatic

break with the traditional teaching of control theory in this department, and we believe that it is a unique program at the undergraduate level in chemical engineering. Teaching in process control formerly consisted of an introductory process dynamics course for all students, a graduate course when there was sufficient demand, and an occasional special undergraduate course in response to demand. We now provide the coordinated sequence which is described in this paper.

One of us has had industrial experience in process control, and the other is knowledgeable in real-time computer hardware, software, and interfacing. Neither of us has much interest in pure theory divorced from application. Hence, the en-



John C. Hassler is currently an Associate Professor of Chemical Engineering at the University of Maine at Orono. His degrees are in physical chemistry from Kansas State University. He spent several years in the "post-doc holding pattern," including four years in the Electrical Engineering Department at the University of Illinois, working on lasers. He joined the Chemical Engineering faculty at Virginia Polytechnic Institute and State University in Blacksburg, Virginia, in 1972, and moved to Maine in 1977. His research interests are process instrumentation, modeling, and control, with an emphasis on the hardware and software involved in the application of computers to real-time problems. (L)



Kenneth I. Mumme' is an Associate Professor of Chemical Engineering at the University of Maine-Orono. He received a B.S. in physics from Lawrence College (1954) and the M.S. and Ph.D. degrees in Chemical Engineering from the University of Maine (1970). He worked for eight years in the pulp and paper industry and has spent two years doing research at the Institute for Engineering Cybernetics in Trondheim, Norway. His research, publications, and patents are in the general area of instrumentation, process control, and system modelling. (R)

tire sequence tends to be strongly applied in nature.

THE COURSES

CHE 152: INTRODUCTION TO PROCESS DYNAMICS AND CONTROL

This is the typical required course for all students in the department. It covers LaPlace transform theory, transfer functions, PID control, etc. The text in current use is by Luyben [3]. Because this course is required of all students, it is not actually part of the Process Control option, although it is a prerequisite for the option.

CHE 154: INTRODUCTION TO DIGITAL PROCESS CONTROL

This course considers single-input single-output (SISO) systems using the Z-transform. The text used is by Kuo [4]. The course covers all of the sections of the text which do not involve state variables. (The reason for this rather uncomfortable division of material is the scheduling problem created by our coop program. This will be discussed later.) The use of fully interactive computer methods for design is emphasized. Many of the "standard" algorithms, such as the Smith Predictor, the Dahlin algorithm, etc. are presented and compared with direct Z-transform design methods.

Unfortunately, there is no formal laboratory with this course. However, we both feel very strongly that practical experience is an essential part of learning, so we "steal" some laboratory time by omitting a certain number of lecture periods. Although we continue to look for good experiments, the system used this past year worked very well. It consists of a series of interacting tank levels, with the series ranging from one to four tanks. The levels are controlled directly by a PDP 11/60 computer programmed in FORTRAN. The students were asked to identify the process by any means they wished and then to control the process on the basis of one of the design methods learned in the lectures. For example, this year they were asked to design a digital PID-exponential filter controller for a third order system, a dead beat controller for a first order system, and to apply any technique they wished, other than PID, to a third order system.

The experiments can take a long time, far more than the class time allotted, for several reasons. One group was very slow because of poor planning. Another group got very interested, tried all sorts of control schemes, and produced a truly excellent report. All of the students agreed later that the laboratory, in spite of the great amount of time spent on the experiment, was an absolutely essential part of the course.

CHE 156: ADVANCED PROCESS CONTROL

This course concentrates on multivariable systems. The text in current use is the portion of Kuo [4] not covered in ChE 154. Virtually none of the students who enter this course have taken mathematics beyond the normal requirement of 16 semester hours. Thus, they know little about linear algebra and are inexperienced in the use of the computer for matrix manipulations. Therefore, some

The Process Control Option is a dramatic break with the traditional teaching of control theory in this department, and we believe that it is a unique program at the undergraduate level in chemical engineering.

time must be used to remedy these deficiencies. Once this has been accomplished, we can proceed to the representation of systems by state variables. This leads naturally through such concepts as controllability, observability, multivariable systems, and control of linear (or linearized) multivariable systems.

CHE 158: ADVANCED PROCESS CONTROL II

The major emphasis of this course is on system identification through filtering and estimation. A portion of this course must be devoted to developing the practical concepts of probability and stochastic systems. Following this, we consider system identification through techniques such as the Kalman filter, least squares, maximum likelihood, etc. Applications of these techniques are examined through case studies, the modelling and control of estimated parameter systems, feedforward systems, model reference systems, and adaptive control systems. Laboratory work is used to reinforce the lecture material but, unfortunately, here again we must "steal" lab time from the lecture schedule. We have not found a truly suitable text for this course, but have based much of the material on the books by Gelb [5] and Meditch [6]. Current literature is also an essential source for this course.

ELECTIVE

To complete the process control option, the student must take one more course related to process control. We have been very liberal in this matter. For many students, it is advantageous to take a processing course, in polymers or pulp and paper for example. This gives better insight into the problems which a control engineer might be expected to solve within a processing industry. We do not encourage co-op students to make this choice, as these students already have two semesters of professional work experience behind them. Many students will elect a course in mathematics, computer science, or electrical engineering. The remaining students will usually choose to do a thesis within the honors program (directed to a control problem), or an individual senior project having something to do with control. The actual choice which any particular student makes depends upon his interests.

FACTORS IN TEACHING

We feel that there is a need for suitable textbooks for this program. We look forward to the publication of a chemical engineering text suitable for the first course, ChE 152, which covers the introductory material from the "modern control theory" point of view. For ChE 154 and 156

The program is . . . unique and valuable. There is a high demand for our graduates, and they seem to fill an obvious industrial need which is not being met by graduate schools. The sequence blends with the other options within the department so that all students can find something of interest to them.

the text by Kuo is quite suitable. It is only a minor handicap that the text is not oriented towards chemical engineering or the process industries. The most serious text problem is the lack of a suitable text for the final course, ChE 158. This lack can only be partially offset by lecture notes and the use of the periodical literature.

Within the department, we have excellent computer facilities, and we are developing laboratory experiments suitable for the program. We have interested and capable students, and a good mesh of faculty interests and expertise. On the other hand, teaching loads in the department are very high, making it difficult to teach, do research, and to find the time to continue to develop and improve the sequence of courses in the program. It has required an almost fanatical belief in the importance of what we are doing to push the courses to their current state of development. According to Waller, this would probably be true anywhere in the country, as control theory has not been much appreciated [2].

About half of our students are in the co-op program. It is impossible for these students to take the control sequence in four consecutive semesters. Because we cannot offer extra sections of any of the courses, we have had to design the sequence so that students could take either ChE 154 or ChE 156 as the first course beyond the introductory course. This is the reason for the artificial division of the material in Kuo [4]. Though this is less than ideal, it seems to work. It should be mentioned that the work experience of the coop students, about half of the class, tends to raise the level of effort and understanding of the entire class.

The constraints of university, college, and departmental requirements so far have made it impossible to develop and include a formal laboratory course in the program. Therefore, we must sacrifice lecture time in order to provide essential laboratory process experience. Laboratory is very time consuming for students and faculty. Because of this pressure, we feel that we must provide more setup and laboratory instruction than we would like. This problem will be alleviated somewhat by development of more experiments which can be run simultaneously by different groups.

The problem here is instrumentation cost. Available computing power is more than sufficient.

GENERAL OBSERVATIONS & CONCLUSIONS

The program is, we believe, unique and valuable. There is a high demand for our graduates, and they seem to fill an obvious industrial need which is not being met by graduate schools. The sequence blends with the other options within the department so that all students can find something of interest to them. It is important to recognize that the option programs work within what most curricula consider to be technical electives. Therefore, every student completes the full ABET-AIChE accredited program in Chemical Engineering.

The "critical mass effect" has been very important. It is not only necessary that more than one faculty member be closely involved in the program, but it is equally important that the faculty have interest and expertise in certain specific areas. We found it necessary that the following areas be fully covered: mathematics, instrumentation hardware, computer hardware and software (on-line, real time system), interfacing of computer and process, computer operating system maintenance, industrial experience, and the areas of process control covered by the courses. Without skill in the above "auxilliary" areas, our program simply would not exist.

Although we feel we have developed an excellent program, we have certain constraints which we have been unable to overcome. Our students generally lack background in statistics, probability, and linear algebra. Although we do consider these topics within the sequence, we cannot spend enough time on them. We do not have sufficient time to spend on hardware, and we have no time to spend on microprocessors or assembly language. We agree with our industrial advisors that these topics are important, but we feel that the material we do cover is more important, and that any time we can "steal" must be used for laboratory work. Those students keenly interested in any of the topics mentioned above can learn more about them through courses given by the mathematics and electrical engineering depart-

ments. These courses can be taken as the fourth elective or as overload courses.

Industrial response to our process control program has been positive and encouraging. Industrial representatives have helped us to choose the material to be presented and have helped with financial support for our computer facility. Positive feedback from instrument and control system vendors and from manufacturing companies, especially pulp and paper companies, has consisted not only of verbal approval but also the ultimate test: They need, want, and hire the graduates of the program. □

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ChE book reviews

ADVANCED PROCESS CONTROL

By W. H. Ray

McGraw Hill, NY, 1981

Reviewed by John C. Friedly
University of Rochester

There are few available books suitable for a graduate-level course in chemical process control, although there are a number of more general as well as a number of more specialized advanced control texts. That fact alone would make this text a useful addition to the literature. However, this book has more to appeal to students and practitioners alike.

