

# CHE

chemical engineering education

VOLUME XV

NUMBER 1

WINTER 1981

CHEMICAL ENGINEERING DIVISION OF AMERICAN SOCIETY FOR ENGINEERING EDUCATION

## **CHE AT NOTRE DAME**

IMPRESSIONS OF PROCESS CONTROL EDUCATION AND RESEARCH IN THE U.S.

*Kurt V. Waller*

INFINITE POSSIBILITIES FOR THE FINITE ELEMENT

*Bruce A. Finlayson*

A SIMPLE TUBULAR REACTOR EXPERIMENT

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CHE SYMPOSIUM AT CARNEGIE-MELLON

*Michael Locke*

TEACHING MARKET ANALYSIS

*J. T. Ryan, Bret Haugrud*

SODALES PRINCETONIENSES

*Rutherford Aris*

### *Award Lecture*

A NEW LOOK AT AN OLD FOSSIL: KINETICS OF COAL PROCESSING

*D. D. Perlmutter*

**RICHARD  
FELDER**  
**OF N.C. STATE**



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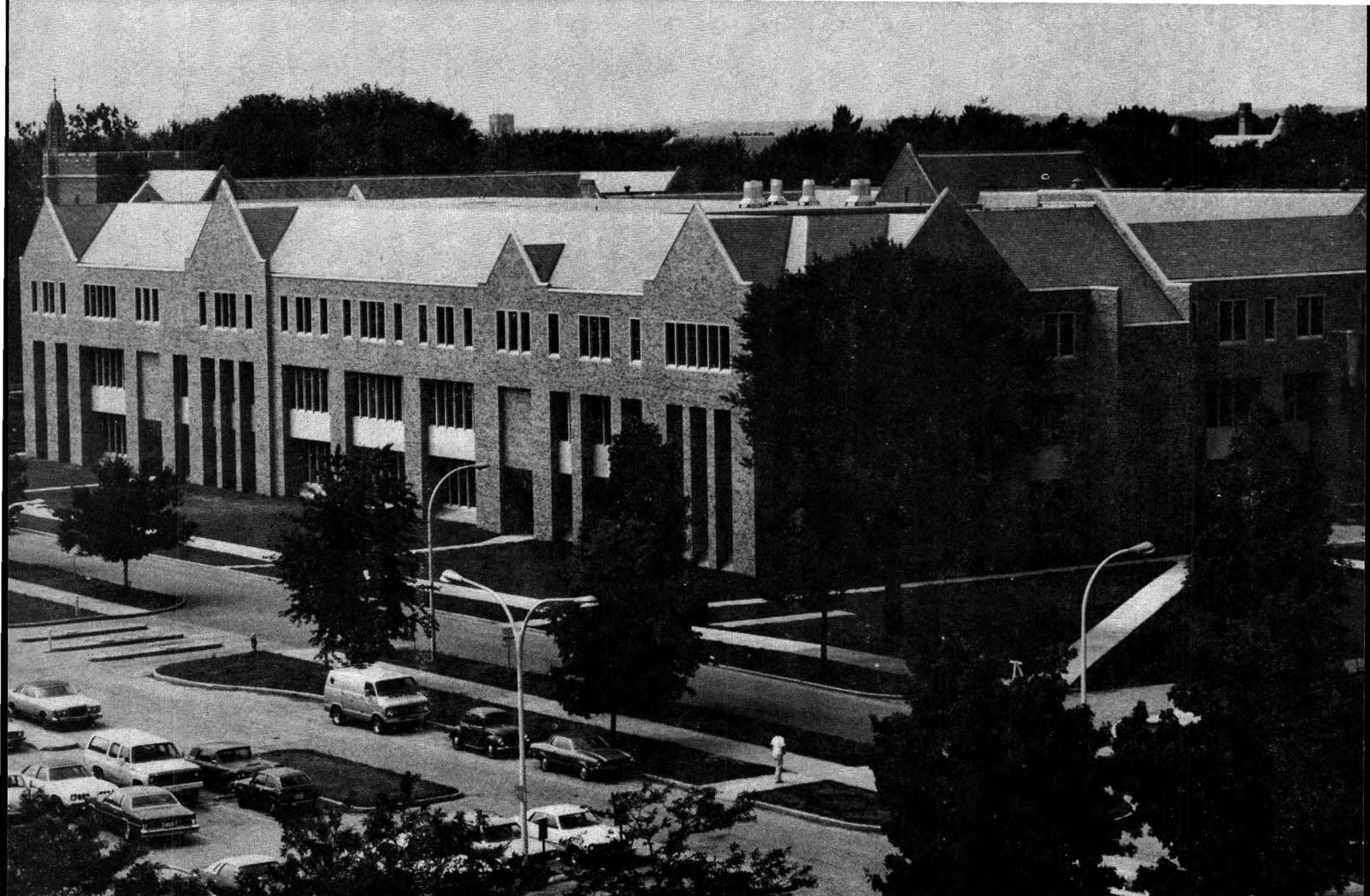
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The ChE department is located in the new Fitzpatrick Hall of Engineering, completed in July 1979.

## ChE department

# CHE AT NOTRE DAME

PREPARED BY THE FACULTY  
*University of Notre Dame*  
Notre Dame, IN 46556

**T**HE CHEMICAL ENGINEERING PROGRAM at Notre Dame began in 1909. The 1908-9 Bulletin published in July 1909 noted that "chemical manufacture has developed so rapidly and grown so exacting that there has arisen a demand for men who not only can create and improve chemical processes strictly so called, but who can deal with the problems of construction and maintenance as far as they are related to chemical industries. To prepare young men for such work, the course in Chemical Engineering has been designed." There were no specific courses in chemical engineering per se; of the total 167 semester credit hours in

the curriculum there were various courses in chemistry (58 cr hrs), mechanical engineering (30 cr hrs), drawing (15 cr hrs) and shopwork (14 cr hrs). By today's standards, the university was small then, with all students numbering 995, and only 42 faculty of which two were in chemistry. (Current total enrollment is 8500 and faculty number about 700). The first undergraduate "degree of chemical engineer" was awarded in June 1911 at the 67th annual commencement to Guillermo Patterson, Jr. of New York City. (Incidentally, ours is the only Chemical Engineering Department in the world which can boast of an alumnus named Jacques Rousseau. He did not minor in philosophy.)

It was in the 1920-21 academic year that the university was reorganized in a form that exists to this date, with four undergraduate colleges in Arts

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The early chemical engineers at Notre Dame were taught chemistry by the brilliant chemist J. A. Nieuwiand, CSC—who with H. H. Carothers of du Pont is credited with inventing the first synthetic rubber “neoprene” . . . —and by Knute Rockne, who was on the chemistry faculty during 1916-22 before moving on fulltime to some other activity.

and Letters, Science, Engineering, and Business Administration (then Commerce)—each with its own Dean—and a separate Committee on Graduate Study, which preceded formal establishment of the Graduate School in 1932. A department of Law, now the Law School, was established in 1869. The heads of various departments were also appointed in 1920-21, and the first Head of Chemical Engineering (1920-41) was Henry B. Froning. Froning was a distinguished chemist who joined Notre Dame in 1920, and also served as Head of Chemistry (1920-41) before becoming Dean of Science (1940-43). The course “Principles of Chemical Engineering” based on the pioneering book of the same name by Walker, Lewis and McAdams (1923) was added to the curriculum in 1921, replacing its predecessor course in Industrial Chemistry. The early chemical engineers at Notre Dame were taught chemistry by the brilliant chemist Rev. Julius A. Nieuwland, CSC—who with W. H. Carothers of du Pont is credited with inventing the first synthetic rubber “neoprene” in the late 20’s—and by Knute Rockne, who was on the chemistry faculty during 1916-22 before moving on fulltime to some other activity.

By 1920, there were only 11 graduates of the department. The present undergraduate degree “bachelor of science in chemical engineering” was instituted in 1925. The number of graduates rose steadily; 59 degrees in the 20’s and 156 in the 30’s. The headship of the department passed to Ronald E. Rich in 1941 when Froning left to

devote fulltime as Dean of Science. Rich had joined the faculty in 1933, and was a Notre Dame alumnus (B.S. Ch.E. ’28, M.S. Chem. ’36); he guided the department until 1959 when Julius T. Banchemo arrived from Michigan as Head. Other Chemical Engineering faculty during this period were P. J. Byrne, Jr. (1920-22), H. Wenzke (1922-39), E. G. Mahin (1926-33), H. Hinton (1929-38), A. Boyle (1929-39), G. Hennion (1933-40) and E. J. Wilhelm (1938-71). The Chemical Engineering Department also moved to a then new building in 1941.

#### GRADUATE PROGRAM

PRIOR TO 1945, THERE WERE NO graduate courses offered within the Chemical Engineering Department. Several graduate courses including lectures and a laboratory in Applied Electrochemistry, Advanced Thermodynamics, Advanced Unit Operations lectures and laboratory, and Advanced Plant and Equipment Design were initiated in 1945-46 to accommodate the returning WWII veterans who were anxious to renew their engineering background. Allen S. Smith (Ph.D. Michigan, ’40), who joined the Chemical Engineering faculty in 1946 and remained here till his death in 1967, was a major factor in this development. He introduced additional graduate level courses in 1946 on analysis of Distillation and Extraction, and Applied Chemical Kinetics; these along with a Heat Transmission course by Rich and Corrosion of Metals and Alloys offered by Wilhelm, plus

#### CHAIRMEN OF CHE AT NOTRE DAME



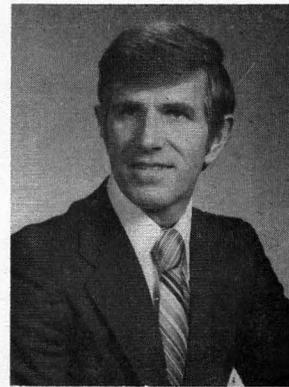
Henry B. Froning  
1920-41



Ronald E. Rich  
1941-59



Julius T. Banchemo  
1959-79

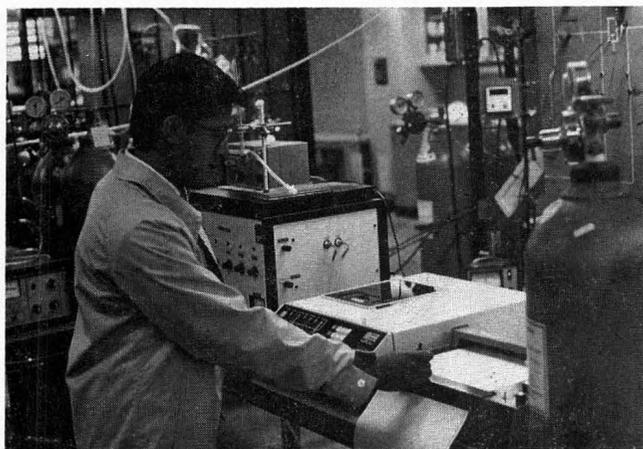


Roger A. Schmitz  
1979-

those initiated the previous year provided sufficient offerings to begin a formal master's program with required thesis research. Other engineering departments were also beginning their master's programs at this time. The very first master of science in engineering was awarded to a mechanical engineer in June 1947; the first wave of ten masters of science in Chemical Engineering graduated in August 1947.

Other than Rich, it was Wilhelm and Smith, F. L. Benton (1940-56), M. T. Howerton (1949-56), J. Treacy (1950-56), G. Parravano (1956-59) and J. P. Kohn (1955-present) who taught Chemical Engineering at Notre Dame during the 40's and 50's. A total of 212 bachelors degrees in Chemical Engineering were awarded during the 40's, and 336 in the 50's. By 1959, 77 master's degrees had also been awarded.

Due to Rich's failing health, J. T. Banchemo was acquired as Head in 1959. He came with assurance from the administration that a doctoral program in Chemical Engineering could be started. By this time, G. S. John (1958-63) had already joined the faculty, but the major addition was that of E. W. Thiele—well known for his pioneering contributions to two major areas of Chemical Engineering science; the McCabe-Thiele method for graphical design of distillation columns for binary separations and the Thiele modulus in the problem of simultaneous diffusion and reaction in porous catalyst pellets. Thiele had just retired after a long and productive research career with American Oil Company in 1960, and was persuaded to take on a second career at Notre Dame. Thiele retired from active teaching in 1970 at age 75, and was awarded an honorary doctor-



Kinetics and reactor studies are conducted in the Catalysis and Reaction Engineering laboratory.

ate in 1971 in recognition of his contributions to Chemical Engineering and Notre Dame.

The next addition to the faculty was J. J. Carberry in 1961, a former Notre Dame undergraduate, who had been with du Pont after receiving his Ph.D. at Yale in 1957. Along with Banchemo, Kohn, Smith, Thiele and Wilhelm already present then, his addition provided a major thrust towards the growth of the graduate program. A total of 55 Ph.D. degrees in Chemical Engineering have been awarded since the first one in June 1963 to Joosup Shim who did his thesis research with Jim Kohn.

During the sixties and much of the seventies, undergraduate enrollments were about 30 in each class, and fulltime graduate students in residence averaged 22 per year. The graduate program was considerably strengthened during this period. Several other faculty members, A. H. P. Skelland (1963-69), E. D. Crandall (1965-69), T. G. Smith (1969-75), N. D. Sylvester (1969-73), F. H. Verhoff (1969-74) and K. D. Luks (1967-79) played a major role in this development. Various new graduate courses were added to the program. Three other present faculty members, W. Strieder (1969), A. Varma (1975) and E. E. Wolf (1975) also joined during this period.

The department moved to its present location in the new Fitzpatrick Hall of Engineering in July 1979. Our classroom and laboratory facilities are now among the best and most modern available anywhere.

## THE PRESENT

WITH THE RETIREMENT and elevation to emeritus status of Julius Banchemo in 1979, the department was very fortunate to attract Roger A. Schmitz as Keating-Crawford Professor and Chairman. Schmitz had taught at the University of Illinois-Urbana since 1962, and is widely known for his pioneering experimental research on dynamics and control of chemical reactors.

As with other Chemical Engineering departments, we are also experiencing a large growth in our undergraduate enrollments. We had 30 bachelor's degree graduates in 1978—the average per year for the preceding twenty years—and 50 in 1979. Our current senior class is 70, and we have 87 sophomores! Female students were first admitted to Notre Dame at the undergraduate level in 1972; our first batch of female bachelor's degree holders graduated in 1975. Today 22% of our

undergraduate students are female, which almost equals the university figures and is significantly higher than the rest of the College of Engineering.

Three new tenure-track faculty, all fresh Ph.Ds, have been hired this year; C. F. Ivory and J. C. Kantor from Princeton, and M. A. McHugh from Delaware. We have 31 fulltime graduate students in residence this year—which with the present faculty strength permits excellent student-faculty interaction.

#### CURRICULA

**T**HE B.S. DEGREE IN CHEMICAL Engineering is a four year program requiring 128 semester hours. The 24 hours of liberal arts required, are well in excess of ECPD requirements. We hope to increase that number as Notre Dame deems a



**Professor James J. Carberry providing valuable tips on reactor design.**

liberal education to be of paramount importance whatever be the students professional calling. In addition to the usual Chemical Engineering and allied chemical and physical sciences, there is an engineering core including a course in the Freshman year, *Introduction to Engineering* in which engineering methodology is taught along with computer training, including use of FORTRAN. The remaining core engineering courses are in probability, engineering mechanics, electrical engineering science, thermodynamics, materials science, and applied mathematics. Chemical Engineering courses include mass and energy balances, stagewise operations, transport phenomena, chemical reaction engineering, thermodynamics, process design, process modeling and control, transport processes laboratory and unit operations laboratory.