The book covers nearly all of the most used ideas of modern process control, from multivariable control, through optimal control, to state estimation. Ray tries to present a balanced coverage of control of both lumped and distributed parameter systems, linear and nonlinear systems, theory and practice. From the large literature

available, choice of the basic principles has been skillfully made. As in most of Ray's work the concepts are illustrated with a wealth of rather detailed examples, all pertinent to chemical engineering. In addition, there is a summary of several more elaborate case studies taken from the literature. The only noticeable omissions are parameter estimation and adaptive control.

The style is mainly expository with approaches to solving the problems stressed rather than an axiomatically rigorous mathematical treatment. As should be expected, vectors and matrices are used throughout and the manipulative skills of linear algebra are essential. For the most part, mathematical methods are introduced where needed as unobtrusive digressions in the text. The prose is eminently readable and the typescript is free of obvious errors.

The bulk of the material is jammed like meat on a delicatessen sandwich into just three rather long chapters. The advanced control concepts are first introduced in Chapter 3 on control of lumped parameter systems. Multivariable control, non-interactive control, modal control and optimal control are all covered in some detail. Both the theoretical basis and the more practical implementation of the control is discussed, including computation and approximation problems. The following chapter attempts to give the same type of coverage for control of distributed parameter systems. This is done to the extent possible and the distinctive problems associated with the more complex distributed systems are covered well. The coverage of optimal filters and observers in Chapter 5 is complete, but the concepts of stochastic control are only paid lipservice. In the same chapter both lumped and distributed, linear and nonlinear systems are included. These meatier chapters are contained between two which, while appropriate, suggest that the sandwich could well have been served open-faced. Chapter 2 gives an overview of the hardware and practical details of the use of minicomputers for process control and is virtually not referred to again in the text. The final chapter reviews several case studies from the literature that use many of the concepts covered earlier, but is also somewhat disconnected from the rest of the material in the text.

The text is not without its faults however. In using many parts of the text for a course in process control, students found that it contained a

Continued on page 46.

DIRECT DIGITAL CONTROL LIQUID LEVEL EXPERIMENT

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DIRECT DIGITAL CONTROL OF liquid level was developed at the New Jersey Institute of Technology as an experiment in the undergraduate process control laboratory. The objective of the experiment is to give the students exposure to the area of digital control which is widely used by industry, although not much attention is given to it in most undergraduate process control curricula. Students can be exposed to writing their control program, and can experimentally determine the transfer functions for all system components. They can compare the actual response of the controlled system with the theoretically predicted response following a step disturbance in the feed rate and also study the effect of sampling time on system response.

APPARATUS

The experimental set-up consists of a plexi-glass tank 0.14 meter in diameter, fed with water from the bottom through a rotameter with a maximum capacity of 0.0015 m³/s or 24.5 gpm. A Fisher Governor control valve type 657A, 3-15 psi is located on the tank outlet pipe. The original set-up, designed for pneumatic analog control includes a Foxboro Model 58P5 controller, and a 3-15 psi type 13A-1 Foxboro transducer. To provide direct digital control, a Devar Inc. air to electric converter (A/E) type 18-118L, 0-5 volts was connected to the transducer, and a Devar Inc. electric to air converter (E/A) type 18-150, 0-5 volts was connected to the control valve. Plumbing was done in such a way that the system can either be operated by the controller or by the digital computer. The digital computer installed was a

Students can be exposed to writing their control program and can experimentally determine the transfer functions for all system components.

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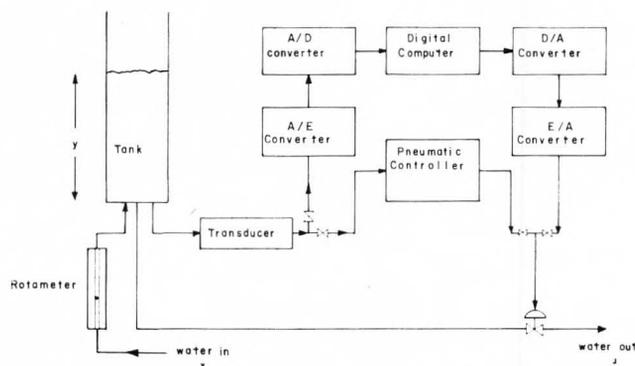


FIGURE 1. Schematic drawing of System.

Digital MINC-11 minicomputer equipped with four laboratory modules: a preamplifier, an analog to digital (A/D) converter, a clock, and a digital to analog converter (D/A). A schematic drawing of the system is shown in Fig. 1.

PROCESS TRANSFER FUNCTION

A material balance in terms of deviation values can be written as

$$A \frac{dY}{dt} = X - U \quad (1)$$

where A = tank cross sectional area; X = feed flow rate; U = outlet flow rate.

The outlet flow rate "U" is a function of the pressure to the valve "P" and the liquid level "Y". This can be written as

$$U = (\partial u / \partial y)_{ss} Y + (\partial u / \partial p)_{ss} P \quad (2)$$

where the subscript "ss" represents steady state value. Combining the above equations, transforming to the Laplace domain and rearranging gives

$$Y(s) = \frac{k_p}{(\tau s + 1)} [X(s) - k_v P(s)] \quad (3)$$

where $\tau = A / (\partial u / \partial y)_{ss}$; $k_p = 1 / (\partial u / \partial y)_{ss}$; $k_v = (\partial u / \partial p)_{ss}$.

CALIBRATION OF CONTROL ELEMENTS

1. τ , k_p can be determined by making a step change of magnitude "a" in the feed rate while the analog controller is placed on manual status.



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The two parameters can be calculated from the equation

$$Y = ak_p[1 - \exp(-t/\tau)] \quad (4)$$

2. With liquid level being kept constant, and the controller on manual status, Eq. (3) can be written as

$$\frac{P(s)}{X(s)} = k_v \quad (5)$$

The valve transfer function k_v can be obtained by changing the flow rate to the tank and varying the pressure to the valve to keep the liquid level at a specified value.

3. In a closed loop experiment with proportional control only, the proportional band was set at 25, and the set point on the recorder controller was set at 9 psi. From the chart recorder, values of the error and pressure to the valve were obtained and the proportional control gain k_c can be calculated.
4. The transducer transfer function was obtained by changing the water level in the tank and recording the resulting transducer output (in psi as obtained from the chart recorder).

THEORETICAL RESPONSE FOR CONTINUOUS SAMPLING

The closed loop transfer function for a proportionally controlled system can be written as

$$\frac{Y(s)}{X(s)} = \frac{k_p}{(\tau s + 1) - k_c k_p k_v T} \quad (6)$$

For a step change from 18% to 30% on the rotom-

eter scale and utilizing the following experimentally determined parameters.

$$\begin{aligned} k_p &= 17.85 \text{ min/ft}^2, (1.153 \text{ s/m}^2) \\ k_v &= -0.151 \text{ ft}^3/\text{min}\cdot\text{psi}, (-1.034 \\ &\quad \times 10^{-3} \text{ m}^3/\text{s}\cdot\text{Pa}) \\ k_c &= 3.53 \text{ psi/psi}, (3.53 \text{ Pa/Pa}) \\ T &= 2.98 \text{ psi/ft}, (6.74 \times 10^4 \text{ Pa/m}) \\ \tau &= 176.40 \text{ s} \end{aligned}$$

The solution of the above equation for liquid level deviation in the units of meters can be written as

$$Y = 0.0729 [1 - \exp(-0.1664t)] \quad (7)$$

where the time units are seconds.

DIRECT DIGITAL CONTROL

Liquid level was converted to an air pressure signal through the transducer, then to an electric voltage signal through the A/E converter, and finally to a digital signal through the A/D converter. The developed computer program compares the measured liquid level to the set point, thereby generating the error. Control actions provided in the software were; proportional (P), proportional-integral (P-I), proportional-derivative (P-D), and proportional-integral-derivative (P-I-D).

For continuous sampling an ideal P-I-D controller is described by the following equation.

$$V = V_o + k_c \left[e + \frac{1}{\tau_I} \int_0^t e dt + \tau_D \frac{de}{dt} \right] \quad (8)$$

Where

$$\begin{aligned} V &= \text{controller output signal at time } t \\ V_o &= \text{controller output signal at } t = 0 \\ e &= \text{error signal} \\ \tau_I &= \text{integral time} \\ \tau_D &= \text{derivative time} \end{aligned}$$

The discrete equivalent of the above equation can be obtained by replacing the derivative with finite difference, and using rectangular integration for the integral. The computer output at the n th sampling instant can, therefore, be written as

$$V_n = V_o + k_c \left[e_n + \frac{T}{\tau_I} \sum_0^n e_n + \frac{\tau_D}{T} (e_n - e_{n-1}) \right] \quad (9)$$

where

$$\begin{aligned} T &= \text{sampling periods, seconds} \\ V_n &= \text{computer output at the } n\text{th sampling instant} \end{aligned}$$

e_n = error at the nth sampling instant
 e_{n-1} = error at the (n-1) sampling instant

Similarly at the (n-1)th sampling instant, the equation for the output is

$$V_{n-1} = V_o + k_c \left[e_{n-1} + \frac{T}{\tau_I} \sum_0^{n-1} e_n + \frac{\tau_D}{T} (e_{n-1} - e_{n-2}) \right] \quad (10)$$

Subtracting Eq. (10) from Eq. (9) gives

$$V_n = V_{n-1} + k_c \left[(e_n - e_{n-1}) + \frac{T}{\tau_I} e_n + \frac{\tau_D}{T} (e_n - 2e_{n-1} + e_{n-2}) \right] \quad (11)$$