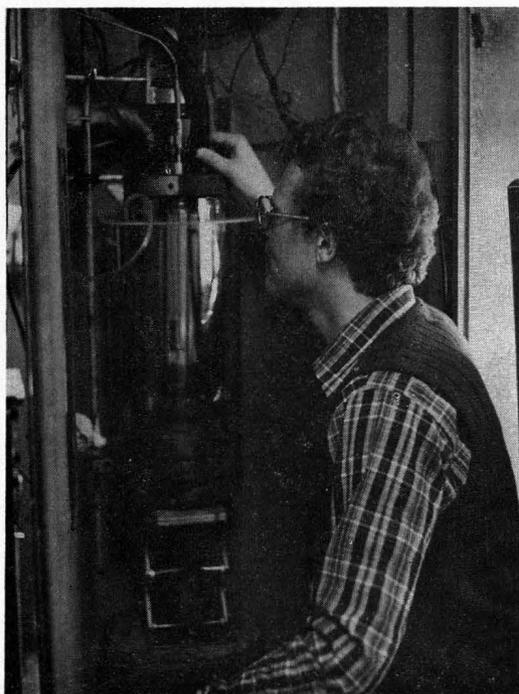
The graduate curriculum includes courses in

advanced thermodynamics, statistical thermodynamics, mathematical methods (2 courses), transport phenomena (2 courses), advanced reaction engineering, heterogeneous catalysis, polymer engineering, numerical methods, process control and modeling, dynamics of reaction processes (2 courses), heterogeneous phase equilibria, and equilibrium state operations. In addition to the formal courses, there is a Chemical Engineering seminar, advanced topics in Chemical Engineering, advanced studies projects, and research projects leading to M.S. and Ph.D. degrees. There is a research M.S. degree which requires 24 hours of course work and a thesis. However most students elect to pursue the non-research M.S. degree which requires 30 hours of course work. Graduate students are encouraged to take graduate level courses from outside the department, particularly in chemistry, physics, mathematics, or engineering. First year graduate students are required to take a 3 credit special topics course in which they choose an advisor and devote themselves to solution of an original problem.

The Ph.D. degree requires the course work for the M.S. degree plus additional courses in Chemical Engineering and science deemed important to the candidate's research area. The progress of each Ph.D. student is reviewed periodically by his or her research committee. Normally the M.S. degree can be obtained in one calendar year of fulltime study, while the Ph.D. degree ordinarily takes from three to four years of fulltime study beyond the undergraduate degree.



**A casual discussion of important issues among faculty members, from left: Arvind Varma, James Kohn and William Strieder.**



Graduate research in the Thermodynamics and Phase Equilibria laboratory.

#### FACULTY AND RESEARCH INTERESTS

**J. T. Banchemo**, Professor Emeritus, Ph.D. University of Michigan, 1950. Co-author of textbook "Introduction to Chemical Engineering" with W. L. Badger, McGraw-Hill Company (1955), and "Unit Operations" with G. G. Brown et al., J. Wiley Company (1950). Dr. Banchemo has interests in liquid-phase epoxide reactions, design of chemical reactors, and thermodynamics of solutions.

**J. J. Carberry**, Professor, Dr. Eng., Yale University, 1957. Author of textbook "Chemical and Catalytic Reaction Engineering," McGraw-Hill Book Company (1976), and co-editor of the journal "Catalysis Reviews." Dr. Carberry has concentrated his research interests in chemical reaction engineering and heterogeneous catalysis, and in 1976 was recipient of the Wilhelm Award in Chemical Reaction Engineering (AIChE).

**C. F. Ivory**, Assistant Professor, Ph.D., Princeton University, 1980. Dr. Ivory has wide-based interests in transport phenomena and bioseparations.

**J. C. Kantor**, Assistant Professor, Ph.D. Princeton University, 1980. Dr. Kantor is interested in process analysis, dynamics and control, and applied mathematics.

**J. P. Kohn**, Professor, Ph.D. University of Kansas, 1955. Dr. Kohn has interests in applied thermodynamics, heterogeneous phase equilibria,

transport phenomena, and solar energy.

**M. A. McHugh**, Assistant Professor, Ph.D. University of Delaware, 1980. Dr. McHugh has interests in high pressure phase equilibria, supercritical solvent extraction, and application to coal utilization.

**R. A. Schmitz**, Keating-Crawford Professor and Chairman, Ph.D. University of Minnesota, 1962. Dr. Schmitz has interests in dynamics and control of chemical reactors; instabilities and oscillatory phenomena in chemically reacting systems and in kinetics of gas-liquid reactions. He won the Colburn Award of AIChE in 1970, and the Westinghouse Award of ASEE in 1977.

**W. C. Strieder**, Associate Professor, Ph.D., Case Institute of Technology, 1963. Co-author with Rutherford Aris of the monograph "Variational Methods Applied to Problems of Diffusion and Reaction," Springer-Verlag, (1973). Dr. Strieder has interests in diffusion in porous media, kinetic theory, surface phenomena, and molecular theory of transport processes.

**A. Varma**, Professor, Ph.D., University of Minnesota, 1972. Dr. Varma has interests in chemical and catalytic reaction engineering, modeling and simulation and applied mathematics. Varma, with Aris, recently co-edited "Mathematical Understanding of Chemical Engineering Systems—Selected Papers of Neal R. Amundson," Pergamon Press (1980).

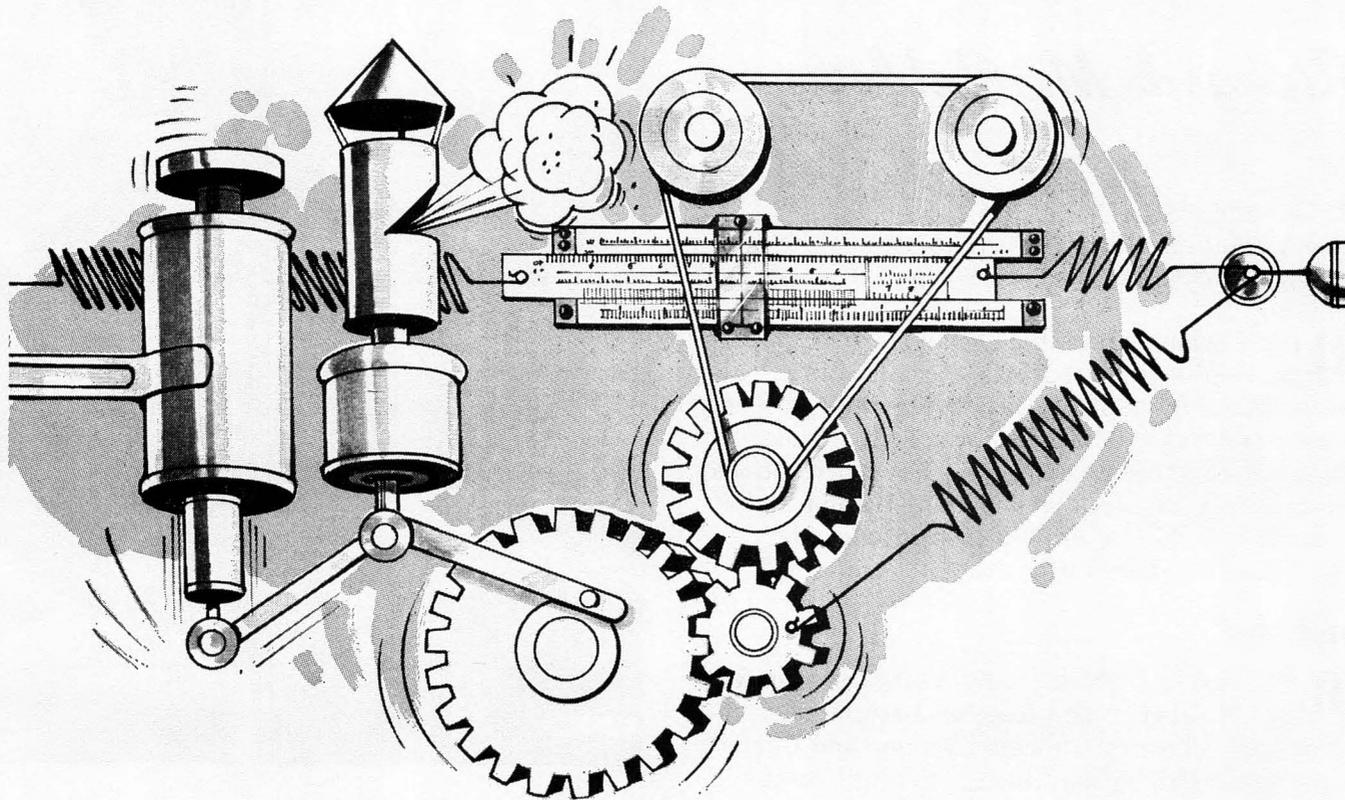
**E. E. Wolf**, Associate Professor, Ph.D., University of California, Berkeley, 1975. Dr. Wolf has interests in heterogeneous catalysis, chromatographic separations, and chemical reactor engineering. Wolf recently translated Carberry's text into Spanish.

In sum, the Chemical Engineering program at Notre Dame has evolved through three stages:

- An exclusively undergraduate program, 1909-1946.
- An undergraduate and master's program, 1946-1960.
- A B.S., M.S., and Ph.D. program since 1960.

With the appointment of Roger Schmitz as Chairman in 1979, and the addition of three assistant professors in 1980, a fourth stage of advancement is manifest insofar as our research strength has been broadened: chemical and catalytic reaction engineering, heterogeneous catalysis, applied mathematics, thermodynamics and phase equilibria, transport phenomena, and process dynamics and control. We are happily charged by our administration in the spirit of Verdi's Falstaff: "Continua!" □

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## Richard M. Felder

R. W. ROUSSEAU  
North Carolina State University  
Raleigh, NC 27650

**R**ICH FELDER JOINED the Department of Chemical Engineering at North Carolina State University in July 1969. He holds the rank of Professor and has established himself as a leader in chemical engineering education. His contributions in teaching, research and administration reflect commitment to the profession and engender appreciation and admiration from his colleagues.

### TEACHING

**R**ICH TEACHES UNDERGRADUATE courses in Reaction Kinetics and Reactor Design, Thermodynamics, Chemical Process Systems and Chemical Process Principles, which is the first course in chemical engineering. In addition he teaches graduate courses in Chemical Kinetics, Reactor Design, Optimization, Process Modeling and Special Topics in Coal Gasification.

His ability to establish rapport with students makes him one of the most popular faculty members in the Department. Undergraduate and graduate students have consistently evaluated his courses as being among the best they have taken. In recognition of his teaching performance he has received a School of Engineering Outstanding Teacher Award and has been named to the NCSU Academy of Outstanding Teachers.

Students particularly compliment the clarity with which Rich can present a lecture. Course evaluation forms describe him as "always prepared," "clear and easy to follow" and a "great teacher." More than any other faculty member,



he is responsible for glowing compliments consistently used by students to describe the introductory course in chemical engineering. The demanding nature of this course makes such attitudes remarkable.

Rich has a classroom style centered about what might be called a present-and-probe approach. The "present" part always consists of a routine in which the class is told first what is going to be covered and why it is important. The concept is subsequently presented clearly and concisely and, finally, an example is used to illustrate its application to a practical problem. The "probe" part actually occurs during his presentation; he sprinkles an oversupply of "okay" and other rhetorical questions throughout the lecture, somehow sensing which points have been grasped by students and which need additional coverage.

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**The reorganization of the  
Ph.D. qualifying exam is one of Rich's  
most significant administrative accomplishments.**

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His work with students outside the classroom is also exemplary, both in his official capacity as Graduate Administrator and in his unofficial role of confidant and consultant. His concern for the development of the complete person fosters statements on student evaluations like "he is always willing to discuss a problem, even if it is a personal one."

In recent years Rich has given numerous industrial short courses in Basic Principles of Chemical Engineering, Process Maximization, Polymer Reactor Technology and Separation Process Technology. In participant critiques of these courses he draws raves for his clarity, style and quantity of material covered.

Finally, no description of Rich's teaching would be complete without mentioning his work with countless elementary and junior high school students. It is not unusual to see him charging out of his class on chemical kinetics and into a meeting with a third grade class from one of Raleigh's magnet schools for extraordinarily gifted and talented kids. He will have volunteered to discuss something like coal gasification with these children, and will do so with the same clarity and enthusiasm he has for his senior class in reactor design. It is believed that he could, given a little notice, walk into a class on almost any subject and present a lecture that would result in students learning the material he presented.

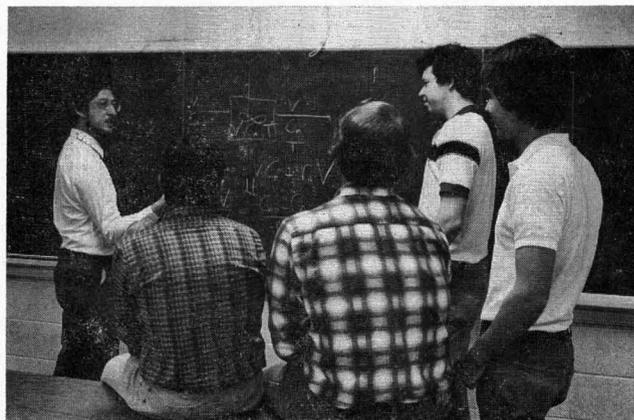
#### **ADMINISTRATOR**

**A**S GRADUATE ADMINISTRATOR, Rich coordinates all graduate student activities in the Department, including applications for admission, admission of new students, selection of a research advisor and graduate committee, selection of a minor, administration of the Ph.D. qualifying examination and scheduling of final oral examinations. Graduate students recognize him as their most important contact, outside of their thesis supervisor, during their stay at North Carolina State University. The reorganization of the Ph.D. qualifying exam is one of Rich's most significant administrative accomplishments. It has been given in its present format for almost 10 years without significant complaint.

#### **RESEARCHER**

**R**ICH'S RESEARCH IS BASED on his interests in modeling chemical processes and the effects of chemical processing on the environment. These broad concerns have led to a variety of research programs, including radioisotope applications to process analysis, photochemical reactions, use of polymeric interfaces for stack sampling, modeling of electrostatic precipitators and, most recently, environmental effects associated with coal gasification. He has published forty-five articles in refereed journals as a result of research in these fields and he was recently awarded a patent for the novel use of polymeric interfaces in stack gas monitoring.

The Environmental Protection Agency supports his research on the development of a collection tube for use as an interface in stack sampling, modeling the performance of electrostatic precipitators and the environmental effects of coal gasification. His research on the evaluation of trace metals and sulfur gases from coal is supported by the Department of Energy. The NCSU Faculty



**Professor Felder giving impromptu lecture on CSTR's.**

Research and Professional Development Fund has supported the construction of a batch photoreactor, measurement of beta spectra emitted by a slab source, and dynamic simulation of a pulp chlorination tower.

The research efforts described above have been marked by the same thoroughness and quality as Rich's teaching. He was given the 1974 NCSU Sigma Xi Research Award for superior accomplishments in the field of scientific research.

Rich has unselfishly contributed to other research programs in the Department. His library of computer programs is extensive and he makes



Felder with colleagues, Hal Hopfenberg (Department Head) and Ron Rousseau.

them available to colleagues and students. Furthermore, he can generally be counted on to have the latest information on analytical instrumentation. When the coal gasification research project got underway, there was a need for someone to learn capabilities of various instruments available for analyses of coal and char, waste water and gases found in the gasification/gas cleaning pilot plant. Rich accepted the responsibility and maintains an expertise in the use of an array of instruments, including atomic absorption spectrometer, ion chromatograph, gas chromatographs, sulfur analyzer, nitrogen analyzer, etc.

Despite the enthusiasm Rich has for these research efforts, he never loses sight of the proper relationship between university research and graduate students. He is concerned with their total professional and personal development, as well as their accomplishment of short range goals like accumulating data points and, ultimately, a degree.

None of Rich's students has the slightest reluctance to take their "problem of the day" to him. His mortality and temper have been observed, however, when a student has just broken the third *calibrated* rotameter in a single day.

#### WRITER

NO DESCRIPTION OF RICH FELDER would be complete without mentioning his enjoyment of

the written word. (That's not to say he doesn't like the spoken one, too.)

Although the 45 publications mentioned earlier and the textbook *Elementary Principles of Chemical Processes* may be indicative of the quality of Rich's writings, they are not true indicators of the quantity. He is prolific. It is common knowledge among graduate students that any question may result in being given a handout specially prepared for such occasions. A look around his office will reveal stacks of documents he has written on everything from "What is Chemical Engineering" to "Radiotracer Applicators in System Analysis."

Writing a paper or a book with him can be both excruciatingly painful and exhilarating. It can be painful because Rich's search for just the right word or phrase can result in numerous rewritings. None of his students or colleagues can escape his trusty scissors, tape and stapler. His saving grace in this regard is that he is just as likely as not to rewrite one of his own drafts. And the exhilarating part is that the document always sounds and reads superbly.

It seems only fitting that I say a few words about Rich's unique contribution to our joint authorship of *Elementary Principles of Chemical Processes*. This textbook was published in 1978 and has been adopted for use at approximately 80 Departments of Chemical Engineering in the United States, several European universities, and will be translated into Spanish and Chinese. Two characteristics of the book which have been a factor in its widespread adoption are its pedagogical approach and style of writing. Quoting from a review of the book that appears in the *AICHE Journal*, 25, 382 (1979), "... the style and level of presentation of the content is excellent, and the subject matter represents the ideal body of knowledge which should be imparted to students in the first year of a chemical engineering curriculum." These features are primarily the result of Rich Felder's insight into what students need to facilitate learning and his very special gift with the written word. In addition, the exploits of Sebastian Goniff, Johann Sebastian Farblunget,

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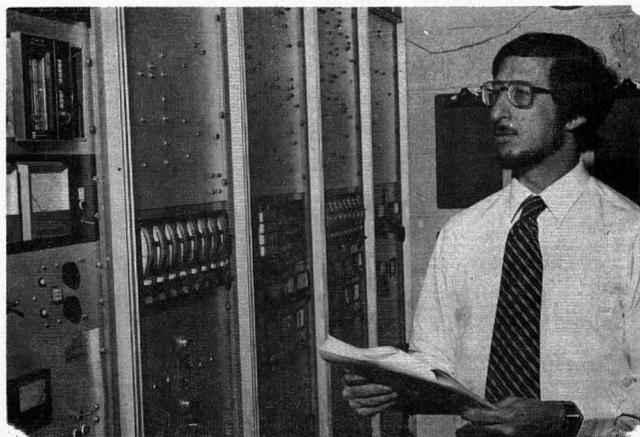
It is not unusual to see him charging out of his class on chemical kinetics and into a meeting with a third grade class from one of Raleigh's magnet schools for extraordinarily gifted and talented kids. He will have volunteered to discuss something like coal gasification with these children and will do so with the same clarity and enthusiasm he has for his senior class in reactor design.

---

Edd Seddera and other seedy but colorful characters sprinkled throughout the text, are illustrations of his sense of humor and his ability to couple wit with the illustration of chemical engineering principles.

#### LIFE AND TIMES

**A**FTER A CHILDHOOD IN Manhattan, Queens, Buffalo and North Miami, Rich settled down to make good grades and enter the City College of New York to study chemical engineering. Why Chemical Engineering? (a) Everyone who knew anything in 1957 was going into engineering and (b) he was intrigued by the idea of mixing colorless liquids to produce a bright orange (his favorite color and the reason for his subsequent



**Felder posing (i.e. acting like he's doing something) in front of coal gasification/gas cleaning pilot plant control panel.**

matriculation at Princeton) fluid. Why CCNY? He didn't like the letter MIT wrote to him, and think of all the carfare he saved.

He graduated from City College No. 2 in engineering and entered graduate school at Princeton. His interests became chemical physics, Barbara Cowl (whom he married), and hopeless liberal causes, not necessarily in that order. He was Morton Kostin's first graduate student, but he claims his major achievement was a catch in a softball game for which he is still revered by old timers on the Princeton faculty like Ernie Johnson and Bob Axtmann. He also tried Electrical Engineering at Princeton but, on falling through the ceiling at 224B Halsey Street while installing air conditioner wiring, he decided his future remained in Chemical Engineering.

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**He enjoys music ranging from Mozart to McCartney and is especially fond of playing classical guitar, but he likes to play in groups so that his mistakes are less obvious . . . he also memorizes Gilbert and Sullivan patter songs, believing that someday they will come in handy.**

---

Following his Ph.D., he spent a year at Harwell, England as a NATO postdoctoral Fellow, and two years at Brookhaven National Laboratory. His research interests had now shifted to photo-reactor design and analysis, and mixing effects in reactors. Letting it become known that he was interested in an academic career, some enlightened soul recommended he interview for a vacant position at North Carolina State University. With his interest in United States geography confined to the blighted land mass east of the Hudson River and the hedonistic environment surrounding the San Francisco Bay, he is reported to have uttered the famous quote for which many New Yorkers later claimed credit: "North Carolina??? Get serious, wouldja!!". Nevertheless, being basically curious, he came, he saw, he stayed. Why? He fell in love with the school, faculty, and (you guessed it) North Carolina. He claims never to have regretted the decision, except when he finds himself almost enjoying eating grits with red eye gravy.

He maintains his passion for hopeless liberal causes, bialys with whipped cream cheese and Chivers Olde English Marmalade. He enjoys music ranging from Mozart to McCartney and is especially fond of playing classical guitar, but he likes to play in groups so that his mistakes are less obvious. He is often awed by our friend and colleague Jim Ferrell, who makes and plays classical guitars. You're not going to believe this, but he also memorizes Gilbert and Sullivan patter songs, believing that some day they will come in handy.

Rich is also the devoted father of Kenneth, Elena and Gary, ages 14, 12 and 10. Despite his tireless professional efforts, he always seems to have enough energy left over to spend time with his children. One of his passions that he indulges in frequently is being beaten in chess by these budding Bobby Fishers. As a father, he exhibits a degree of patience and concern which reflects his feelings about children and, in fact, all people. □

## ChE stirred pots

UNIVERSITATIS MINNESOTENSIS  
COLLEGIUM FABRORUM CHYMICORUM  
SODALES PRINCETONIENSES,  
NUNC ANNUM FORUM QUINQUAGESIMUM  
FELICITER AGENTES,  
GRATULATUR,  
MAGNO CUM GAUDIO,  
GRATUITO CUM CONSILIO,  
VENIAMQUE W. S. GILBERTI POSCENS

EDITOR'S NOTE: We are grateful to Prof. John Seinfeld (California Institute of Technology) for bringing our attention to the following poem, written by Prof. Rutherford Aris of the University of Minnesota to congratulate Princeton University's Chemical Engineering Department on their fiftieth anniversary.

*When you're taking a whack,  
in your orange & black,  
at a problem defying solution  
In kinetics or flow,  
or the ways that bugs grow,  
or just how to get rid of pollution.  
When you're wracking your brain  
& you cannot obtain  
a result that fulfills your intentions  
Remember that Chem.E.s  
do nothing by semis,\*  
and always get rid of dimensions  
Recollect that p'raps Schmidt's  
is the number that fits  
and that Pelet is Reynolds times Prandtl.  
Just remember your D's,  
it'll come out with ease  
when it's wrapped up in Damköhler's mantel.  
If you wish you could borrow  
relief from your sorrow,  
the Ohnesorge number we'll mention,  
Into Reynolds you shoot  
the good Weber's square root—  
it accounts for the surface's tension.  
For tubes in the boiler,  
use t'number of Euler  
and for drag use the factor of Fanning,  
Which in matters of fiction  
was used for the friction  
'twixt Newman and Cardinal Manning.  
But it's really quite rude  
to rhyme Froude with St. Jude  
or to mess up a grave patronymic,*

*To dress up in gingham  
the number of Bingham,  
or regard Boussinesq's as a gimmick,  
While to think that Biot  
has to do with the glow  
that both heat and hard work often foster,  
Or that Deborah's song  
has the permanent pong  
of an overly ripe double Gloucester.  
To madden a Hatta  
or exchange for the latter  
the group that's been named Svant Arrhenius,  
To mock at the balding  
of Sherwood or Spalding;  
these are all of 'em crimes hyperheinous.  
If none of these fit,  
just reflect for a bit,  
devise one of your own—  
it's a sine qua non—  
for there's many a name  
that has brought Princeton fame.  
For size of reactor,  
use great Wilhelm's factor;  
for hard computation,  
'tis Leon's equation;  
and if that don't fit well  
the number of Whitwell.  
If you've pulled a slight boner,  
be absolved by Dick Toner;  
your problem's all garbled?  
Why, Dean Elgin's not marbled;  
While, if biking's your goal,  
use the Johnson Control.  
You've got Schowalter (Bill),  
and there's Dudley Saville,  
Andres, Russel and Hall,  
Prud'homme, Ollis et al.\*\*,  
for from such you can scoop  
a dimensionless group  
and you'll out of your fix be  
with some help from Ms. Bixby.  
But away cerebration.  
Now 'tis your celebration  
and we all think it's nifty  
that you flourish at 50.  
So we wish you good cheer  
for full many a year.*

RUTHERFORD ARIS

\*Except Centenaries, of course.

\*\*With due apologies to those not mentioned.



# Chevron Oil Field Research Company

## PhD Chemical Engineers

For Research And Development  
In Enhanced Oil Recovery

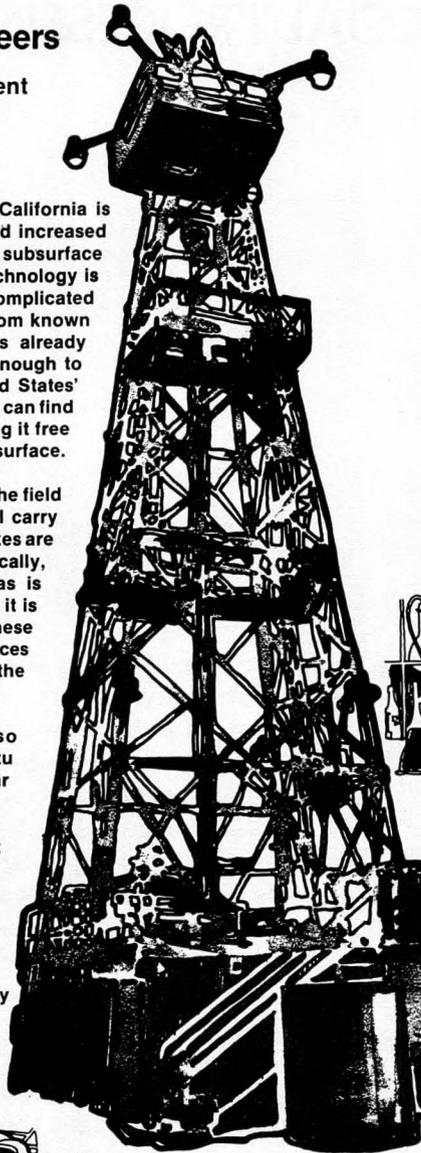
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*Greg D. Sackett '80*

# Award Lecture

## A NEW LOOK AT AN OLD FOSSIL: KINETICS OF COAL PROCESSING

*The 1979 ASEE ChE Division Lecturer was Dr. Daniel Perlmutter of the University of Pennsylvania. The 3M Company supports this annual award.*

*Dan Perlmutter earned his Bachelor's Degree (Magna Cum Laude) from New York Univ. and his Doctorate in ChE from Yale Univ. From 1955 to 1958 he worked for the Exxon (then Esso) Standard Oil Company. His academic career began in 1958 at the U. of Illinois, Urbana, and moved to the U. of Pennsylvania in 1964. Following a reorganization of the College of Engineering and Applied Science, he became the first Chairman of the department of Chemical and Biochemical Engineering, a position he held from 1972 to 1977. He has been a visiting Professor at Harvard U., the U. of Manchester, the U. of Zagreb, and the Hebrew U. of Jerusalem, in the capacity of a Fulbright Professor in England and Yugoslavia and as a Guggenheim Fellow in Cambridge.*

*He has developed new course materials in chemical reactor control, optimization, and stability problems. His textbook, Introduction to Chemical Process Control, was one of the first available in its field, and was widely adopted in the U.S. and abroad. His monograph on Stability of Chemical Reactors provided a unified view of a wide range of questions by combining some original work with an integrated survey of material only available in scattered journal articles. His most recent research has been on the kinetics of gas-solid reactions, prompted especially by their connections with energy-related problems in coal drying, oxidation, and gasification, as well as reversible storage in the form of heat of reaction.*



D. D. PERLMUTTER  
*University of Pennsylvania  
Philadelphia, PA 19104*

THE WIDELY PROCLAIMED energy crisis that so profoundly affects world affairs should be understood to be caused not by a lack of fossil fuel resources, as much as by a shortage of fuel in the highly desirable gaseous and liquid forms. It is accepted in all quarters that proved coal reserves are ample to supply anticipated world energy needs for at least several hundred years and further that no geographic monopoly is possible, since the deposits are very widely distributed over virtually every continent. It is evident in this context that the technology of the so-called gasification and liquefaction processes are central to handling the crisis: techniques for coal conversion are being sought that will supply transportation, space heating, chemical feedstocks, and industrial needs at prices comparable to petroleum sources. The objective moves closer as OPEC prices continue to rise.

It is convenient to think of gasification as composed of three steps: (i) coal pretreatment, (ii) pyrolysis, and (iii) char reaction, even though a particular process may circumvent one or more of these, or may be designed to accomplish several objectives in a single reactor. The step-wise view-

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point leads most smoothly into an examination of the appropriate chemical and physical properties of coal, and of the changes that need to be sought and monitored.

## PRETREATMENT

THE PRIMARY MOTIVATION for a study of coal pretreatment is a practical processing difficulty. When common bituminous coals are subjected to high temperature gasification conditions they tend to soften and swell, and can plug reactors and transport lines before ultimately resolidifying as a porous char or coke. This process is commonly referred to as caking; it must be controlled if the solid fuel is to be successfully gasified. A mild oxidative pretreatment is commonly used to reduce or eliminate this coal caking propensity, providing two steps in one: drying to re-

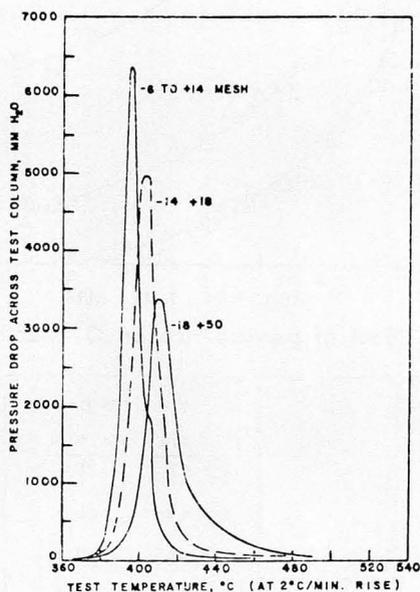


FIGURE 1. Caking test results for feed coal samples.

move naturally occurring water on the coal surfaces, and the chemical oxidation.