In the sampling method adapted in this experiment one point (y_2) was collected at the start of each sampling loop and the error e_n was calculated. This error was used along with the errors e_{n-1} and e_{n-2} according to Eq. (11) to formulate the computer output signal. The next loop began with the collection of a new data point (y_2) and calculating a new error e_n the old value of e_n was transferred to e_{n-1} , the old value of e_{n-1} was transferred to e_{n-2} , and the old value of V_n was transferred to V_{n-1} . The fastest sampling rate was approximately one sample every 0.12 second for proportional control. A pause statement was also incorporated in the program to introduce a time delay, thus varying the sampling rate. The software also contained a program for calibrating the "transducer + A/E" converter, and a program for calibrating the "E/A converter + valve." Fig. 2 represents the block diagram for the digital control loop. The output of the A/E converter which is a continuous electric signal of the measured variable is fed to the A/D converter. The A/D converter changes the continuous signal to a discrete form (series of impulses of varying

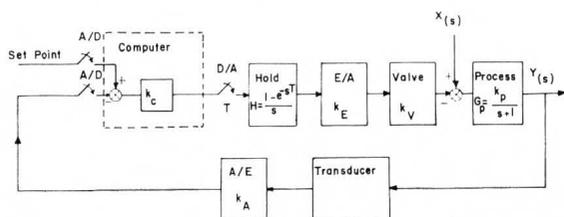


FIGURE 2. Block diagram representation of the digital control loop.

strength). The computer compares the discrete forms of set point and measured value to produce the error, and acts on the error by the appropriate control algorithm. The output of the computer generated every "T" seconds is sent to the D/A converter where a continuous signal is produced. In effect, the D/A converter clamps on the signal until the next one comes along; i.e. the output voltage of the D/A converter remains at a constant value over the sampling period. The D/A converter, therefore, acts as a holding device. For a zero-order holding device, the transfer function is

$$H = \frac{1 - \exp(-sT)}{s}$$

The analysis of a discrete system is conveniently done in terms of z-transforms, defined as

$$F(z) = Z[f(t)] = \sum_{n=0}^{\infty} f(nT) z^{-n} \quad (12)$$

The use of the z-transform in discrete systems is analogous to the use of Laplace transform for continuous sampling, and the Laplace transforms are usually tabulated alongside the time function and the corresponding z-transforms [1]. This allows direct conversion from the Laplace transform of a continuous function to the z-transform of that same function.

The closed loop transfer function for the system

$$\frac{Y(z)}{X(z)} = \frac{G_p(z)}{1 - (Tk_A k_c k_E k_V H G_p)(z)} \quad (13)$$

Since T, k_A , k_c , k_E , k_V are constants, they can be combined in one term as K, and the output variable can be written as

$$Y(z) = \frac{(XG_p)_z}{1 - K(HG_p)_z} \quad (14)$$

What is needed are the values of $(XG_p)_z$ and $(HG_p)_z$ to plug in the above equation

$$\begin{aligned} Z(XG_p) &= Z \left[\frac{a}{s} \frac{k_p}{\tau s + 1} \right] = Z \left[\frac{ak_p}{s} - \frac{ak_p}{s + 1/\tau} \right] \\ &= ak_p \left[\frac{z}{z-1} - \frac{z}{z - \exp(-t/\tau)} \right] \end{aligned}$$

Let $e^{-t/\tau} = b$. Then

$$Z(XG_p) = \frac{ak_p(1-b)z}{(z-1)(z-b)} \quad (15)$$

Also

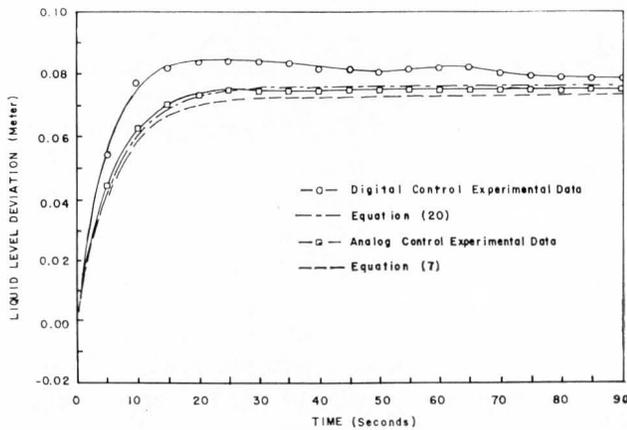


FIGURE 3. Comparison between experimental and theoretical responses.

$$\begin{aligned}
 Z(HG_p) &= Z \left[\frac{k_p}{\tau s + 1} \frac{1 - \exp(-Ts)}{s} \right] \\
 &= Z \left[\frac{k_p [1 - \exp(-Ts)]}{(\tau s + 1) s} \right] \\
 &= k_p (1 - z^{-1}) Z \left[\frac{1}{s(\tau s + 1)} \right] \\
 &= \frac{k_p (1 - b)}{(z - b)} \quad (16)
 \end{aligned}$$

Substituting and rearranging gives

$$\begin{aligned}
 Y(z) &= ak_p (1 - b) z \left\{ z^2 + z [Kk_p (b - 1) \right. \\
 &\quad \left. - (b + 1)] + [b - Kk_p (b - 1)] \right\} \quad (17)
 \end{aligned}$$

with values of

$$\begin{aligned}
 k_A &= 0.358 \text{ volt/psi, } (5.1924 \times 10^{-5} \text{ volt/Pa}) \\
 k_E &= 2.649 \text{ psi/volt, } (1.8264 \times 10^4 \text{ Pa/volt}) \\
 K &= -1.51 \text{ ft}^3/\text{min}\cdot\text{ft, } (-2.3381 \times 10^{-3} \text{ m}^3/\text{s}\cdot\text{m})
 \end{aligned}$$

To examine the effect of sampling time on the stability of the system one has to substitute different values of sampling time in the above equation and find the values of denominator roots. If the roots are located within the unit circle of the z-plane, the system is stable [2]. The following table shows the values of the roots at different sampling time.

TABLE OF ROOTS

Sampling Time	Roots
0.12 sec.	+1.000, +0.981
1.0 sec.	+1.000, +0.842
5.0 sec.	+1.000, +0.220
10.0 sec.	+1.000, -0.563
12.0 sec.	+1.000, -0.831
13.0 sec.	+1.000, -0.982
13.1 sec.	+1.000, -1.000
14.0 sec.	+1.000, -1.128

Notice that second root decreases in value as the sampling time increases and the system becomes theoretically unstable when the sampling time is above 13.1 seconds. It can therefore be stated that increasing the sampling time would destabilize the system.

For a step change from 18% to 30% on the feed rotameter scale, and for a sampling time of 0.12 seconds, Eq. (7) reduces to

$$\begin{aligned}
 Y &= \frac{0.001452 z}{z^2 - 1.98103 z + 0.98103} \\
 &= 0.0759 \left[\frac{z}{z-1} - \frac{z}{z-0.981} \right] \quad (18)
 \end{aligned}$$

The pole 0.981 can be expressed as

$$0.981 = \exp(-aT) = \exp(-0.0192)$$

$$Y = 0.0759 \left[\frac{z}{z-1} - \frac{z}{z - \exp(-0.0192)} \right] \quad (19)$$

Inverting to the time domain gives

$$Y = 0.0759 [1 - \exp(-0.0192n)] \quad (20)$$

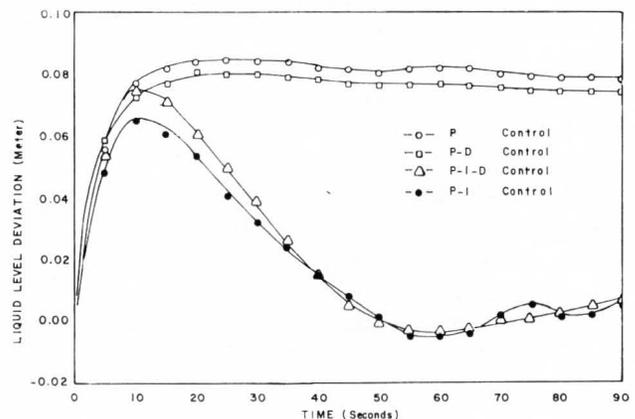


FIGURE 4. System response for different control modes under digital control.

RESULTS AND DISCUSSION

Eq. (7) and Eq. (20) are plotted in Fig. 3 along with experimental data taken with analog proportional control, and digital proportional control at 0.12 seconds sampling interval. Agreement between the equations and the actual response was quite good.

Fig. 4 shows the response of the system at the fastest sampling time to a step change in the feed rate using proportional control ($k_c = 3.53$ volt/volt), proportional-integral control ($k_c = 3.53$ volt/volt, $\tau_I = 20$ seconds), proportional-deriva-

Continued on page 47.

SURVEY: COMPUTER USAGE IN DESIGN COURSES

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WE REPORT HERE THE results of a survey of chemical engineering departments regarding computer usage in senior design courses. All chemical engineering departments in the United States and Canada were polled, and two-thirds responded. That the sample was representative was verified by checking the number of schools reportedly using FLOWTRAN (12) against the actual number (18): (Personal Communication, Prof. J. D. Seader, University of Utah, CACHE Corp.).

FINDINGS

A. COMPUTER USAGE

1. Use of Process Simulators

Forty seven of the ninety eight schools responding used process simulators. The most popular were: CHESS (15), FLOWTRAN (12), CHEMSHARE (5), GEMCS (4), ASPEN (2).

2. Student-Written Programs

Fourteen schools responded that the students write programs in the design courses.

3. Faculty-Written or "Canned Programs"

Four of the five schools using canned

programs included CSMP on their list.

Many schools use mixtures of the above, as follows

- 1. + 2. Number of Schools = 7
- 1. + 3. Number of Schools = 4
- 2. + 3. Number of Schools = 25
- 1. + 2. + 3. Number of Schools = 30

Only seven schools do not use the computer in the senior design courses.