Many laboratory test methods have been used to study the plastic properties of coals, all empirical in nature and devised to characterize the plastic behavior of coal by means of numerical indices. Comprehensive summaries and reviews of the methods have been given by Brewer (1945) and Loison et al. (1963). One common test is the Gas Flow test (Foxwell, 1924; Coffman and Layng, 1927, 1928), chosen for its simplicity in apparatus design and operation and for its close resemblance to the caking of coal in a packed bed

... techniques for coal conversion are being sought that will supply transportation, space heating, chemical feedstocks, and industrial needs at prices comparable to petroleum sources.

reactor. In this test, a sample of the coal is heated at a constant rate of temperature rise ( $2^{\circ}\text{C}/\text{min}$ ) inside a tube with a constant flow of nitrogen through the coal sample. The differential pressure drop across the sample is monitored, as the sample goes through its plastic range. Pressure drop vs. temperature readings are taken as data, as shown in Figure 1. After the oxidizing pretreatment the same test shows a sharp reduction in pressure drop as in Figure 2, reflecting a lesser degree of softening, swelling, and "caking."

Changes recorded as mechanical properties need to be matched to chemical effects, if one is to understand the details of the preoxidation. For this purpose, a HVA bituminous coal was oxidized in a packed-bed reactor with a once-through mixture of  $\text{N}_2$  and  $\text{O}_2$ , monitored by analyzing the composition of the feed and product gases with a dual-column Gas Chromatograph.

Typical results on overall reaction rates are shown in Figures 3 to 7, emphasizing the effects of flow rate, particle size, oxygen concentration, pressure, and temperature, respectively. In addition, the chromatographic analysis run on each sample of reactor effluent provided a record of carbon dioxide and carbon monoxide production to match

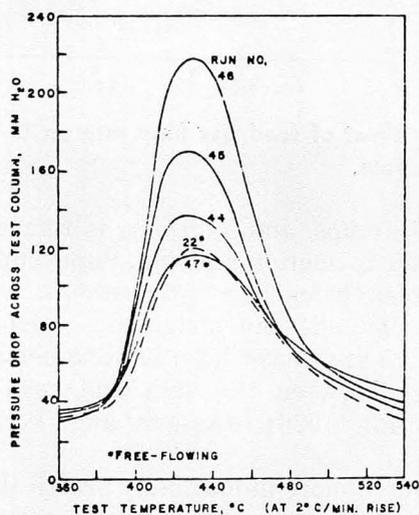


FIGURE 2. Caking test results for -18 to +50 mesh oxidized coal samples.

the rates of oxidation. Cross plots are presented as Figures 8 and 9 to illustrate the linearity and to demonstrate that the correlations for the various coals do indeed persist as flow rate, particle size, and conversion vary. Evidently, the two carbonic gases are formed in a constant ratio, presumably by the same mechanism.

Correlation of all these findings by means of a comprehensive argument requires formulation of a model that includes several steps. The two carbonic gases appear to form together by a direct burnoff reaction. Simultaneously, oxygen is adsorbed by the coal to form any of a series of oxy-

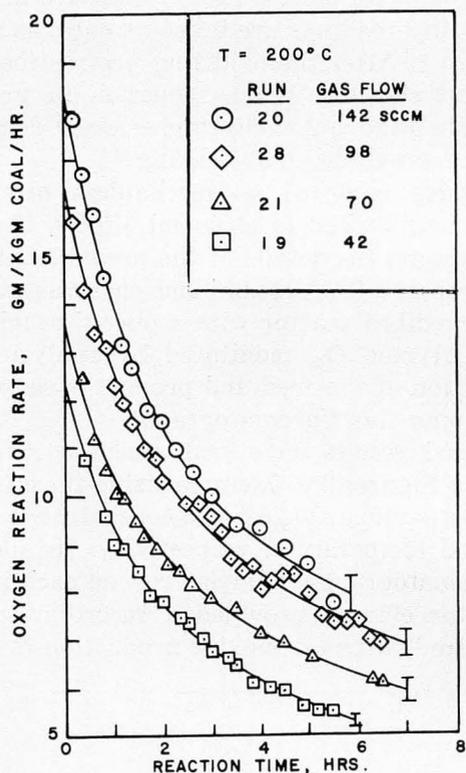


FIGURE 3. Effect of feed gas flow rate on  $O_2$  reaction rate.

functional groups, and hydrogen is removed in a direct water formation reaction. Superimposed on this complex chemistry are possible transport limitations outside and inside the coal particles. Quantitative tests have been used to demonstrate consistency between the data and such models (Kam *et al.*, 1976; Karsner and Perlmutter, 1980).

Turning to more immediately practical results, it is of interest to relate oxidation rates to the geologic history of various coals. In Figure 10 comparable rates are presented as a function of

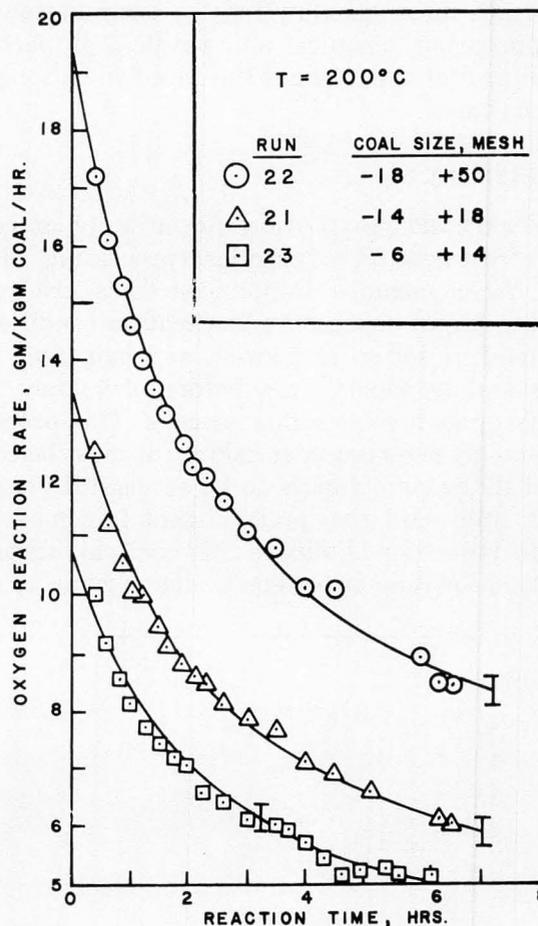


FIGURE 4. Effect of particle size on  $O_2$  reaction rate.

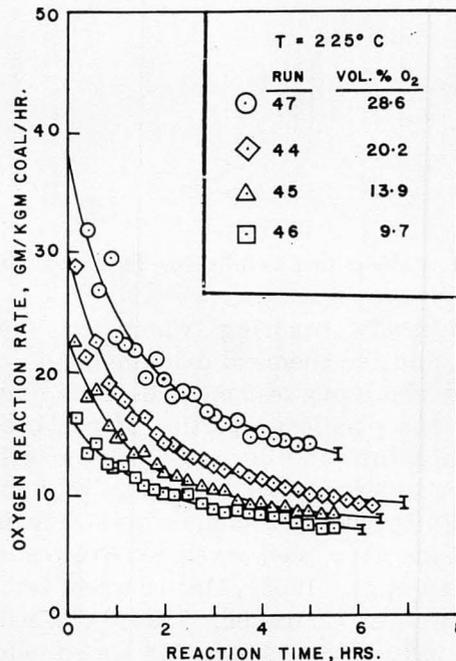


FIGURE 5. Effect of feed  $O_2$  concentration on oxygen reaction rate.

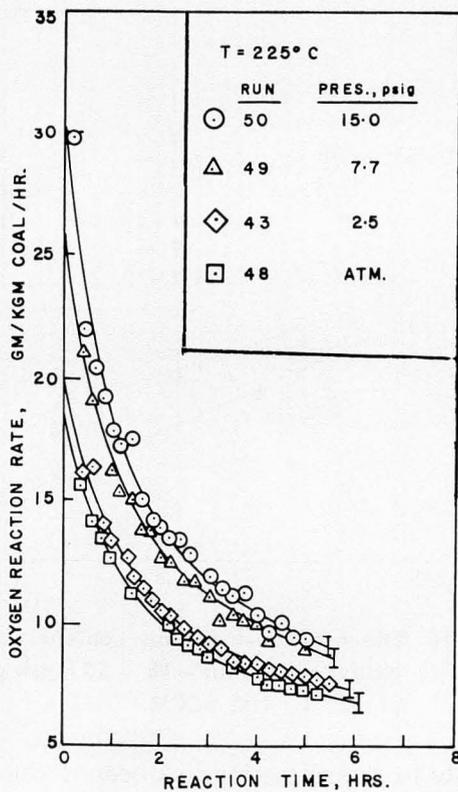


FIGURE 6. Effect of pressure on oxygen reaction rate.

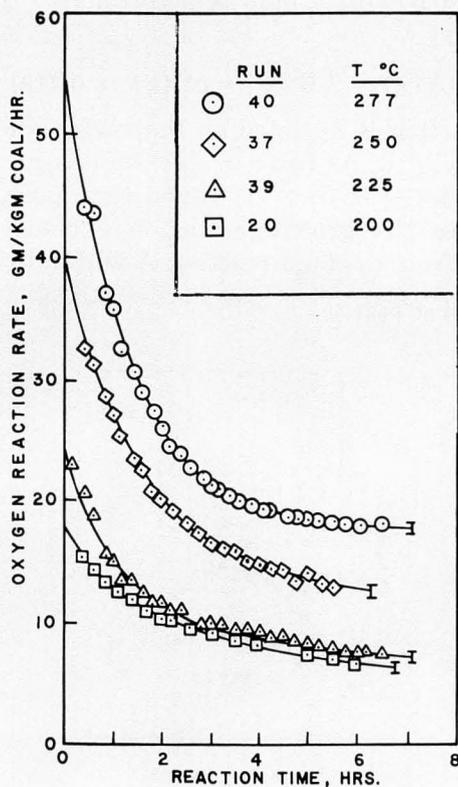


FIGURE 7. Effect of temperature on oxygen reaction rate.

carbon content, a commonly used index of a coal's rank. As shown, by the duplicate runs, the cross-hatched band is primarily a reflection of variability among coals and only in minor part caused by experimental scatter. A balanced evaluation of pretreatment must also consider the economic losses that accompany any reduction in heating values. The data show a strong correlation with the carbon content of a sample. Regardless of particle size, the heating value of a material changed upon oxidation primarily as the carbon changed for a wide range of coals of different types. There is also a suggestion in the data that

Regardless of particle size, the heating value of a material changed upon oxidation primarily as the carbon changed for a wide range of coals of different types.

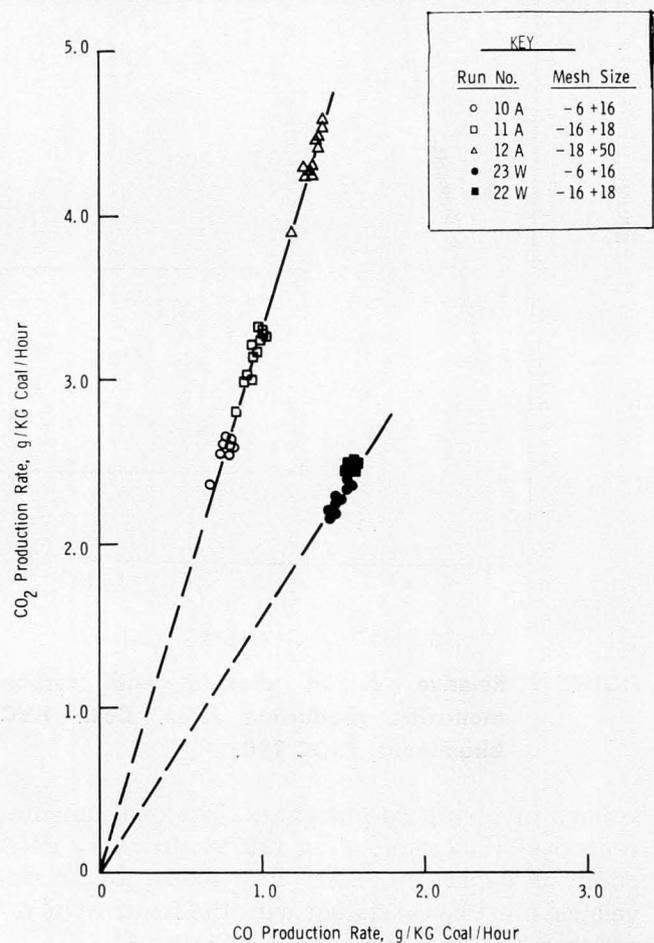
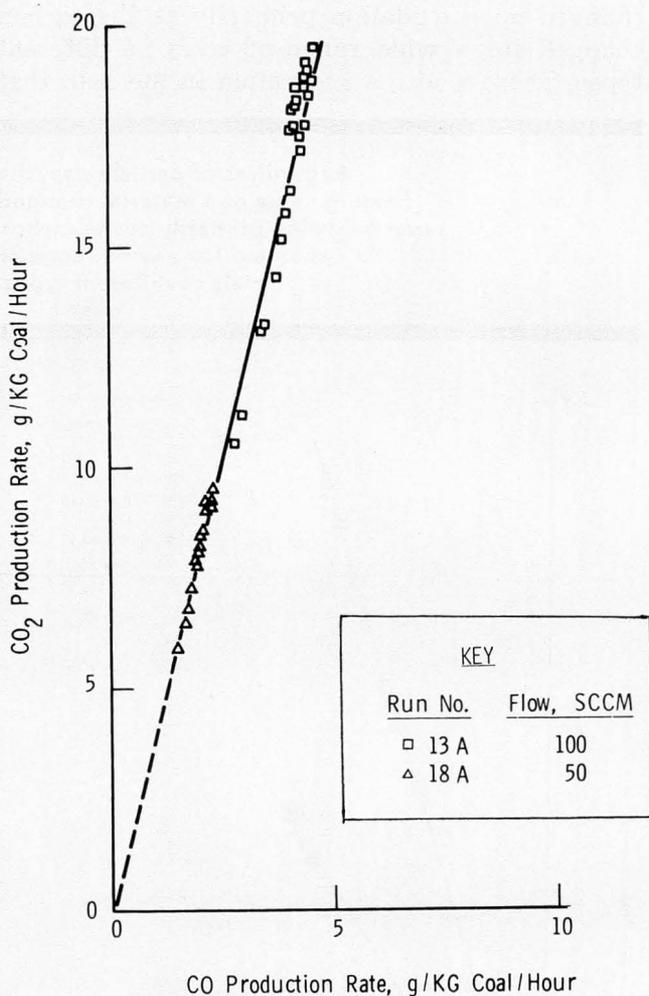


FIGURE 8. Relative carbon dioxide and carbon monoxide production rates. Coal: MV bituminous, PSOC 135.

generalizations regarding the fixation of oxygen that occurred for all the various bituminous coals do not apply to the lignite (PSOC 87) and the anthracite (PSOC 80) coals.

### CHAR REACTION

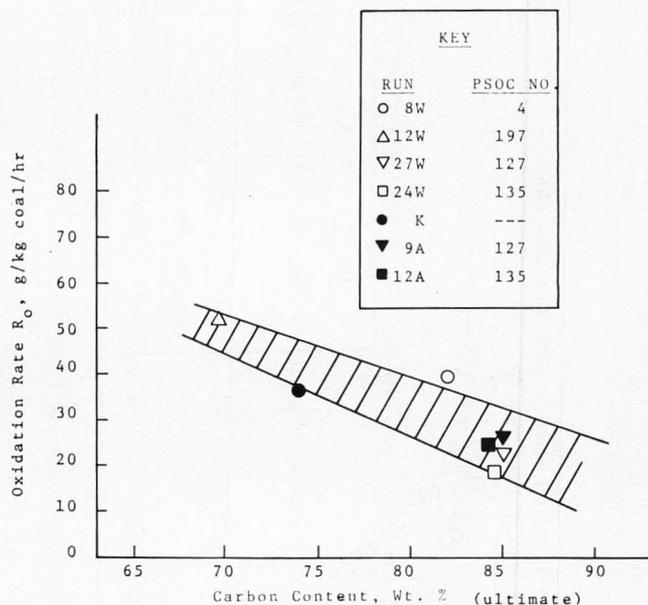
**T**URNING ATTENTION TO the downstream side of a coal gasification process, models are needed to describe kinetics of the several gas-solid re-



**FIGURE 9. Relative carbon dioxide and carbon monoxide production rates. Coal: HVC bituminous, PSOC 190.**

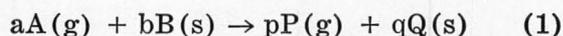
actions involving porous chars. The experimental reports of Hashimoto et al. (1979) provide a good point of departure, since any model to be developed must be consistent with the features of reaction such as are presented in Figure 11.

Above all a viable model must permit the development of a maximum in rate (or reactive surface) as a function of conversion. A promising



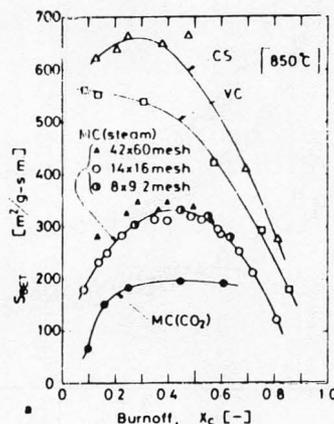
**FIGURE 10. Effect of coal carbon content on initial oxidation rate for -18 + 50 mesh particles at 225°C, 100 SCCM.**

candidate in this direction has been developed by Bhatia and Perlmutter (1980), who considered the isothermal chemical reaction of particles of the solid B with a fluid A according to the stoichiometry



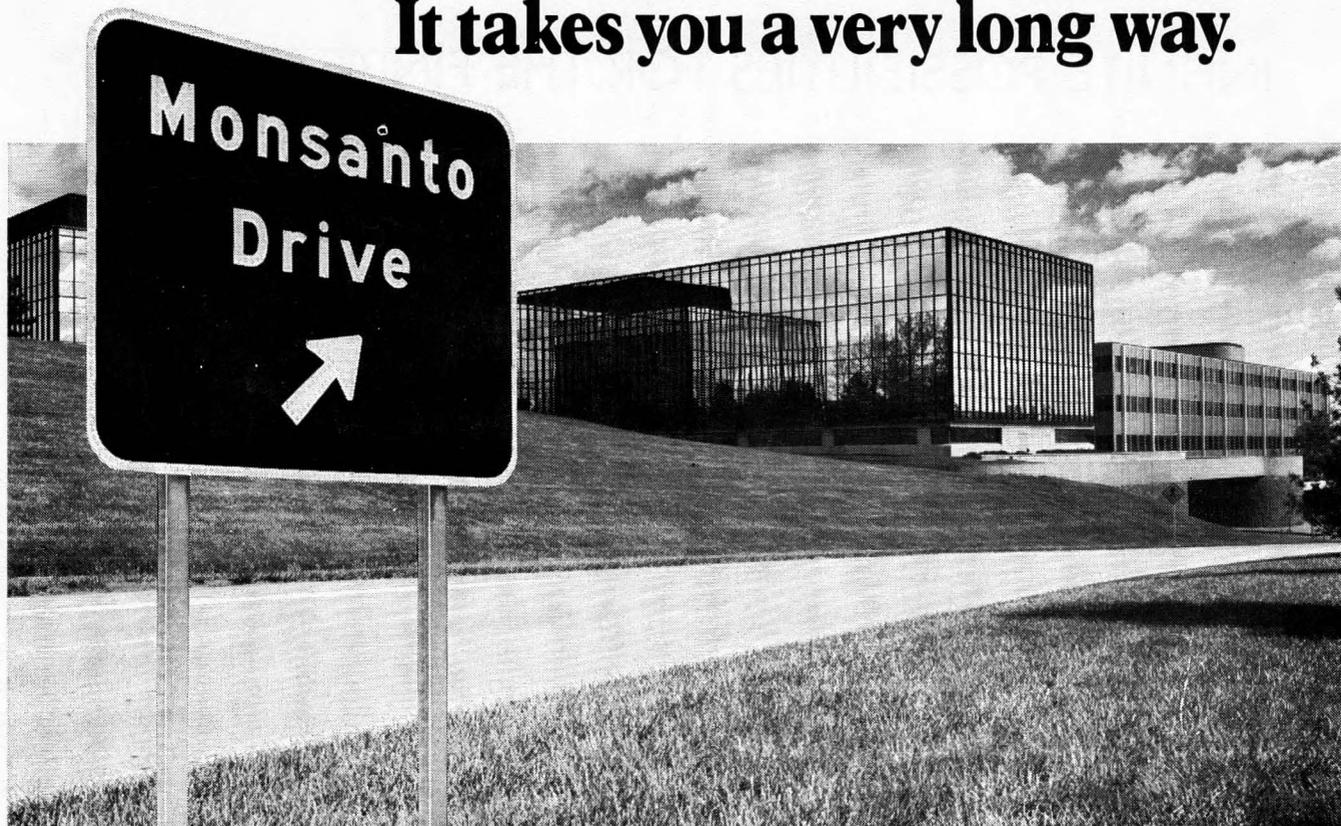
The reaction is initiated on the surfaces of pores in the solid B. As further reaction occurs, a layer of product Q is formed around each pore, which separates the growing reaction surface of the solid B from the fluid reactant A within the pores.

Continued on page 49.



**FIGURE 11. Effect of char conversion on surface area, after Hashimoto et al. (1979).**

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# INFINITE POSSIBILITIES FOR THE FINITE ELEMENT\*

BRUCE A. FINLAYSON  
*University of Washington*  
*Seattle, WA 98195*

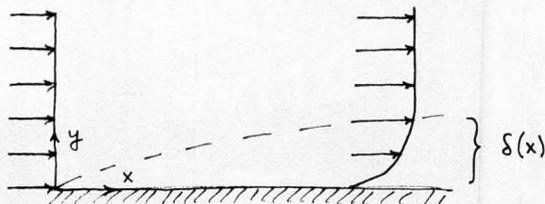
**F**INITE ELEMENT METHODS are being used increasingly for engineering studies of structures, heat transfer, fluid flows, design of dams and flow of water in aquifers. Because of this widespread use the well-educated engineer should have some experience applying the finite element method.

Finite elements are most effective for solving two-dimensional problems on irregular domains, but their use is sometimes warranted in one-dimensional problems. Chemical engineers have used finite element methods in 1-D, without calling it a finite element method. Sometimes finite elements are not needed, and an analyst should know when to use finite elements and when not. This



**Bruce Finlayson** has extensive experience modelling chemical engineering systems. He is well known for developing the orthogonal collocation method as an efficient computational tool for modelling chemical reactors with both radial and axial dispersion and monolith, wall catalyzed reactors. More recently he is known for work in finite element methods solving heat transfer and flow problems, particularly viscoelastic polymeric fluids and flow in porous media. He is the author of two books: *The Method of Weighted Residuals and Variational Principles*, Academic Press, 1972, and *Non-Linear Analysis in Chemical Engineering*, McGraw-Hill, 1980.

\*This paper was presented at the ASEE meeting in Baton Rouge, LA, on June 24, 1979.



**FIGURE 1. Flow Past a Flat Plate.**

distinction is less important for the practicing engineer who may use an available program.

## ONE-DIMENSIONAL PROBLEMS

**P**ROBABLY THE OLDEST USE of finite element methods is for flow past a flat plate (see Figure 1). In the integral method (1, p. 142) we divide the region of space into two elements: a small element near the plate and a larger element away from the plate. We represent the velocity in these two regions by two functions:

$$\begin{aligned} \text{outer element: } u &= U_{\infty} \\ \text{inner element: } u &= U_{\infty} \phi(\eta), \\ \eta &= y / \delta(x) \end{aligned}$$

The boundary layer thickness is  $\delta(x)$ . It is this division of the region into two, with expansions of velocity in each region, that makes this a finite element method. We must still determine  $\phi(\eta)$  and  $\delta(x)$ .

These expansions are substituted into the boundary-layer equations (see 1, p.142; 2, §4.2 for the details) and the result is called a residual. We would like the residual to be zero since then the differential equation is satisfied. That may not be possible, particularly if the expansions for  $\phi(\eta)$  or  $\delta(x)$  are simple. In the integral method we integrate the differential equation over the domain—in this case over the inner element—and set the result to zero, thereby making the differential equation zero “on the average.” The result is an equation for the boundary layer thickness.

$$(B - A) \delta \frac{d\delta}{dx} = \frac{\nu}{U_\infty} C \quad (1)$$

The numbers A, B, and C can be calculated once  $\phi(\eta)$  is known, and Eq. (1) is easily solved.

The expansion for  $\phi(\eta)$  is made as simple as possible: a polynomial. There are certain conditions it must satisfy: The velocity should be zero at  $y = 0$  (on the wall) or at  $\eta = 0$ :  $\phi(0) = 0$ . The velocity should match at the node between the inner and outer element, which occurs at  $y = \delta(x)$  or  $\eta = 1$ :  $\phi(1) = 1$ . Likewise it is convenient to have the slopes match at  $\eta = 1$ :  $\phi'(1) = 0$ . Applying these conditions to a quadratic function,  $\phi = a + b\eta + c\eta^2$ , gives the expansion for  $\phi(\eta)$ .

$$\phi = 2\eta - \eta^2$$

Ref. (1) uses

$$\phi = \frac{3}{2} \eta - \frac{\eta^3}{2} \quad (2)$$

which is derived by using a cubic polynomial and adding the condition  $\phi''(0) = 0$ , which is obtained by making the differential equation be satisfied at the point  $\eta = 0$  on the wall. Eq. (2) gives a slightly better result. With this function we have a representation for the velocity field in the whole domain. By satisfying the equation "on the average" we are using the integral method, and by representing the velocity by piecewise polynomials in different regions we are using finite elements. The finite elements are necessary because of the sharp changes of velocity near the wall.

For the next example we turn to diffusion and reaction in a spherical catalyst pellet. Consider the reaction of carbon monoxide with oxygen in an alumina catalyst coated with small amounts of platinum. The rate of reaction has been measured to be

$$\text{Rate} = \frac{kc^*}{(1 + K_a c^*)^2}$$

where  $k$  and  $K_a$  depend on temperature (see 3, p. 461). The equations to be solved are

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dc}{dr} \right) = \frac{R^2}{D_o} \frac{k(T)c}{(1 + \alpha c)^2}$$

$$- \frac{dc}{dr} = \text{Bi}_m (c - 1) \quad \text{at } r = 1$$

where we have written the non-dimensional  $r = r' / R$ , with  $r'$  the dimensional radial position in the catalyst and  $R$  the radius.  $c = c^* / c_o$ , where  $c_o$  is the external concentration of CO, taken here

**Finite elements are most effective for solving two-dimensional problems on irregular domains, but their use is sometimes warranted in one-dimensional problems.**

as 4%, and  $\alpha = K_a c_o = 5$  at 58°C. For purposes of illustration we solve this for  $\text{Bi}_m = 20$  and a variety of  $R^2 k(T) / D_o = \phi^2$ , the Thiele modulus squared. A quantity of interest is the average rate of reaction, compared to the rate of reaction if there were no diffusion limitation. The effectiveness factor is

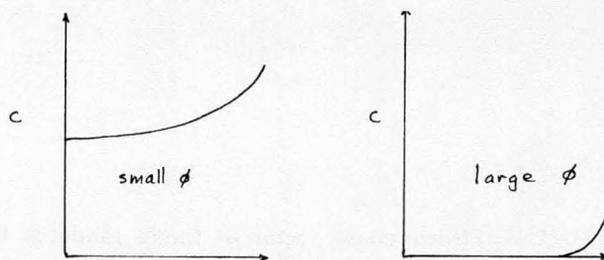
$$\eta = \int_0^1 \text{Rate}(c(r)) r^2 dr / \int_0^1 \text{Rate}(c = 1) r^2 dr$$

Now we know the concentration profile depends strongly on  $\phi^2$ , which is the ratio of diffusion time to reaction time. If the diffusion time is very small (i.e. diffusion is very rapid) then the concentration profile is as indicated in Figure 2a. Under these conditions the concentration can be easily represented by a polynomial in  $r$ , and finite elements are not indicated. By contrast, if  $\phi^2$  is large then the reactants are rapidly depleted in the pellet, and concentration profiles such as Fig. (2b) are possible. Then finite elements are indicated—express the solution as one function in the inner core and another in the outer boundary layer.

For low  $\phi$  we can use the orthogonal collocation method to solve the problem. The concentration is expanded in a quadratic polynomial.

$$c(r) = c_2 + a(1 - r^2)$$

Higher order polynomials are possible but are not needed except for high accuracy. We find it more convenient to solve in terms of  $c_2 = c(1)$  and  $c_1 = c(r_1)$ , where  $r_1$  is the collocation point = 0.65465. The orthogonal collocation equations are given here (for details see 2, §5.3 and 4).



**FIGURE 2. Concentration in Catalyst Pellet.**

$$B_{11}c_1 + B_{12}c_2 = R^2k(T_1)c_1 / D_e(1 + \alpha c_1)^2 \quad (3)$$

$$-(A_{21}c_1 + A_{22}c_2) = Bi_m(c_2 - 1) \quad (4)$$

$$\eta = 3(w_1R(c_1) + w_2R(c_2)) / R(c = 1)$$

$$B_{11} = -B_{12} = -10.5, A_{21} = -A_{22} = -3.5$$

$$w_1 = 0.2333, w_2 = 0.1, r_1 = 0.65465$$

$$T_1 = 1 + \beta\delta + \beta(1 - \delta)c_2 - \beta c_1 \quad (5)$$

$$\delta = Bi_m / Bi = k_g k_e / (h_p D_e)$$

$$\beta = (-\Delta H_R) C_o D_e / k_e T_o$$

The equation for  $T_1$  is exact. (4, pp. 96-97). Here we solve for  $\beta = 0$  (isothermal case) and  $Bi_m = 20$ . This solution is not valid for any  $\phi^2$ , but it is a good approximation provided  $c(r = 0) \geq 0$  (see Figure 2a). Since

$$c_1 = c_2 + a(1 - r_1^2)$$

$$a = \frac{c_1 - c_2}{1 - r_1^2}$$

the approximation is valid for

$$c_2 + a \geq 0$$

$$\text{or } c_1 - r_1^2 c_2 \geq 0.$$

The  $\eta - \phi$  curve is shown in Figure 3 and is indistinguishable from the exact solution when  $\phi < 10$ . This curve is easily calculated, without iteration, simply by choosing a  $c_2$ , finding  $c_1$  from Eq. (4),  $T_1$  from (5) (if non-isothermal), and  $R^2k(T_1) / c_1$  from (3), with  $\alpha$  evaluated at  $T_1$ .

For large  $\phi$  we must use the Paterson-Cresswell (5) approach using finite elements. In the inner element of Figure 2b we take  $c = 0$  and we let the inner element have length  $b \leq 1$ . In the outer element we use the trial function

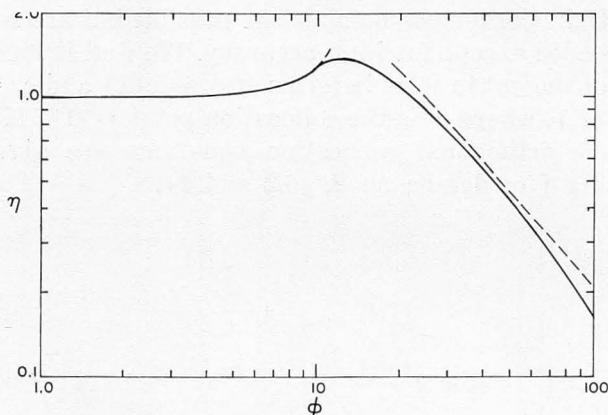


FIGURE 3. Effectiveness Factor — Thiele Modulus for Carbon Monoxide Reaction,  $Bi_m = 20$ ,  $\alpha = 5$ . ——— exact, - - - approximate.