B. Cost of Computer Usage

The schools were asked how much they spend on computing per student, and whether the funds came from "soft" or "hard" sources. The replies were

Soft Money

- \$ 10 - 30 : 13 schools
- 31 - 70 : 12 schools
- 71 - 150 : 18 schools
- 151 - 300 : 9 schools
- 301 - 500 : 6 schools
- 501 - 1500 : 3 schools

Average: \$178/school

Average for Schools Using Simulators:
\$221/school

Hard Money

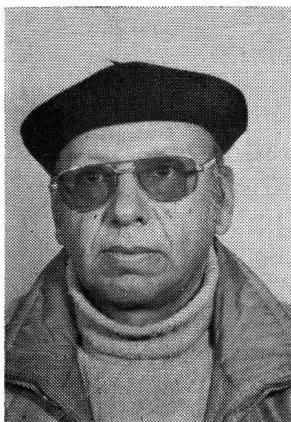
- \$10 - 30 : 4 schools
- 31 - 100 : 7 schools (4, partial soft)
- 331 : 1 school (partial soft)
- 500 : 1 school

C. Available Software

One of the questions was whether the schools had software they would share with other schools. This produced the list shown in Table I. Entries 14-17 reflect the recent decision of the four major purveyors of industrial-level simulators to make their products available to Universities. Except for the case of ASPEN, only load models are being provided. These, of course, are computer dependent.

CONCLUSIONS

The use of large simulators in senior design courses is clearly established. Over sixty five percent of the schools will be using them in 1983. Computing costs are high. Unmonitored student use can easily result in expenditures of over \$1,000/student. □



Ernest J. Henley has been a professor of chemical engineering at the University of Houston since 1964. He received his Ph.D. from Columbia University in 1953 and has been on the faculty of Columbia University and Stevens Institute of Technology.

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TABLE 1. Programs Offered

NAME	UNIVERSITY	DESCRIPTION
1. Dr. R. D. Weir	Royal Military College of Canada	CALYPSO—Neutron Diffusion Code
2. John A. Meyers	Villanova University	Activity coeff. from data. Tray efficiency Antoine constants from data HTU in packed column. Multipass ht. exch. Non-ideal binary x-y. Linear and non-linear regression. Tray by tray by relaxation. Multicomponent distillation.
3. Jim Douglas	University of Massachusetts	Process synthesis programs (in preparation)
4. John H. Erbar Jan Wagner	Oklahoma State University	PAS, MINISIM (General purpose simulators similar to CHESS, FLOWTRAN, etc.)
5. Paul Babcock	University of Connecticut	GEMS, FLOWSIM under restrictive agree- ments
6. R. L. Motard	Washington University, St. Louis	CHESS (\$1000/school)
7. M. V. Svrcek	University of Calgary	HYSIM, HYDIS, (property of Hydrotech Ltd. of Calgary)
8. W. D. Seider	University of Pennsylvania	GIBBS, Chemical and phase equilibrium. HETDIS, three-phase distillation
9. B. A. Finlayson	University of Washington	DISTIL—Shortcut distillation
10. E. J. Henley	University of Houston	BCOST—Equipment costing and economic analysis
11. Alberto I. LaCava	City College of City University, NYC	Parametric Estimation. Dynamic Simulator. Nonlinear Equation Solver.
12. John L. Potter	New Mexico State University	Economic Evaluation. PCS (written by J. Erbar)
13. R. F. Benenati	Polytechnic Institute of New York	Comprehensive collection covering unit ops suitable for microprocessors (Fall, 1982)
14. Vickie Jones	CACHE, #3062MEB University of Utah	FLOWTRAN (Load Module Only)
15. Larry J. Lesser	CHEMSHARE, P. O. Box 1885, Houston, TX 77001	DESIGN/2000 (Load Module only)
16. Jim Byrne	Simulation Sciences, Inc. 1400 North Harmor Blvd. Suite 250, Fullerton, CA 92635	SIMSCI (Load Module only)
17. Margaret Butler	National Energy Software Center 9700 South Cass Ave., Argonne, IL	ASPEN (IBM, UNIVAC and VAX Ven- sions)

TUTCHE - A PROGRAM PACKAGE FOR TUTORING CHEMICAL ENGINEERS*

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J. ALONSO
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ALL ENGINEERS, AND particularly chemical engineers, have needed to bring to their professional activities a blend of inspiration, information and perspiration. A common complaint about the academic training of engineers is cogently expressed in the Finneston Report where it is concluded that not enough attention has been paid, in the recent past, to developing the inspirational aspects of design. This report recognizes the need for more time and effort to be devoted to training in design methodologies but, apart from one brief reference and recommendation, it fails to anticipate the impact that developments in computing techniques would have in the areas of training and design methodology.

As computer technology has evolved in the directions of large efficient time-shared machines on the one hand and more powerful desk-top mini-computers or micro-processors on the other we are witnessing significant changes in the ways in which we tackle the design both of individual units and of integrated systems. It is particularly in the opportunities that we now have for examining alternatives in large scale "integrated" designs that we can see the greatest impact.

All the major chemical manufacturers, oil refiners, plant contractors and design offices have built up their computer-aided engineering activities over the past fifteen years so that they now possess significant libraries of well proven programs for use by their staff. The smaller firms may not have been able to spare the effort to develop the soft-ware themselves but in many instances make use of bureaus which have established themselves as reliable sources of design capacity on large, shared, computers.

*A revised version of a paper originally presented to the 1979 Montreux Conference—"Computer Applications in Chemical Engineering."

The smaller firms may not have been able to spare the effort to develop the soft-ware themselves but in many instances make use of bureaus which have established themselves as reliable sources of design capacity on large, shared, computers.

Clearly, the universities have a responsibility to ensure that when their graduates emerge they are prepared to work in this new manner and many academic institutes have not been slow to recognise the potential for using computers to improve their teaching and training activities. The original CACHE committee which published a well-known set of some 112 programs in 1972 is now a Corporation which is fostering these activities in the U.S.A. Of these the most ambitious is the CHEMI project which aims to produce some 500 tried and tested instructional modules. CACHE also supports the use of FLOWTRAN as a networked flow-sheeting package and has now initiated a project to develop and exchange Micro-computer Aids for Chemical Engineering.

CHICHEE and EURECHA have encouraged parallel but smaller scale activities in the United Kingdom and Europe.

Most of the activities referred to above were directed to exploiting batch computing facilities but it became apparent in the late '70's that developments in low-cost interactive computing were going to have the most significant impact on Computer-Aided Design (in all its shades of meaning) and that, potentially, this mode of computation could be of equal importance for the development of Computer-Aided learning. It was these considerations which led the authors to examine the problems of constructing a package which would be designed to take advantage of the vibrant characteristics of this mode of working.

After some initial trials using an existing Cyber 72, the hard-ware described in the next section was acquired to evaluate the package under conditions which would provide some 250 chemical

engineering students (3 years of B.Sc. and 1 of M.Sc.) with a novel experience and also permit colleagues in other departments to take advantage of the facility in order to develop teaching packages appropriate to their own disciplines.

HARDWARE

The hardware to be described is as it will be at the completion of the first phase of the project and is the best that we could afford and most appropriate for the computers available to us. It should be stressed that the TUTCHE package does not depend on this hardware and could be run on any interactive system ranging from a single-user mini with a 10 char/sec teletype to a multi-user main frame provided with a large number of (colour) graphics terminals. We had outgrown the former but could not afford the latter.

The compromise was to set up three clusters of five terminals arranged as shown in Fig. 1. In any one cluster all five terminals have an upper and lower case alphanumeric capability, three have a graphics capability which is required to give a full Tektronix 4010 emulation and one of these has a micro-processor capacity (twin 5½" floppies) so that it can work in "stand alone" mode or in transparent mode when it behaves as an α /graphics terminal. All five may be connected by a simple multi-pole switch to an α /graphics printer with extended buffer storage that enables any one user to dump a "page" as displayed at the terminal onto the printer. (We should remark,

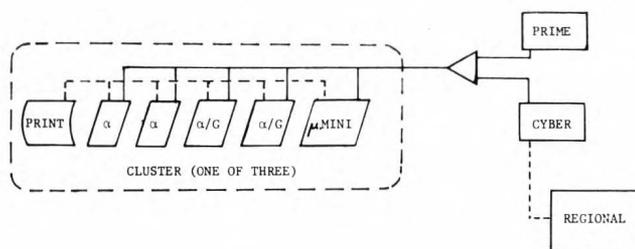


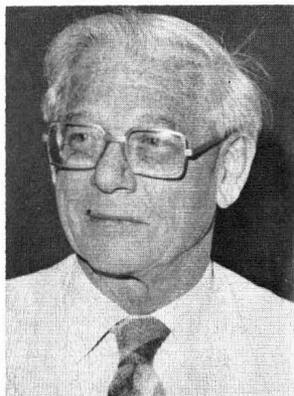
FIGURE 1

here, that we have had no problems with α -numeric displays and printing, but we are still not satisfied with the copying of graphics display and are currently examining alternatives.) The ambition is to progressively upgrade the alphanumeric terminals as funds and graphics requirements increase.

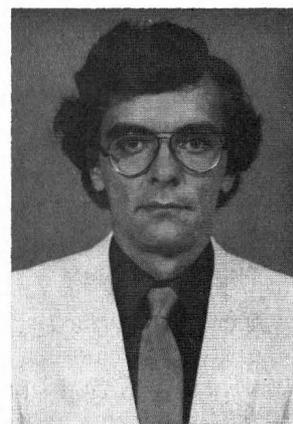
Any of the fifteen terminals in the suite will be connected via a "Gandalf Switch" to various machines and currently we may access either a Prime 750 or a Cyber 172 both of which provide time-shared interactive operation at linespeeds of 2.4kB which is just about the lowest acceptable rate for graphics work and is a very comfortable rate for conventional dialogue.