The advantage of the finite element method is that the elements can easily be deformed, small elements can be used in important regions, and irregular domains are easily handled.

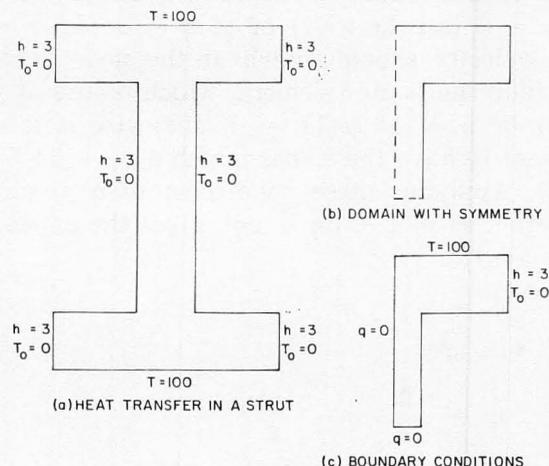


FIGURE 4. Heat Transfer Problem.

$$c = u^2 c_3,$$

$$u = (r - b) / (1 - b)$$

which satisfies  $c = 0$  and  $dc/du = 0$  at the node between elements. The collocation equations are now (see 4), for planar geometry,

$$\frac{1}{(1 - b)^2} (B_{21}c_1 + B_{22}c_2 + B_{23}c_3) = R^2k(T_2)c_2 / (D_e(1 + \alpha c_2)^2) \quad (6)$$

$$- \frac{1}{1 - b} (A_{31}c_1 + A_{32}c_2 + A_{33}c_3) = Bi_m (c_3 - 1). \quad (7)$$

Now  $c_1 = c(u = 0)$ ,  $c_2 = c(u = 1/2)$ , at the mid-point of the outer element, and  $c_3 = c(u = 1) = c(r = 1)$ . We have  $c_1 = 0$  and  $c_2 = c_3 / 4$ , so we can solve (7) for  $c_3$ .

$$c_3 = \frac{(1 - b) Bi_m}{2 + (1 - b) Bi_m} \quad (8)$$

For various  $b$  from 0 to 1 it is easy to see the influence of external diffusion resistance. When  $c_3 = 1$  there is no concentration drop across the boundary layer surrounding the pellet, and this condition depends on  $(1 - b)Bi_m$ . For large  $Bi_m$ , we have  $c_3 = 1$ . These equations are solved without iteration by choosing  $b$ , finding  $c_3$  by (8),  $c_2 = c_3 / 4$ , and then using (6) to get  $\phi_p^2 = R^2k(T_2) / D_e$ . Choosing  $b = 0$  gives the dividing

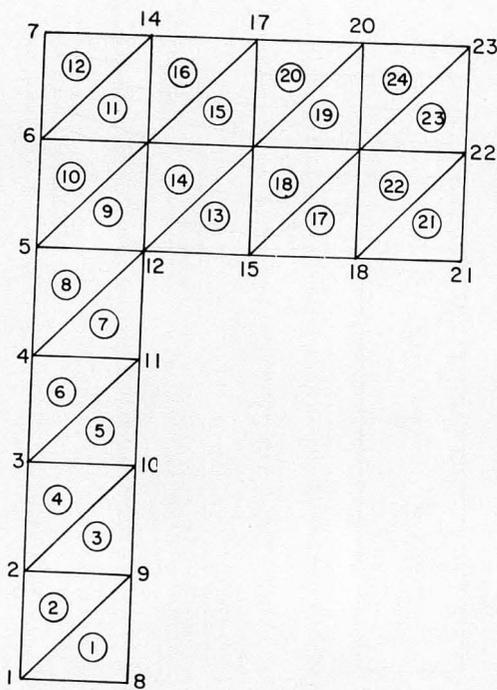


FIGURE 5. Mesh for Heat Transfer Problem.

line between the orthogonal collocation solution and the finite element solution. Here we have solved the finite element solution for planar geometry (it is easier than spherical geometry), and we use

$$\phi_p = \frac{\phi}{3}$$

to get the results for spherical geometry. The  $\eta - \phi$  curve is shown in Figure 3. Over the whole range of  $\phi$  we get a reasonable solution; compared to much more difficult numerical solutions. Certainly the solution exhibits all the important phenomena, usually within experimental accuracy. This example clearly shows the importance of using finite elements when the solution is sharply

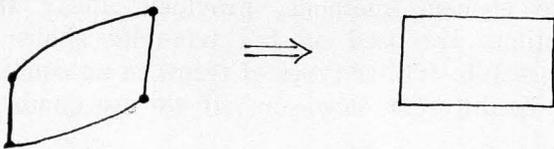


FIGURE 6. Element Deformation.

changing, Figure 2b, whereas non-finite element methods are suitable for smooth solutions; Figure 2a.

## TWO-DIMENSIONAL PROBLEMS

**A** MORE IMPORTANT USE of finite element methods is for two-dimensional problems. Consider heat transfer in the region shown in Figure 4. The boundaries are maintained at temperature = 100 and the interior is cooled with a heat transfer coefficient  $h = 3$ ,  $T_o = 0$ . We wish to solve  $k\nabla^2 T = Q$  in strut,  $T = 100$  on top and bottom boundary,  $-kn \cdot \nabla T = h(T - T_o)$  on side boundaries. Space does not permit a complete discussion of all aspects of the finite element method but the highlights can be given.

We first discretize the space, as shown in Figure 5. We can divide the region into triangles,

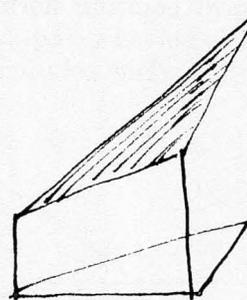


FIGURE 7. Trial Function, Linear on Triangle.

rectangles or quadrilaterals. Because of the way finite element programs are written it is very easy to use deformed elements, as shown in Figure 6. The actual calculations are made on the square element, with appropriate account taken of the transformation properties. Within each element we expand the unknown function in a polynomial—either linear or quadratic, usually (see Figure 7). Having decided on the trial function (here linear functions on triangles) we number the nodes and elements (see Figure 5). Now in two adjacent elements the equations are similar when written in terms of the local coordinates (see Figure 8). The appropriate equations must be assembled properly. The equations are solved with

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Since finite methods are being used increasingly by industry for design of structures, heat transfer, fluid flow, design of nuclear reactors, etc., it is important that the modern student be exposed to them. It is not necessary that the engineer be familiar with the details . . . but (he) should know the general idea.

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an LU-decomposition or a Gaussian elimination (6). These techniques are beyond the scope of this article.

The user then specifies the thermal conductivity and heat generation rate in each element. Here we have

$$k_e = 1, Q_e = 0.$$

Finally the boundary conditions are specified as

$$\begin{aligned} T_1 &= 100 \\ \text{nodes } i &= 7, 14, 17, 20, 23 \\ h_i &= 3, T_{oi} = 0 \\ \text{nodes } i &= 8, 9, 10, 11, 12, 15, 18, 21, 22, 23. \end{aligned}$$

For a boundary node at which temperatures are *not* specified by the user the boundary condition is automatically the natural boundary condition

$$\begin{aligned} \partial T / \partial n &= 0 \\ \text{nodes } i &= 1, 2, 3, 4, 5, 6, 7, 8 \end{aligned}$$

with  $n$  the outward pointing normal.

This problem is solved using the program in Huebner's book (7). The solution is shown in

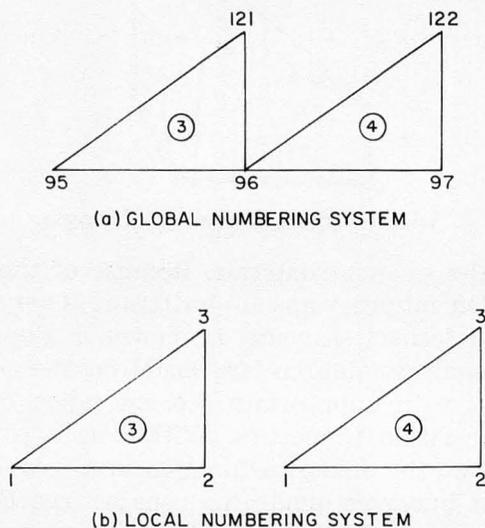


FIGURE 8. Finite Element Numbering System.

Figure 9. Naturally more elements are needed for good accuracy, but the essential elements are clear in Figure 9.

The advantage of the finite element method is that the elements can easily be deformed, small elements can be used in important regions, and irregular domains are easily handled. The reason for these features is that the computer programs are written on an element-by-element basis, since each element is similar. The user, then, has complete freedom in how the elements are to be arranged.

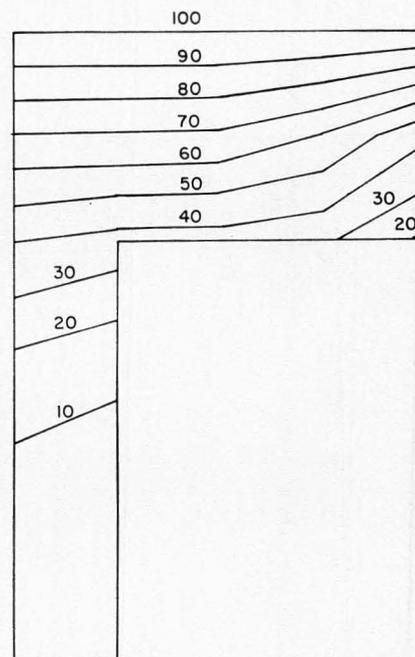


FIGURE 9. Solution to Heat Transfer Problem. Contours are for each 10 degree increment.

#### COMPARISON TO FINITE DIFFERENCE

THERE ARE BOTH SIMILARITIES and differences between finite element and finite difference methods. For the heat conduction problem

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

a finite difference grid is shown in Figure 10a. The finite difference method uses the following equation representing the differential equation at node 5.

$$\nabla^2 T|_5 = (T_6 + T_4 + T_2 + T_8 - 4T_5) / h^2.$$

The same equation results from application of the finite element methods, provided linear trial functions are used on the triangles shown in Figure 10b. (Other types of terms in an equation may be different, however). If we use quadratic

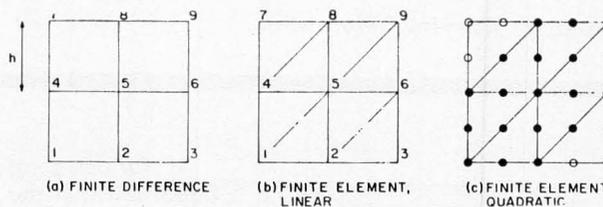


FIGURE 10. Comparison of Finite Difference and Finite Element Methods.

polynomials in the finite element method, then we have more nodes and the equation at node 5 involves terms at each node represented by  $\cdot$  in Figure 10c. Because the equations are derived in different ways the finite element method is, however, easy to apply with the irregular geometries shown in earlier figures. In addition, certain types of boundary conditions are easily handled in finite element methods, particularly boundary conditions involving derivatives and/or free surfaces, whose location is to be determined.

#### SUMMARY

SINCE FINITE ELEMENT methods are being used increasingly by industry for design of structures, heat transfer, fluid flow, design of nuclear reactors, etc., it is important that modern students be exposed to them. It is not necessary that the engineer be familiar with the details of the method, but the engineer should know the general idea and be able to apply the method. The author has found students are quick to learn how to use finite element programs, and once experienced will always know what someone means when they say Finite Element Methods.

#### FURTHER INFORMATION

COMPARISONS OF finite element, collocation, and finite difference methods are given in Ref. (8). One-dimensional cases are emphasized since that allows the easiest description of the methods and details of applications. Two-dimensional problems are treated there as well as books by Huebner (7) and Chung (9). Huebner's book contains a simple finite element program for heat transfer problems. More elaborate programs are available (10). Applications to engineering design are widespread, and one concentrated source is the *International Journal of Numerical Methods in Engineering*. Probably there are published accounts of research applications of the finite element method in the journals related to your area of interest. □

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## ChE letters

#### FOREIGN STUDY PROGRAM

Dear Sir:

We read with interest about the successful Study-Travel Program at Virginia Tech (Summer 1980 issue).

I would like to briefly mention two intensive foreign study programs which are open to selected Chemical Engineering undergraduates at Case Western Reserve. They may also serve as examples for other Departments who wish to initiate such programs.

Each year since 1978, three of our undergraduates have spent their junior year at the University of Edinburgh. There they are regular full time students in the third year Chemical Engineering program. The students normally live in university student housing and can participate in the usual range of student activities. Full academic transfer credit for a years work is granted upon successful completion of the third year course at Edinburgh. This arrangement has been extremely successful, primarily due to the excellent and continued cooperation of the Edinburgh faculty. The experiences of the students have been uniformly good and there have been minimal academic re-entry problems after returning to Case for their senior year.

We also participate, with Iowa State University and Georgia Tech, in a summer laboratory course at University College London. This very well run program lasts for approximately one month and, in addition to the intensive laboratory course, includes a one week bus tour of various British chemical industries. Credit for our Unit Operations Lab is given upon completion of the course. Part of the reason for the success of the program is the dedicated work of the faculty representatives from Iowa State and Georgia Tech that accompany the students.

Overseas study has been an area in which we in engineering education have lagged behind our colleagues in the liberal arts. Part of the reason has been the necessity of meshing requirements from two highly structured curricula. Despite these difficulties, the remarkable benefits to the students involved make the effort worthwhile. More programs of this type should surely be offered.

Sincerely yours,  
John C. Angus  
Case Western Reserve University

## A SIMPLE TUBULAR REACTOR EXPERIMENT

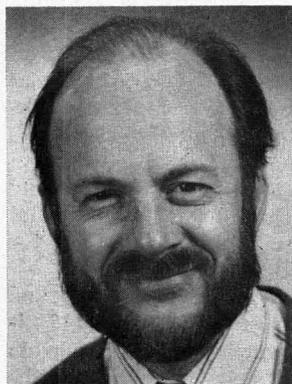
ROBERT R. HUDGINS

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BERTRAND CAYROL

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USING AS A REACTION system the hydrolysis of acetic anhydride, Anderson [1] developed a laboratory demonstration of tubular reactor behaviour. In this article, another such demonstration is presented with two novel additions: (i) a color change is added as a visual reinforcement of the measured results and (ii) the temperature constraint is removed in order to provide an experiment operable at room temperature. The



**Robert R. (Bob) Hudgins**, born in Toronto, Canada, obtained all his degrees in Chemical Engineering; B.A.Sc. and M.A.Sc. at the University of Toronto and the Ph.D. degree at Princeton University. He came to the University of Waterloo in 1964 where he has remained except for study leaves at Polysar, Sarnia, Ontario, Université de Sherbrooke, Sherbrooke, Quebec, and most recently (1979) at the Swiss Federal Institute of Technology (EPF), Lausanne. His research studies have focused upon the influence of inert diluent gases in heterogeneous catalytic reactions, and on the behavior of chemical reactors under forced cycling. (L)

**Bertrand Cayrol** received his Ph.D. from McGill University, Canada, in 1972. He has been a Research Visitor at Chalmers University of Technology, Sweden, and a Research Assistant at the Université d'Orsay, France. Presently he is Assistant Professor at the Université de Sherbrooke, Canada, with special interest and work on the viscoelastic properties of polymers synthesized by micro-organisms. (R)

latter innovation reduces the complexity and thus the cost of the apparatus.

Corsaro [2] described the hydrolysis of crystal violet dye by sodium hydroxide. Reaction is first order in the concentrations of each of the reacting species. If the base is in great excess, the kinetics of reaction become pseudo-first order,

$$-r_{\text{dye}} = k' [\text{dye}]$$

where  $k' = k[\text{NaOH}]$ . The dye concentrations needed for this experiment are of the order of  $10^{-5}$  mol/L. Thus, a 0.01 mol/L solution of NaOH is in 1000-fold excess and in a concentration readily achieved at low cost. Also, NaOH concentrations can be varied considerably in order to achieve a desired pseudo-first order rate constant  $k'$  at room temperature. This feature of the experiment eliminates the expensive temperature control equipment of the sort used by Anderson [1].

Another advantage of this system over that using acetic anhydride hydrolysis is that the system remains isothermal during reaction. The fact that the reagents are also very dilute means that there is little safety hazard if the reagents are spilled, though safety glasses are recommended.

The results of this experiment may be approximated by idealized models, such as the plug flow tubular reactor (PFTR) and laminar flow tubular reactor (LFTR).

### THEORY

The PFTR model is widely used, (see Levenspiel [3] for example) and is related to the inlet and outlet dye concentrations as follows.

$$\tau = \frac{V}{v_0} = \frac{1}{k'} \ln \frac{[\text{dye}]_i}{[\text{dye}]_0} = -\frac{1}{k'} \ln(1-x)$$

The LFTR model has been developed by Cleland and Wilhelm [4]. The radial mean conversion at the exit from the tube is given by the expression.

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$$\bar{x} = 1 - 2 \int_1^{\infty} \frac{e^{-\nu y}}{y^3} dy$$

$$= 1 - \nu^2 \text{Ei}(\nu) + e^{-\nu} (\nu - 1)$$

where  $\nu = k'\tau_0$ ,  $y = t/\tau_0$   
and  $\tau_0 = L \pi r^2 / (2 v_0)$

Ei is the exponential integral, available in mathematical handbooks.

## APPARATUS

The principal components required for this experiment are listed below; code letters refer to the schematic in Figure 1.

**Tanks:** (T1) 200-L polyethylene tank bottle with 3/4-in spigot for draw-off. (T2) 10-L Nalgene aspirator bottle with spigot.

**Pumps:** (P1) Century type SPS (1/4 HP); available from Flotec Inc., Norwalk, California. (P2) Magnetic-drive variable speed micropump; Cole-Parmer Cat. No. 7004-92.

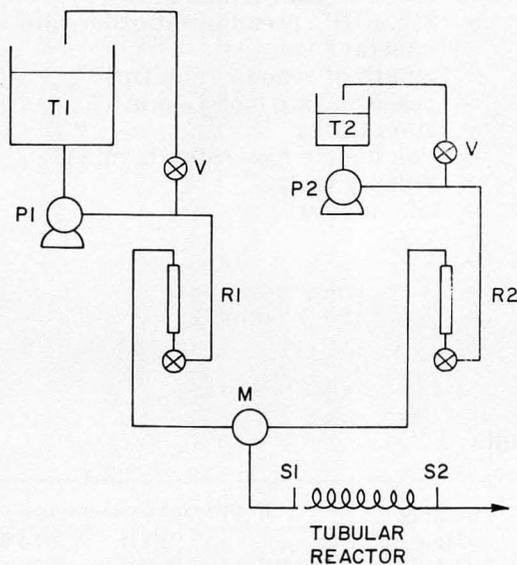
**Mixer:** (M) Graphite impeller pump (whose impellers have been removed for use as a mixer); Eastern Pumps, LFE Fluids Control Div., Hamden, Conn.

**Rotameters:** (R1) Brooks type R-6-15-A. (R2) Brooks type R-2-15-B.

**Reactor:** 40 m of 3/8-in I.D. Tygon tubing, wound on a spool 28 cm in diameter and 55 cm in length.

**Valves:** (V) any adjustable valve to adjust flow in the recycle lines.

**Spectrometer:** Spectronic 20 (Bausch & Lomb) fitted with a "Flow-Thru Accessory" for rapid sampling.



**FIGURE 1: Schematic Diagram of Apparatus.** T1, T2 — tanks for NaOH solution, dye solution respectively; P1, P2 — pumps; R1, R2 — rotameters; V — adjustable valves; M — mixer; S1, S2 — sample points.

A 200-L reservoir (T1) is used for the caustic solution and a 10-L reservoir (T2) for the crystal violet dye solution. These are metered into a mixer (M) at the entrance to the tubular reactor. Samples may be withdrawn from the entrance (S1) to the reactor and from the exit (S2) from it at tee-junctions. These tees are fashioned by welding short lengths of 1/8 in O.D. stainless tubing to 3/8 in O.D. stainless tubes used as connectors at the entrance to and exit from the reactor tube.

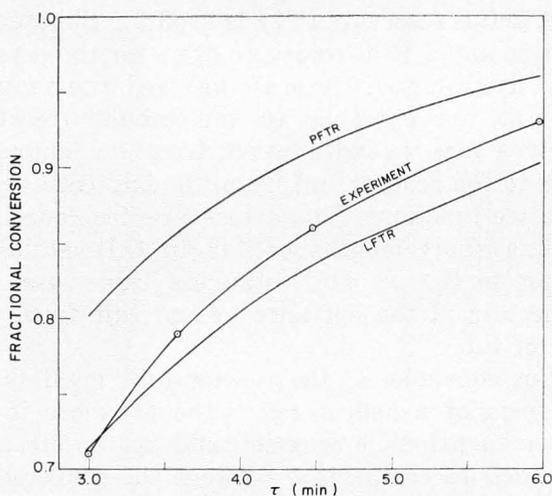
For convenience, the reactor tube itself takes the form of a helical coil, although there is no reason in principle why it could not be straight or folded (a comparison between the conversions using helical coils vs. straight tubes might make an interesting variation of this experiment, to investigate the importance of secondary flow in the helical reactor). During operation, a strong change in color may be observed along the reactor tube between inlet and outlet.

The analysis of crystal dye at both the inlet to and outlet from the reactor is readily done with a spectrometer, and the method is given by Corsaro [2]. The Flow-Thru Accessory of the Spectronic 20 consists of a vacuum system to draw small samples through a fine tube into cuvette, and then to empty into a waste jar. Since the sampling time is brief, and reproducible, errors in measuring the concentration of the reacting sample are kept to a minimum. The concentration is readily obtained by calibration with known concentrations of the dye. Occasional sampling of methanol or ethanol will prevent the build-up of adsorbed crystal violet dye on the walls of the cuvette.

## EXPERIMENTAL PROCEDURE

**T**HE MAXIMUM FLOWRATES of crystal violet dye solution and caustic soda solution are 50 mL/min and 1000 mL/min respectively. Thus, in the reactor volume, the holding time is just a few minutes, and since plug flow is approximated, little more than a single filling of the reactor is needed to obtain steady state conditions after a change is made in the input flows and/or concentrations.

For purposes of illustration of the behavior of this reactor, several points may be obtained at different space velocities. This is done by deciding on the range of flowrates available and then keeping the two feed pumps in the same ratio. Concentrations are measured at a sample point just at



**FIGURE 2: Comparison of Experimental Conversions with those Predicted from PFTR and LFTR Models.**

the entry to the reactor, and just at the exit. Some student data are presented in Table 1, for the experiment at Université de Sherbrooke. Note that the volume of the reactor was 2780 mL, and the concentration of NaOH (from the titration tests) was 0.04 mol/L. In addition, batch tests of dye with caustic soda solution of this concentration provided a pseudo-first order rate constant  $k' = 0.54 \text{ min}^{-1}$ .

Using this information in the reactor models provided, the model conversions of Table 1 were calculated and the graphs in Figure 2 prepared for both PFTR and LFTR. The conversion data from Table 1 are also plotted in Figure 2. It appears that the behavior of the reactor lies between the LFTR and the PFTR. No particular significance is attached to the fact that the conversion curve crosses the LFTR curve at short holding times; the conversion data of most student groups appear to lie between the two theoretical curves. A wider range of flows might be used in order to

discern trends in the behavior of the real reactor with holding time.

Finally, we offer a comment or two on student reaction to the experiment. The change in color of the reactants across the reactor is quite a novelty in a chemical engineering laboratory experiment. This visual effect helps to reinforce what is learned from both the measurements and the theory. The measurements are readily made, and the theoretical models used to bracket the expected performance of the reactor are inherently interesting. This happy combination of factors has meant that the experiment has always been well received by students working on it. □

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#### NOTATION

- $e, i$  = subscript symbols for exit, inlet  
 $k$  = rate constant L/mol·min  
 $k'$  =  $k[\text{NaOH}]$ ; pseudo-first order rate constant ( $\text{min}^{-1}$ )  
 $L$  = length of reactor tube (m)  
 $-r$  = reaction rate mol/L·min  
 $t$  = time (min)  
 $v_0$  = volumetric flow rate (L/min)  
 $V$  = volume ( $\text{m}^3$ )  
 $X$  = conversion  
 $y$  =  $t/\tau_0$   
 $\nu$  =  $k'\tau_0$   
 $\tau$  =  $V/v_0$  ( $\text{min}^{-1}$ )  
 $\tau_0$  =  $L/\pi r^2 / (2v_0)$  ( $\text{min}^{-1}$ )

**TABLE 1**  
**Experimental Results**

Run No.	Flow of dye (mL/min)	Flow of NaOH (mL/min)	Dye Concentration		Holding Time (min)	Fractional Conversion		
			Inlet (mol/L x 10 <sup>5</sup> )	Outlet		Exp'tl	PFTR Model	LFTR Model
1	15	450	1.1	0.08	5.98	0.93	0.96	0.90
2	20	600	1.05	0.15	4.48	0.86	0.91	0.84
3	25	750	1.05	0.22	3.59	0.79	0.86	0.77
4	30	900	1.05	0.30	2.99	0.71	0.80	0.72

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# IMPRESSIONS OF CHEMICAL PROCESS CONTROL EDUCATION AND RESEARCH IN THE USA\*

KURT V. WALLER  
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**T**HE FIELD OF CHEMICAL process control was heavily criticized in 1973. Foss [1] wrote a much cited critique of the theory research. Athans' critique[2] pointed in a different direction when he stated: "It is indeed unfortunate that the process control engineers have disassociated themselves from the mainstream of modern control theory. . . In this manner, the tremendous advances during the past three years in system identification, adaptive control, sensor location, and accuracy tradeoffs have probably gone unnoticed by the very profession that stands the benefit most."

Athans was aware of the difficulties: "I do believe that far greater care and finesse is required to apply modern control theory to process control problems than missile autopilotes," but his opinion about what action should be taken is clear: "Everybody knows that chemical process control systems are inherently less understood in their dynamic behaviour than Newtonian systems. But it seems to me that this should be viewed as a challenge, rather than an outcry that the theory is no good."

It is easy to criticize. This is especially true of process control research, which is in the

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**In design of control systems there are two basic approaches. The first, in this paper referred to as the forward approach . . . The second here called the backward approach, starts from the process operator.**

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\*This is a condensed version of Prof. Waller's original paper published in the Finnish journal *Kemia-Kemi*, Vol. 7 (1980), page 85.



**Kurt V. Waller** was born in Mariehamn, Finland, in 1940. After studying in Finland and West Germany he got the degrees M.Sc., Tech. Lic. and Tech.Dr from Abo Akademi, Finland, in 1966, 1970, and 1972. A member of the faculty of Chemical Engineering at Abo Akademi since 1970, Dr. Waller was appointed full Professor in 1975. Professor Waller has written about 50 scientific papers, mainly on process dynamics, optimization, and control.

difficult position that it [3] "must compete for funds with such endeavors as process de-bottlenecking, process improvements, new plant construction, and other undertakings. Returns from these latter efforts are usually more easily proven or at least more readily believed."

Still, has the critique from 1973 been seriously considered by the chemical engineering profession? Is the field of chemical process control in USA today a vital field, or does it lack enthusiasm and perspectives?

## STATE OF THE ART

### Education

A good picture of how established process control has become in chemical engineering education in the United States and Canada is obtained from Seborg's recent survey [4]. It shows that the basics of process control is now taught at practi-

cally all chemical engineering departments. The main part of the teaching is, however, concentrating on very basic facts only and using surprisingly old textbooks, the clearly dominating one (by Coughanowr and Koppel [5]) written over 15 years ago.

The vast majority of departments have only one faculty member in process control. There are some departments, however, which put more emphasis on control and which can offer quite advanced programs. One example of a two-person process control program was recently described in [6].

### Research and Development

In design of control systems there are two basic approaches. The first, in this paper referred to as the *forward approach*, is to take a theory with potential for the specific process in question and apply it after a possible adaptation to the class of problems at hand.

The second, here called the *backward approach*, starts from the process operator. In this approach the goal is more or less to imitate a skillful and experienced operator by the automatic control system. In many respects the automatic system can perform better than the manual, since it is not influenced by the many sources for human errors, it won't get tired, etc. It is natural to improve the system continuously by extending it to include more and more new and abnormal situations, making the reasons for the operator to switch to manual less frequent.

It seems natural that a sound design includes elements from both the forward and the backward approach. The impression obtained is that applications in the U.S. industry have a stronger emphasis on the backward approach than is the case in Finland (and Scandinavia).

One explanation for such a difference is easily found. The connections between the universities and industry seem to be much closer in Finland than in U.S.A., as also indicated by Foss and Denn [7] in summing up the 1976 Asilomar Conference on Process Control: "The ties between industry and the university appear closer in Europe than in North America, and the closeness seems to have afforded European university researchers opportunities to implement and test their control methods on industrially significant processes." There are, however, a few university groups in the U.S. sponsored by and working in

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**The connections between  
the universities and industry seem  
to be much closer in Finland than the U.S.A.**

---

close cooperation with industry. One is the group at the Case Western Reserve University directed by I. Lefkowitz.

If there is a gap between industry and the university on the one hand, there also seems to be quite a gap between the control researchers in U.S. electrical and chemical engineering departments. The electrical engineers are often very theoretical while their chemical colleagues are quite oriented towards applications, often even to that extent that they rather work on specific problems than on concepts. Thus there seems to be a certain vacuum in the study of the applicability of the more advanced theory, seemingly the most natural process control field for activity in chemical engineering departments. However, there seems to exist a strong controversy concerning this latter statement.

There are some workers in the field though. At the University of California, to provide just one example, Foss at the Berkeley campus has for many years studied a packed bed chemical reactor, the studies including state space modeling by orthogonal collocation [8] and recently [9] [10] the applicability of LQG-theory to the reactor, which exhibits inverse response. At the Santa Barbara campus Seborg and Mellichamp are working both on reactor and distillation control, two of the applications in chemical process control which seem to have a large potential for modern multivariable estimation and control theory.

There is also quite an interest in exploring the potential of the frequency response methods for multivariable systems developed in Great Britain by Rosenbrock, MacFarlane and coworkers. Indeed, such an interest was already expressed by Fisher [11] in 1973. The largest advantage is generally considered to be the insight into and feeling for the system obtained by the methods. Recent applications treat Foss' reactor [12] and Wood's distillation column [13] in Alberta, Canada.

Among new approaches being studied can be mentioned "Inferential Control," studied by Brosilow and coworkers [14]. The goal is to infer unmeasurable product qualities from secondary measurements, and here e.g. standard least squares estimates are used. The novelty is how the secondary measurements are selected so as to minimize

the number of such measurements required to obtain an accurate estimate which is insensitive to modeling errors. A compensator, which is a process model, compensates for the effect of the control effort on the secondary measurements. This leads to the appealing feature of the approach that the control effort is not fed back in the system, only the disturbances and the model mismatching. This fact is said to give the system excellent stability properties. One interesting task would be to exploit the approach systematically for the model mismatching problem, which is of such a central importance in process control. A first step in this direction is taken in [15].