The Prime has proved to be a very effective machine since, up to the limits of the locally set connection limit, it gives a very fast response to "trivial" dialogue—i.e. during data input sessions. An important feature that we have been able to exploit is a "shared code" facility which means that when all fifteen terminals are used by students on the same tutorial exercise we can arrange

F. P. Stainthorp graduated in chemical engineering from Manchester in 1941. After eight years in industry he was transferred to University College, London to work for his doctorate and then returned to chemical industry for a further six years. He was recruited to Manchester, UMIST, at a time of expansion with a special remit to cultivate the growing fields of process control and digital computation. He is chairman of CICHEE and directs the chemical engineering computing service at UMIST. (L)



David Lomas is a member of the British Computer Society and has spent most of his working life in University engineering departments first as a programmer but lately as the supervisor of the chemical engineering computing service at UMIST. He has made a special study of the problems of transferring nominally 'standard' programs between different computing systems. (C)



J. Alonso received his Chemical Engineering and MSc. degrees from the Universidad Central Venezuela in 1972 and IVIC 1976, and his Ph.D. degree from the University of Manchester England in 1979. He currently is lecturer of process simulation at the Universidad Central Venezuela and his interests have generally been in software developments. (R)

for only one copy of the program to be resident in the machine. This has the big advantage of enabling the normal load of other users to be satisfied without them seeing a significant impact from the student users.

The Cyber 170, having nearly 200 terminals connected across two campuses, tends to get overloaded at peak times, but a scheduling facility in the switch should ease this problem in the future. The big advantage of this machine is that it is linked to a CDC 7600 which is used to process the largest design packages. In this mode of working the intention is to use the interactive machine for validation and preprocessing activities that generate a suitable data file for subsequent batch processing in the larger machines. The interactive system is also used for post-processing the output files resulting from the batch machine so that only selected material required for permanent record need be printed.

SOFTWARE

Fig. 2 is a diagrammatic representation of the overall structure of the package which is shown in this manner for ease of discussion of the various components. There is some correspondence with the actual system since many of the programs need to use common data files and in general only one program will be in use by a student at any

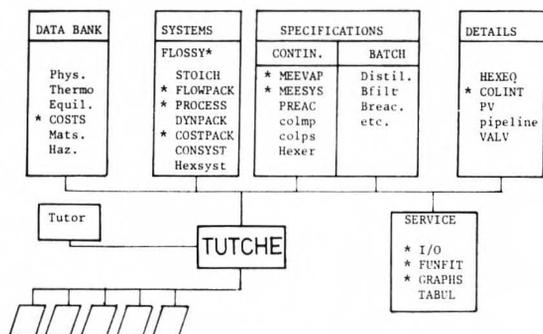


FIGURE 2

one time. We think of four banks which contain, respectively, common data, overall systems related programs, unit design specification programs, and detail design programs. Another bank contains a library of service programs or sub-routines which can be used to deal with input/output problems, graphical interactions, function fitting etc. Each component of the total package communicates with the user via a dialogue that is appropriate to the application. On the first occasion that a

On subsequent occasions abbreviated prompts are used but the student may always ask for "Help," whereupon the abbreviations are explained and amplified if further requests for help are made.

program is used the requests are full but not verbose. On subsequent occasions abbreviated prompts are used but the student may always ask for "Help" whereupon the abbreviations are explained and amplified if further requests for help are made. We also find it convenient to include a switch that enables the frequent user of a particular program to suppress the dialogue.

TUTCHE/TUTOR

Students gain access to the suite via a program named TUTCHE. This program is a purpose written data base management system which serves to control and record the use of the various programs by the students. It also tidies up the student's own data and results in files on exit so that they may be retrieved reliably on re-entry.

TUTOR is a separate interactive program which enables a tutor to examine and modify the record held in TUTCHE. The use made by all students of any one program may be displayed or the record of programs used by any one student may be examined. In some cases a permit has to be set and continued use of a program may be contingent upon monitored successes at selected points. The tutor may insert, examine and modify these controls through TUTOR.

This control is not a case of "Big Brother watching" since, in the main, the programs are directed to use by responsible and mature students who each work at their own pace but within constraints imposed by the capacity of the resources. Examples of the regulation of use will be given later but in general they either ensure that the student has understood the fundamentals of the tutorial exercise and is not using the program as a "black-box" or they serve to curb extravagance on open-ended exercises. This discipline is intended to correspond to that which they will find necessary in industrial environments when the use and time has to be paid for.

The titles shown in Fig. 2 are those that form the current basis for the package. Those marked with an asterisk have reached the stage of regular student use, those in capitals but not starred are undergoing trials and those in lower case are still

ics of various alternatives and ends up with a design which satisfies some agreed criterion.

With MEESYS, access to which may be contingent upon demonstrated successes with MEEVAP, the student can explore the economic benefits of introducing heat-exchangers to preheat the feed and/or the addition of condensate flash recovery.

Automatic optimisation is deliberately excluded from these packages but the student needs to be able to compare several designs so an essential component of the package is a facility to generate tables which collate nominated variables for a sequence of runs. Fig. 4 is an example of

NR	FS	NE	AE	PS	ULE
6 BAC	0.581	5.00	65.0	257.	2.50
5 BAC	0.660	5.00	65.1	273.	7.50
7 BAC	0.665	4.00	65.0	254.	2.50
4 BAC	0.702	5.00	72.9	240.	7.50
3 BAC	0.772	4.00	71.2	240.	7.50
2 BAC	0.910	3.00	69.6	240.	7.50
1 FOR	0.984	3.00	69.7	240.	7.50
NR	FS	NE	AE	PS	ULE

FIGURE 4

such a table in which the runs have been ranked in order of increasing flow of steam to the first effect.

EXPERIENCES AND OBSERVATIONS

After two years experience at using the package at UMIST and some attempts to transport parts of it to other departments with different systems we can comment on some aspects which seem to us important.

There is no doubt that the impact made by a well-prepared interactive exercise can be substantially greater than a conventional tutorial. The opportunity for the student to examine aspects of design which calculation time would hitherto have prevented is particularly welcome. We would certainly endorse the experiences of those such as our colleagues at Illinois, who find the PLATO system so effective. However, we also recognise that a considerable effort is required to generate the program, exercises and support documentation needed for each module in the packet. We believe that the only solution to this problem is to ensure that the packages receive wide distribution and use by generating modules to agreed standards and by enlisting the co-operation of several authors in many departments so that modules may be exchanged.

The original version of the package was written, as far as possible, in strict FORTRAN4

(ANSI 66) but we have now rewritten it to conform to strict FORTRAN77 (having looked at PASCAL and rejected it). There are still several machine dependant features, however, connected with file creation, opening and closing, I/O procedures, graphics or quasi-graphics. Our solution to the problems in these areas is to confine them to a few sub-routines which have been coded so that the local peculiarities may be incorporated during the initial setting up. Particular attention has been paid in writing the I/O procedures to making the dialogue "user friendly" and to trapping spurious or invalid responses.

The students need to be prepared for this type of tutorial work by providing them with concise documentation which sets out clearly the initial objective and encourages them to extend the exercises in an imaginative way. We arrange to schedule the terminals so that their use coincides with other practice and laboratory classes and find sessions of about 45 minutes to be about optimal. □

WILHELM'S INFLUENCE

Continued from page 15.

gave in Montreal in 1961 so much sums up his work that it is worth examining in a little more detail. The flavor of the argument and its presentation will have been gained from the lengthy extraction which was quoted above; here I would like to lay out its main lines. After an historical introduction Wilhelm divided the field of reactor studies into three parts. These were classified according to the difficulty of applying design objectives and the first was that part which seemed beyond immediate *a priori* design objectives because of incomplete theory. The second was the domain of moderately well-understood processes and the third was that part which was already developing rapidly. In 1962 he saw flame theory with its rapidity of reaction and complicated thermodynamics and other systems in which turbulent fluid dynamics plays a part as in the first category. Fortunately, the second category was larger and comprised most of the conventional reactors for which sensible models had been constructed. The incorporation of some of these reactor types into the third area of well-understood systems was the thrust of his own concern and, as he said, "I have chosen the packed bed reactor, a device which clearly falls in the third category, as the specific subject of my paper."

He commented that historically the packed

bed reactor is one of the oldest arrangements for conducting gas-solid or liquid-solid chemical reactions on an industrial scale, but that the component parts which he proceeded to analyze had only more recently come under investigation. He divided this into the external field model, the interparticle field, the interphase field and the intraparticle field. In the first case he summarized, with masterly touch, the state of knowledge on axial and radial dispersion in the packed bed, an area to which he had himself contributed so much. He then turned aside to comment on the Lapidus-Dean cell model, recognizing its potentials and limitations. He also mentioned in passing the currently exciting work of correlating experimental data on kinetics with scientific, rather than empirical, expressions for the reaction rate. Non-linear estimation of constants was at that time a comparatively new topic and he draws attention to some of the work that was going on. In connection with the interparticle field he remarked on the calculation of temperature and other profiles in the bed, the subject of one of his earlier papers (1943). However, he quickly turned to the question of the interphase field by which he meant the diffusion-reaction problem at the surface of a particle, then to the internal diffusion problem, showing how the Thiele modulus could be recognized by considering the relative rates of reaction and diffusion. In particular he rejoiced in the practical test for diffusional effects which had been proposed by Weisz [38].

To sum up I think it is fair to say that of the pioneers of chemical reaction engineering Wilhelm stands out for his marriage of the concept of *a priori* design, as he called it in his 1962 review, and the laboratory-scale experiments that would be needed to understand the physical effects. In contrast to Hougen and Watson and their school he did not pursue reaction kinetics or attempt to fit these data in any systematic way, though he had a keen appreciation of the importance of catalysis as shown, for instance, by the early appointment of Boudart to his department. He saw the interaction of chemical and physical rate processes as central to the design of chemical reactors and established a research program that would elucidate the different factors which might bear upon it. He was not so concerned, as was Amundson, with the dynamics or behavior of the reactor though he was interested in the fluctuating processes as they gave insight into the transport properties. In the dominant part of his research

he chose to investigate the properties of the tubular and packed-bed catalytic reactors, but this did not prevent him from looking at other types as in his work on fermentors and, more especially, in his continued interest in fluidized beds. His 1962 plenary lecture represents his mature reflection on the whole question of design. It is not his last publication, for he was about to turn to a fruitful preoccupation with parametric pumping, but it may serve as a *terminus ad quem*. "I wish to suggest," he there said in conclusion, "that substantial progress has been made, in the case of packed-bed reactors toward the goal of being able to design such reactors from basic principles, rapidly and for realistic systems. The supporting physical and engineering sciences and the development of computational capabilities are sufficiently well advanced to encourage computational design explorations, at least in selected cases. A major problem, always, is to secure reliable chemical rate data and any wide-spread trend toward computational simulation may well serve to encourage the undertaking of basic laboratory chemical rate studies even more than at present. A need for continuing research in certain engineering aspects of chemical reactors is indicated." And indeed, the work has gone on well,* it is now celebrated by a biennial International Symposium and perhaps, more than any other branch of chemical engineering, has shown its intrinsic vitality—a spur to engineering research, an incentive to physical and chemical experimentation, and both the stimulator and benefactor of applied mathematics.

CONCLUDING UNSCIENTIFIC POSTSCRIPT

The last time I recall meeting Wilhelm was in the spring of 1965. His thoughts had been turning to parametric pumping for some time and in connection with this he had more to do with biological workers than before. In May of that year a conference was held under the auspices of the International Society for Cell Biology at the Villa Falconieri. A very pleasant villa it was, situated above the hill town of Frascati and overlooking the plain that was once the northern end of the Pomptine Marshes and, in the distance, the southern aspect of the city of Rome. We assembled there from all sorts of places one Sunday evening in May, seeing old friends and meeting new acquaintances. I remember Wilhelm's eager interest in what

*This growth is illustrated by the multiplication of texts and monographs on chemical reaction engineering.

each was doing and the unpretentious enthusiasm with which he spoke of his own work. I recalled that occasion when, a few years later, I read Dick Toner's beautifully written Memorial Statement in the issue of I. and E.C. Fundls. in May of 1969. He drew attention to the very meetness of an issue filled with papers written by former students, colleagues and friends who had worked with Wilhelm during his lifetime. "For it is through what these men are now doing", Toner wrote, "and will continue to do that his influence on chemical engineering will continue to be exerted. It is likely that he would have regarded this Memorial Issue as the greatest honor ever accorded to him." □

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APPENDIX

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INTEGRATING CHEMISTRY, ENGINEERING

Continued from page 19.

quently means that the difficulty of performing calculations obscures the importance of the chemistry. The examples which are chosen must therefore involve some simplifying approximations. These simplifications may be introduced by the instructor, but in many cases the key idea in making the simplification can be suggested by the students. For example, feedstocks for petroleum refining consist of a very large assortment of paraffins, naphthenes, aromatics, and heteroaromatics. Reforming this complex mixture involves many reactions. However, a grouping of these reactions into paraffin isomerization, naphthene isomerization, paraffin dehydrogenation, naphthene dehydrogenation, hydrocracking, and dehydrocyclization permits a reasonable choice of temperatures and pressures to be made on the basis of thermodynamics. Students can calculate the effect of temperature and pressure on equilibrium constants for the reaction of representative components in a naphtha stream. Similarly, calculations for coal processing routes cannot proceed quickly without significant simplifications in the representation of the composition of coal. One of the most drastic suggestions (which can be used most successfully) is to consider coal to be essentially carbon. There are pitfalls in these calculations, and the tentative nature of this approach must be emphasized. However, such methods can successfully reinforce the importance of quantitative reasoning. In addition, they illustrate that crucial chemical insights concerning composition and reactivity guide the calculations.

Fundamental concepts of stoichiometry, thermodynamics, kinetics, reactor design, and heat and mass transfer provide a basis for performing calculations. The calculations are not as detailed as those encountered in a traditional design course; rather, an emphasis is placed on "screening" calculations, the precursors of equipment design calculations. These are in close juncture with the processing chemistry. Thermodynamic calculations are useful in evaluating stoichiometry or predicting product distributions. An excellent example is synthesis gas conversion. The stoichiometry may be written to indicate methanol production, but methane, higher alcohols, and paraffins may all be present in significant amounts under industrial conditions. The effect of temperature and pressure on these reactions can be easily

quantified. Similarly, the heat released in the nitration of benzene can be determined; by combining this information with activation energies, students can demonstrate the potential for reaction runaway. The heat released in this reaction clearly illustrates the importance of heat transfer and control in the creation of a process flowchart.

An illustration involving underground coal gasification is given in the Appendix. This problem is typical of systems involving feedstocks with complicated chemical compositions. By using a simplified composition, the stoichiometry of several key reactions can be written. Since the key gasification reactions at low temperature (methane formation) are endothermic, other reactions (such as combustion) are required to provide the necessary energy. The students are asked to determine whether it is feasible to gasify a particular coal. The open-ended nature of this question is intentional. The results depend on the particular choice of reactions. Similar thermodynamic criteria may be introduced in ammonia synthesis in demonstrating the effect of temperature or pressure on equilibrium yields or in determining the importance of carbon monoxide impurities. The importance of the reverse water-gas shift reaction in controlling the temperature in methanol synthesis may also be clarified using elementary thermodynamics.

TEACHING THE COURSE

The emphasis in the course on synthesis and invention creates a sharp contrast with other chemical engineering courses. Classroom activities are similarly distinct. We have scotched the traditional lecture format for a much more informal orientation. Central to the approach are oral expression and exchanges, spontaneity, rapid changes and creation, and competition. All classroom techniques are designed to maximize the students' participation in the conceptualization of processes. The intent is to devise an environment more consistent with industrial experience. The style, language, and pace of industry are much different from those of the conventional classroom, and we have attempted to provide a transition to the industrial environment in this course.

The case study approach is useful in promoting this atmosphere. Typically, only one or two periods are spent on a process. The case studies are team taught, and student participation is encouraged by frequent alternations in faculty

leadership. All participating faculty are usually present in the classroom; their presence is invaluable in posing questions about processes, in suggesting alternatives, and in encouraging informality.

Spontaneity is the most distinctive characteristic of the classroom sessions. The classroom functions as a model of the industrial "brainstorming" session. We attempt to create this atmosphere in several ways. We encourage "off-the-top-of-the-head" ideas; rapid-fire question-and-answer participation is included. Ideas are sorted out and recorded quickly to prevent the loss of any concepts. Critical evaluation is particularly avoided at some points in the course. Ideas are solicited from all members of the class (making small classes helpful). Eventually, the spontaneity must be managed in a give-and-take atmosphere. The instructor can adeptly allow "dull" ideas to be left aside. And absolutely wrong ideas (e.g., fraudulent thermodynamic reasoning) must be clearly identified as being erroneous.

Competitive events are included—again reflecting an industrial flavor. Small groups are frequently formed in the class, and these groups typically present their ideas during the class. The efforts of one group in a particular event are shown in Figure 2. In this circumstance, groups of about five students were required to create a flowchart for reforming of naphtha. The creation was to proceed by stages: there were three time periods of about ten minutes during which the groups could create and modify flowcharts. Each of these periods was followed by an oral presentation of the flowchart and the basis for the reasoning. Critical evaluation by the students and faculty was performed to determine key innovations or errors. (This class period had been preceded by a discussion of the basic chemistry of reforming.) The results for most groups have been very close to the actual flowsheet for reforming.

Other competitive events are also employed. Alternative processes may be presented by faculty advocates. Strong claims and contradictions can be introduced. Students are then asked to present their own evaluations. These roles can also be reversed. Students can be asked to defend specific aspects of given processing chemistry. One successful event has dealt with rival choices for a catalyst. Two instructors (each a "salesman" for a catalyst) were permitted to answer specific questions about their catalysts, but only questions raised by the students. Thus, the students had to

FLOWCHART SEQUENCE KEY CHEMICAL AND ENGINEERING INSIGHT

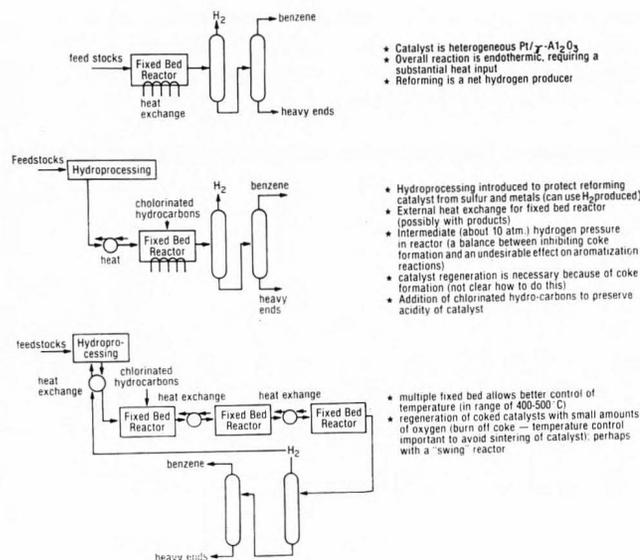


FIGURE 2

cross-examine the instructors, and the successful "purchase" of the catalyst at the end of the class period depended on the students' ability to pose the "right" questions concerning the catalytic chemistry.

USE OF PATENTS

Patents are a helpful tool in generating classroom discussion and in developing homework problems. A brief introduction to patents is provided by local patent lawyers who are active in the chemicals area. The basis for patentable work, reading the patent literature, and patent law are discussed. This portion of the course complements the emphasis on innovation by stressing the creation and recognition of new ideas.

Several industrial processes offer excellent examples of innovations recorded in the patent literature. Processes for converting synthesis gas to methanol and higher alcohols have a long patent history. We have used a short series of these patents for discussing the chemistry and engineering of these processes. The patents illustrate the use of different metal components of the catalyst to reduce the temperatures or pressures required within the reactor. One patent also introduces the ideas of using CO₂ as a moderator (via the water-gas shift reaction) to control the reactor temperature. A controversial patent suggests using water as a replacement for hydrogen in producing methanol. Students were challenged to distinguish between the patents.

We have scotched the traditional lecture format for a much more informal orientation. Central to the approach are oral expression and exchanges, spontaneity, rapid changes and creation, and competition.

Thermodynamics can frequently be used to evaluate the patents and, in some cases, kinetic information is available.

Patents also provide a basis for homework problems. A typical problem involves the creation of a flowchart based on a patent for acetic acid or ethylene oxide. Several longer term projects of this nature have also been used.

EVALUATION OF STUDENT PERFORMANCE

Much emphasis in the course is placed on oral performance and evaluation. This nontraditional method results in a more spontaneous response from students and a better appreciation of the conceptualization process. Oral reports and presentations by students are frequently used to provide opportunities for classroom interactions. Student contributions are further encouraged by the sharing of industrial experience; frequently a rather high proportion of the class has worked in industry during previous summers. Graduate students with industrial experience also participate in the course.

Midterm examinations are conducted orally. Students are assigned a chemical compound and are sent to the library to determine "everything that is important" concerning the processing for its manufacture. Students are assigned topics sequentially to avoid overlap in the library. After two hours, the student returns to give a half-hour presentation to the faculty instructors. We have found that this format works very well with two or three faculty members present, rather than just one; however, the faculty time commitment becomes large. Students are usually able to find relevant resource material and the basic processing information. The majority of students can also reason using basic thermodynamics and kinetics. Of course, much more than this is desired, and the questions posed by the faculty invariably lead the more able student to some aspects of industrial chemistry which were un-researched or which are unknown. These probing questions are the most difficult and also the most instructive. Some students are shaken by the ex-

perience—usually to their benefit! Generally, students have responded favorably to this approach.

A final project is also used in which the students are required to work independently of known solutions. Students are organized into groups, but each individual is required to submit a written report. The projects typically involve new or unconventional processes. Recent patents are used, such as the production of vinyl acetate from carbon monoxide and hydrogen. Another example of a successful final project is the cleanup of chemical dumps. Here the student is confronted with a myriad of possible reactions in an unfamiliar environment (soil). Much discussion centers on identification of the problem (composition of materials and possible reactions) and many alternative solutions are possible. We have also used projects dealing with natural products chemistry, enzyme chemistry, and photochemistry—again, areas relatively unfamiliar to the students.

REFERENCES

While we have found that several references are useful in providing background information, no single book is suitable as a text. Class notes are available for some portions of the course. Students refer frequently to their previous chemistry and engineering textbooks. The following is a list of references which provide some helpful material:

- 1) "Kirk-Othmer Encyclopedia of Chemical Technology," Second Edition, John Wiley & Sons, New York, 1963. (Volumes of Third Edition, 1978, appearing).
provides a good discussion of general processing technology and equipment, some flowsheets provided, limited discussion of processing chemistry.
- 2) A. L. Waddams, "Chemicals from Petroleum," Third Edition, John Wiley & Sons, New York, 1973.
good overview of petrochemical industry, provides good overall flowcharts, some processing chemistry.
- 3) P. Wiseman, "An Introduction to Industrial Organic Chemistry," John Wiley & Sons, New York, 1976.
good perspective on chemistry involved in important organic processes, orientation toward British routes (coal given larger discussion).
- 4) K. Weissermel and H.-J. Arpe, "Industrial Organic Chemistry," Verlag Chemie, New York, 1978.
good collection of industry-wide flowcharts, alternative chemical routes suggested with some processing chemistry included.
- 5) H. A. Wittcoff and B. G. Reuben, "Industrial Organic Chemicals in Perspective," Parts I and II, John Wiley & Sons, New York, 1980.
provides a broad orientation for the chemistry

for industrial process, little discussion of flow-charts or engineering requirements.

- 6) S. A. Miller, Ed., "Ethylene and its Industrial Derivatives," Ernest Benn, London, 1969.
E. G. Hancock, Ed., "Propylene and its Industrial Derivatives," Halsted, New York, 1973.
much of the petrochemical industry is described in these books.
- 7) J. T. Maynard, "Understanding Chemical Patents," American Chemical Society, Washington, D.C., 1978.
an excellent, short introduction to patents.
- 8) E. Mansfield, J. Rapoport, A. Romeo, E. Villani, S. Wagner, and F. Husic, "The Production and Application of New Industrial Technology," W. W. Norton, Inc., New York, 1977.

Although these references provide some useful information, we have found that a very effective method for introducing an industrial orientation is through industrial speakers. These practitioners have had extensive experience with a particular process. Typically, they are industrial organic or inorganic chemists and possess an excellent understanding of industrial technology, economics, the availability of raw materials, and the changing nature of chemical markets. These interactions are also stimulating to classroom discussions.

APPENDIX: COAL GASIFICATION

Problem Statement

Underground coal gasification is typically performed at lower temperatures (for example, 700 K) than the Lurgi process which was discussed in class. The product from such an operation is referred to as "high Btu" gas. The gasification is performed by injecting oxygen and steam into coal beds which have been drilled or fractured. Typical annual consumption rates for a 100 billion cubic feet plant are as follows:

Gas produced	100 BCF
Coal consumed	5.05 million metric tons
Oxygen consumed	1.53 million metric tons
Water consumed	1.54 million metric tons
Drill holes	240

A typical Wyoming coal ("Thunderbird coal") has the following analysis:

moisture	21.4%
volatiles	33.7
carbon	38.6
ash	6.4
S	0.8
H	5.6
C	58.6
N	1.0
O	27.5

The heat of combustion of this coal is 1.33×10^4 Btu/lb (138 kcal/mole, based on the formula weight).

Determine if it is feasible to gasify this coal.

Solution Comments:

In order to solve this problem, the student must determine the meaning of the criterion "feasible". The previous classroom discussion provided an important clue: in a Lurgi gasifier, there are regions of drying and devolatilization, combustion, and synthesis gas production. Similarly in this problem, coal must be combusted to provide the heat required by the endothermic reactions. Perceptive students also realize that there is a significant heat demand due to drying the coal and to heating the coal bed and the surrounding environment; some estimates of these heat effects can be made.

In order to determine the grams of coal which must be combusted per gram of coal converted to produce gas, it is necessary to first determine the stoichiometry of the reactions. The composition of this coal may be expressed as $\text{CH}_{1.15}\text{O}_{0.35}\text{N}_{0.0146}\text{S}_{0.0051}$ (providing the formula weight for heat of combustion). The student may be tempted at this point to write a large number of reactions of this "species" with O_2 , H_2O , CO , CO_2 , H_2 , H_2S , etc. This approach is further frustrated by the difficulty of obtaining thermodynamic properties for the coal and related coal-derived intermediates: such an approach would be useful only if this data were available.

In previous classroom discussion, the possibility of considering coal to be essentially carbon was discussed. (Frequently, this "discovery" is suggested by a student.) The students are much more likely to be able to evaluate this process if such an approximation were made.

The chemical species which therefore are considered to be involved in the gasification process are C , O_2 , H_2O , CO , CO_2 , H_2 and CH_4 . Four independent reactions may be written for these species:

- (1) $\text{C} + 2\text{H}_2 \rightleftharpoons \text{CH}_4$
- (2) $\text{C} + \text{H}_2\text{O} \rightleftharpoons \text{CO} + \text{H}_2$
- (3) $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$
- (4) $\text{C} + \text{O}_2 \rightleftharpoons \text{CO}_2$

The equilibrium composition of the product gas may be determined from thermodynamic calculations. However, an additional simplifying assumption

tion may be used. The fourth reaction involves combustion of the carbon to carbon dioxide. Complete combustion of other product gases also occurs in the presence of oxygen at these temperatures. The equilibrium constants for these reactions are very large; similarly, rate data which was presented in class indicated that the rate constants for reactions between carbon and oxygen were very large. The fourth reaction might be excluded from consideration since the presence of excess oxygen at specific regions in the bed would likely lead to complete combustion products. The heat derived from such reactions, of course, is necessary to balance the endothermic reactions involved in the production of high Btu gas.

The composition of the product gas may be determined by thermodynamic calculations. At 700 K, the equilibrium constants are $K_1 = 22.6$, $K_2 = 1.60 \times 10^{-3}$ and $K_3 = 7.31$. The corresponding gas phase composition is $y_{\text{CH}_4} = 0.20$, $y_{\text{H}_2\text{O}} = 0.44$, $y_{\text{CO}_2} = 0.25$, $y_{\text{H}_2} = 0.094$, and $y_{\text{CO}} = 0.0074$.

The results of the calculation indicate that the heat required due to the overall endothermic nature of the gasification reactions is relatively low. Substantial amounts of energy are required to heat the coal to 700 K and vaporize the moisture in the coal bed. Students are also capable of providing a rough estimate of the heat loss to the surrounding environment. The effect of approximating the coal composition is relatively small. The results of the calculations vary as a result of the particular assumptions made, but roughly 15-20% of the coal would have to be burned. □

BOOK REVIEW: PROCESS CONTROL

Continued from page 27.

curious mixture of brevity and detail. A great deal of straightforward algebraic detail is given in many places while in others mastery of far more difficult concepts is assumed. For example, knowledge of eigenvalues and eigenvectors of matrices is assumed in the earlier part of Chapter 3, but is reviewed in some detail later in the same chapter. Far more background in stochastic processes is assumed than the typical chemical engineer has. Although little theory of stochastic processes is actually needed, the jargon is used extensively. The reader is not given enough background for even a clear physical interpretation of the results. Such a commonly used concept as the expected value of a stochastic variable is

never even defined. Notation is also a problem in places, with the same symbols being used for different quantities or different symbols used for the same quantities within the same chapter.

In spite of some shortcomings Ray's latest book is highly recommended. It is by far the best book available for a graduate-level level course in modern chemical process control. □

DESIGN OF INDUSTRIAL CHEMICAL REACTORS FROM LABORATORY DATA

By J. Horak & J. Pasek

Heyden & Son, Philadelphia, PA

Reviewed by Moin Ahmed
Union Carbide Corporation

This book is an addition to a large number of books on the design of chemical reactors. However, this book differs from many other text books by emphasizing the practical aspects, sometimes at the expense of needed theory. The book touches some subjects like analytical methods and statistical methods of data evaluation which most books on reactor design do not address.

The book delves into useful qualitative discussion of many design principles, design methods and reactor descriptions. However, in a number of places a more mathematical and less empirical approach would have been useful. Most of the examples are of a qualitative nature, and there are very few examples which emphasize more than one principle at a time. At least on one occasion the book is misleading, referring to free energy of reaction as enthalpy of reaction. The translator has often used terms that are not familiar to American readers (like technological properties of a reactor).

The book is not well organized and is divided into too few chapters. After an introductory chapter, there is a chapter on Reactions in Solutions which is actually a chapter on homogeneous reactions. This chapter is followed by a chapter titled, Types of Reactors. In addition to the title, it describes data collection, treatment and regression of data, determination of specific heats and heats of reaction, and a very good description of scale-up techniques referred to by the authors as Data Transfer. Chapter 4 deals with the catalytic reactors. This chapter also presents the trickle bed reactors, heat transfer media and construction of heat transfer loops—subjects very useful to practicing which are neglected by most re-

actor design books. On the other hand, the authors have barely touched upon catalyst deactivation, and the discussion of intra particle diffusion limitation and multiplicity in catalyst pellets is very limited. The fifth and the last chapter is on Gas-Liquid and Liquid-Liquid Reaction. The material in this chapter is better presented than in most other books and is very useful to the design engineers.

The authors have completely neglected non-catalyzed gas-solid reactions and a very common class of reactors, namely slurry reactors.

The book can be useful as a reference book for chemical engineers in industry but its utility as an undergraduate or a graduate text seems very limited. This is due not only to the lack of mathematical approach but also because it contains no problems for students to solve. Finally, the book does not represent the state of the art since most of the references are pre-1975. □

J. M. SMITH

Continued from page 9.

in 1973 and 1980; and Pieter Stroeve and Dewey Ryu, are the most recent additions.

While Joe has always emphasized to his colleagues that undergraduate education is a vital part of the UC Davis chemical engineering program, he has also promoted the ideal of strong and varied graduate training. Although Joe is planning a partial retirement to begin in the fall of 1984, he expects to continue to teach and work with graduate students and postdoctoral scholars on chemical engineering research. In view of the personal characteristics he has so far exhibited, it is not anticipated that Joe will retire to a life of leisure and abandon. His single-minded pursuit of achievement in solving chemical engineering problems is probably the critical factor in Joe's success. Undoubtedly, the robust creativity and inexhaustible energy have been important ingredients as well, but his exacting commitment to getting the job done and done well has made the difference between routine and monumental accomplishment.

In all the aspects of chemical engineering education—exemplary research, the writing of textbooks, teaching classes, the guiding of students (graduate and undergraduate) in their research, and administration—Joe Smith has earned and will continue to deserve his Davis title, "Mr. Chemical Engineering". □

DIGITAL CONTROL EXPERIMENT

Continued from page 31.

tive control ($k_c = 3.53$ volt/volt, $\tau_D = 0.1$ seconds), and proportional-integral-derivative control ($k_c = 3.53$, $\tau_I = 20$, $\tau_D = 0.1$). Introduction of integral action eliminates the offset (at much longer time than shown in the graph), and less oscillation is shown with P-I-D control.

Fig. 5 represents the effect of sampling time on the system with only proportional control action.

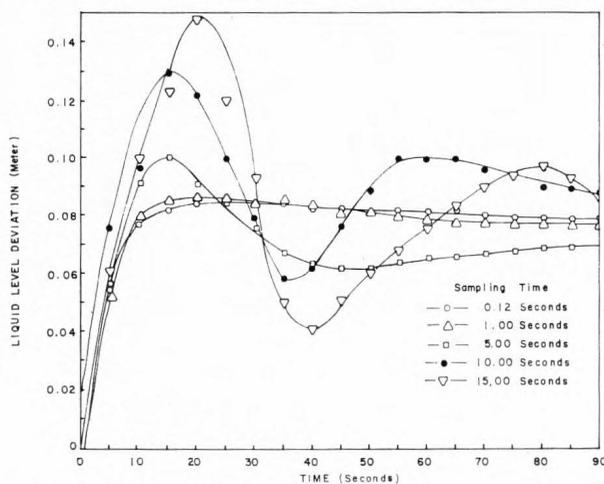


FIGURE 5. Effect of sampling time on system with proportional control.

Increasing the sampling time resulted in higher overshoot and more oscillation. What is interesting is that the system which is first order starts to act like a second order system with decreasing damping coefficient as the sampling time increases. Similar responses are obtained for P-I and P-I-D control.

It should be pointed out that the present undergraduate process control course at NJIT does not cover direct digital control. With this experiment, and the introduction of z-transforms, students can get a very good understanding of discrete sampling and direct digital control. □

ACKNOWLEDGMENT

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CLEMSON

Continued from page 5.

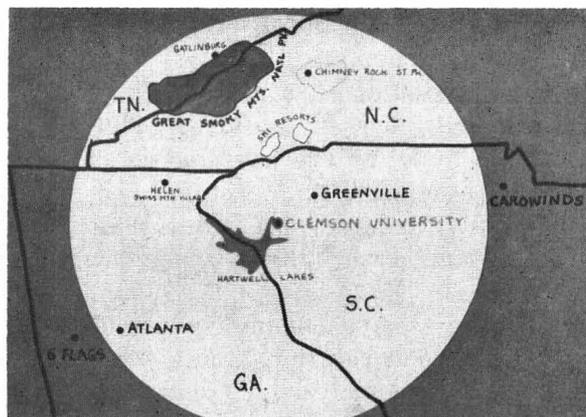
industrially subsidized stipends to pursue full-time graduate study, preferably at the PhD level. Both new programs have already had impact on enrollment; thus, the 1981-82 enrollment of graduate students in the department was twice that of the previous year.

Faculty research interests are divided along traditional lines: F. C. Alley (PhD, North Carolina, 1962), environmental pollution control; W. B. Barlage, Jr. (PhD, North Carolina State, 1960) and D. D. Edie (PhD, Virginia, 1972), rheology and polymer processing; J. N. Beard, Jr. (PhD, LSU, 1971), industrial energy conservation and process control; W. F. Beckwith (PhD, Iowa State, 1963), transport phenomena and kraft-pulping process; R. C. Harshman (PhD, Ohio State, 1951) and R. W. Rice (PhD, Yale, 1972), chemical reaction kinetics and catalysis; C. H. Gooding (PhD, North Carolina State, 1979), separation processes; S. S. Melsheimer (PhD, Tulane, 1969), mass transfer, mathematical modeling, and process control; J. C. Mullins (PhD, Georgia Tech, 1965) and J. M. Haile (PhD, Florida, 1976), thermodynamics and statistical mechanics.

CONCLUDING REMARKS

Sheltered in the southeastern foothills of the Appalachian Mountains, Clemson enjoys a mild, four season climate. The environs of the university provide unlimited opportunities for outdoor recreation, including all types of fresh-water sports, hiking, camping, cross-country running, and hang-gliding. Cultural activities can be pursued in Atlanta—a two hour's drive from Clemson. Furthermore, there is the summer arts festival, Spoleto, held annually in Charlestown, SC. This is an offshoot from Gian-Carlo Menolti's festival held in the Umbrian hill town of Spoleto, Italy, and has evolved into a musical and operatic event of some significance.

The combination of mild climate, moderately priced electrical power, low taxes, and non-unionized labor is attracting important new industry to upstate South Carolina. The cotton mills of the first part of the century have long disappeared from the region and have been replaced with plants producing nylon, polyester, and polypropylene.



Clemson and surroundings.

Today, literally scores of textile mills dot northwest Carolina and eastern Georgia. Moreover, high technology electronic manufacturing companies are moving into the area.

The future of Clemson University also seems particularly promising. The decision of the administration not to expand the student body nor the physical plant during the student boom years of the 1970's seems, in retrospect, to have been a wise decision indeed. The demand for entry into the university, as well as chemical engineering, is higher than ever. Private and industrial support for the university seems to be increasing substantially. In 1981 alone, several important contributions were made to the university: Abney Foundation gave one million dollars for the endowment of a chair in Economics, National Cash Register and Digital Equipment Corporation gave generous research grants to the College of Engineering, and Senator Strom Thurmond donated his public papers to Clemson. Plans are being made for the creation of a Strom Thurmond Center for Excellence in Government and Public Service that will include a library to house Thurmond's papers, a performing arts center, and a continuing education facility.

During its ninety year history Clemson has matured from a local agricultural college to a regional university of some stature. Now, the visions of both the university and its Department of Chemical Engineering are beginning to extend beyond the region to problems and opportunities of national significance. This further maturing process, while not without growing pains, promises to enhance and deepen the educational environment at Clemson University. □

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