At present there does not seem to be much active interest among chemical engineers to try to apply and explore the self-tuning regulator (STR) of Åström and coworkers [16] [17] or Zadeh's fuzzy control concepts [18] [19]. The

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#### **Another use of the interaction analysis is for design of decoupling schemes.**

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common attitude is to wait and see until convincing application studies are presented in which these approaches have turned out to result in something that more familiar and commonly accepted methods have not. Previous studies in North America of the STR and of Fuzzy Control have mainly been done on the north side of the Canadian border.

One of the subjects of great research activity in chemical process control in the U.S. today is interaction analysis, in which coupling between inputs and outputs in multi-input multi-output systems is studied. Interestingly enough the topic is studied by consultants and industrial researchers as well as by university people.

The analysis starts in many cases from Bristol's Relative Gain Array [20] [21] or similar interaction indices suggested by Rijnsdorp [22] or Nisenfelt and Schultz [23]. One of the main uses for the technique is to pair variables, resulting in (interacting) single-input single-output control systems. It should be emphasized that one is not restricted to basic manipulators but can use various combinations of manipulative variables. Interesting examples are given by McAvoy [24] in exploring two-composition control in distillation. Conventional control, in which reflux and boilup are manipulated, is compared to Shinskey's material balance control (with either reflux and

bottoms flow rate or boilup and distillate flow rate as manipulators), and also to Rijnsdorp's suggestion to use the ratio reflux to boilup as one control variable in addition to boilup. The least amount of interaction is found for a hybrid between Shinskey's and Rijnsdorp's suggestions.

While the interaction analysis usually uses only steady-state data, extensions to include dynamics in the interaction analysis in a rational way have been treated in several papers. Witcher and McAvoy [25] as well as Tung and Edgar [26] show by including dynamics in the analysis that it can lead to wrong pairing to take only steady-state properties of the process into account.

While Witcher and McAvoy, Tung and Edgar, and recently Gagnepain and Seborg [27] work in the time domain, Kominek and Smith [28] work with polar plots in the frequency domain. The screening of a dual composition control scheme from 12 potential candidates for an ethylene column is used by Kominek and Smith to illustrate the use of the theory. Use of only steady-state interaction index is shown to result in systems unsuitable for implementation.

Another use of the interaction analysis is for design of decoupling schemes. The discussion is largely concerned with decoupling in two-composition control in distillation. At present the discussion is highly concerned with the question of whether one-way (also called partial) decoupling, advocated e.g. by Shinskey [29], or two-way (complete) decoupling, which is the approach previously investigated, is to be preferred. Strongly related to this question in distillation is the question of degeneracy in decoupling, recently studied by McAvoy and coworkers [30] [31].

Additional papers on the topics of interaction and decoupling analysis are [32] to [34].

Some further research objects of present and/or planned activity are mentioned below in the discussion of trends.

#### **THE FUTURE: TRENDS AND SPECULATIONS**

##### **Education**

Since no major changes concerning process control can be foreseen in chemical engineering departments in U.S.A. in the near future, most departments will continue to have one faculty member who teaches the basics of process control and systems engineering. Advanced teaching programs in process control will probably be given only in the very few departments (the order of 5

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Since no major changes concerning process control can be foreseen in ChE departments in the U.S.A. in the near future, most departments will continue to have one faculty member who teaches the basics of process control and systems engineering.

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schools in the whole U.S.A.) where there is more than one faculty member in the control field.

This scarcity of more advanced programs in process control seems to be very unfortunate, because the correct interpretation and intelligent application of modern control concepts is a task that takes quite a lot of understanding of and familiarity with the theory as well as it demands engineering skill. There are several examples where the application has failed solely because of unsuitable interpretation of the theory. A perspicuous example of the importance of a correct interpretation of the theory is given in [35] and [36] concerning the way of treating the integrals in optimal PI-control of systems with time delay.

What will be taught? There probably won't be much enthusiasm in the teaching of only the basic process control courses, so for that matter the text by Coughanowr and Koppel could be used for another 15 years. It seems likely, however, that it will be replaced by a text which has a much stronger emphasis on computers and digital systems. The text may very well start the treatment directly in discrete time and skip much of the old material used for continuous time treatments. The same goes for the future teaching of process control, which is likely to put less emphasis on equations and more on algorithms than has been done in the past.

What will be taught in the more advanced courses will usually reflect the research.

### Research and Development

Largely the industry is likely to continue to go its own way. Then the "backward approach," i.e. the one in which the operator is translated into the computer system, may be one of the main approaches for design of industrial control systems.

Undoubtedly the approach has its merits. One rationale for it is that things are almost never "normal" in process operation: "the normal state is the abnormal one." Therefore one should start from the process at hand, (and why not) as viewed by the experienced operator.

Important university research in this area will be concerned with plant diagnosis, fault detec-

tion, control under failure, and system reliability. Also, the emphasis will shift towards treating more difficult processes and to be more "devilish" in testing the control systems. The important subject of man-machine communication, however, is probably best studied in industrial environment.

There is, however, also in industry an awareness of the serious drawbacks inherent in the backward approach. It conserves bad habits of the operators and retards the progress. A catalytic reformer is a good example: The operator tends to recycle much hydrogen because the operation is then very stable and safe. However, less hydrogen recycled generally means less energy consumed and more economic operation. Another example [37]: In distillation it is common practice for operators to increase the reflux rate above the design value. Then disturbances in the feed composition seldom cause the top product to fall below specifications, but this advantage is balanced by the excess steam supply needed to overreflux the column.

Today we are faced with a lot of double conservatism in the process industries. Firstly, processes and plants are *designed* to be conservative meaning a lot of capacity for decoupling and disturbance attenuation. And secondly, the processes are *operated* in such a conservative way so that most of the disturbances left by the design disappear into the conservative operation. And this usually means a waste in energy and equipment.

However, it seems quite clear, that industry has to cut down the waste of resources by means of more sophisticated technology. Processes will have to be designed as well as operated in a significantly more integrated way, closer to constraints, than today. It probably won't be possible, and certainly not economic, to operate such plants manually. Or as seen by Evans [38]: ". . . new processes are bigger, more integrated and more highly automated. Operators are at the same time becoming further divorced from the process, removed from the operation of the process, so when it comes time to start up or shutdown, or emergency situations occur, the operator does not have the intimate familiarity with the process which his counterpart in the less automated facility once had."

Closer ties between industry and universities

would, of course, decrease the gap. The industry would get competent help to apply more advanced control concepts and the university people could more easily ask the right questions and attack the relevant problems.

The gap can be illustrated by some views on process modeling [39].

Much of the university research in modeling for process control has been concerned with the small perturbation, linear approach. The tendency has been to include more and more smaller and smaller effects into the model. An industrial response is: These complicated models can never take everything into account anyway, the operator does not understand them since they are so complicated, so they are not used.

Or to put it another way: University people usually suppose a "normal" state for the process. An industrial conception of what is "normal" was expressed as: Things are never normal—or perhaps 2% of the time.

Models will have to become simpler and more robust. (Signs of steps in this direction are already visible [40]). In many cases a simple model structure only will be determined from first principles. In operation there will be a strong shift towards experimental modeling, i.e. towards on-line identification and estimation, with a subsequent reduction in importance of modeling from first principles.

It seems likely that the concept Fuzzy Control will find increased use in the backward approach, since the most important property of a system designed by the backward approach is that it is kept on automatic and not switched over to manual. System performance comes only second in importance. The natural language flavor of fuzzy control seems ideal to prevent the operator from feeling unfamiliar with the concepts used in the computer system. Another rationale for the use of fuzzy logic is that much of the control work going on in industry is done, and will continue to be done, almost without any control theory in the sense of "hard" systems theory. So far, however, use of fuzzy logic has been reported mainly from Europe [41] [42].

For a long time it has been recognized that there is a large potential in an integration between process and plant design and control. Indeed [43], "it is important to consider process control in general—the development and the application of its theory—as an integrated part of the plant design and the process operation." There is quite

a lot of interest in the subject among chemical engineers in the U.S.A. today, and increased research activity can be expected. In this integration the potential of the chemical engineer can be utilized at its very best.

The increased integration of processes and complexity of plants, will make the control aspects more critical. There will be a greater need for, and emphasis on, multivariable control methods. Analysis of plants will to an increased extent rely on efficient simulation methods for large systems. More work in these areas is needed and is likely to be done [44].

What about adaptive control methods? Will, for example, the self-tuner see an increased number of applications? The answer is most likely yes. One of the reasons was formulated, somewhat cynically, by an industrial control system designer: These methods will be used more because university people like to play around with them.

Starting from the single process unit rather than from the concept point of view, no significant changes are visible. Thus the large interest in distillation control of the last decades continues. Today research in distillation control in U.S.A. is concerned with such questions as pressure control, coupling and decoupling in two-composition control, multivariable control in general, and nonlinear control of high-purity columns.

The other "large" process will probably continue to be the chemical reactor, which offers a wealth of challenging design, optimization, identification, estimation, and control problems.

It is also felt by several workers, both in universities and industry, that these two processes, the chemical reactor and the distillation process, have the greatest potential for use of modern control theory.

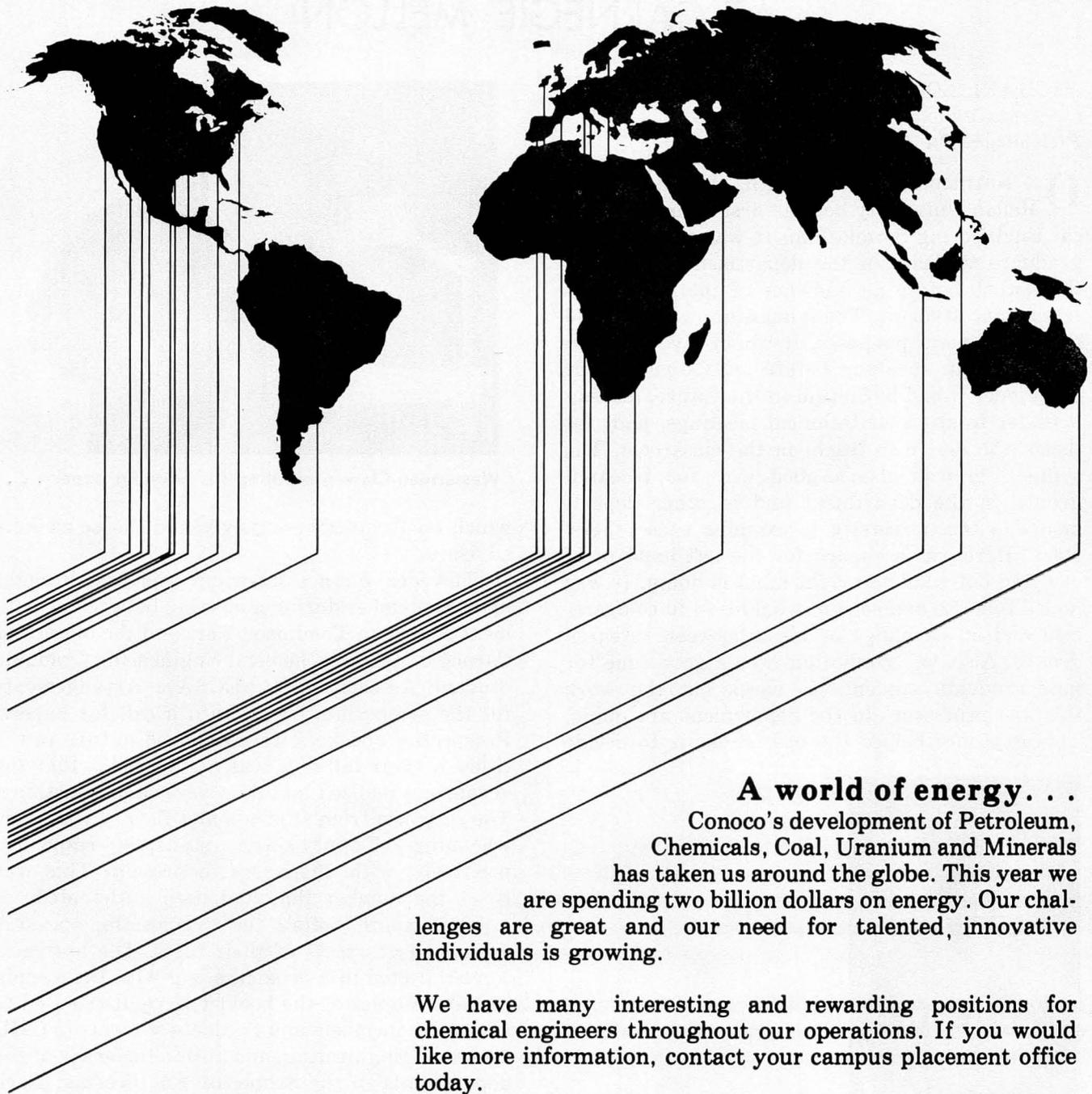
## DISCUSSION

**H**OW HAS THE CHEMICAL process control community responded to the critique expressed in 1973?

Athans' opinion 5 years later is not less critical, when he comments on the—in his opinion sad—state of applications of advanced control in the process industries. He states [45] that the chemical engineers are so conservative that they have only got what they deserve. Shinnar [46] (1977) laconically states: "the state of process control is rather sad."

Continued on page 51.

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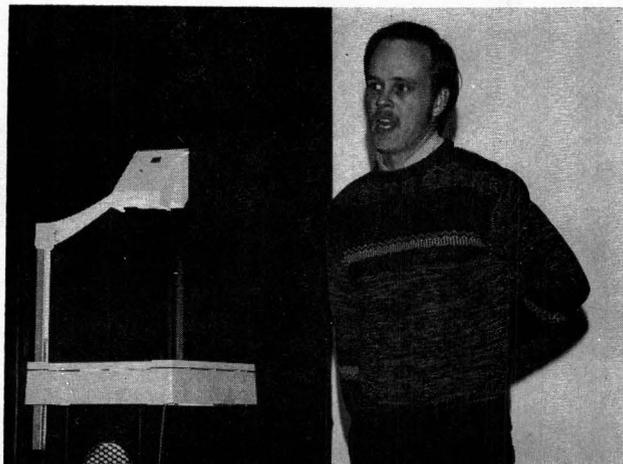
## CHEMICAL ENGINEERING SYMPOSIUM AT CARNEGIE-MELLON

MICHAEL LOCKE  
*Carnegie-Mellon University*  
*Pittsburgh, PA 15217*

ON NOVEMBER 15th and 16th, 1979, Carnegie-Mellon University held its first annual Chemical Engineering Symposium. It was a chance for graduate students in the department to present their work before an audience of interested professors and students. The symposium was intended to serve several purposes. It would give students experience in speaking before an audience. This experience would be helpful in the future, making it easier to speak at technical meetings, and, for those who desire to teach, in the classroom. The symposium was also a good way for research groups in the department and in other departments in the university to examine each others' work. Here was a chance for the left hand to at last find out what the right hand is doing. It was hoped that the symposium would lead to co-operation and an exchange of ideas between research groups. Also, the symposium was a good time for new graduate students to check out the work that the professors in the department are doing. This exposure helped the new students to decide



**Mike Locke** received his B.S.Ch.E. from the University of Massachusetts in 1976, his M.S.Ch.E. from Carnegie-Mellon in 1978 and is presently working on his Ph.D. at Carnegie-Mellon. His areas of interest include Optimization, Computer Aided Design, and Equation Solving. He presently serves as a consultant to NTP Corporation of Pittsburgh.



**Westerman-Clark presenting his winning paper . . .**

which faculty members they would choose as their advisors.

The idea for a symposium was first brought up in September during a meeting between department chairman Tomlinson Fort and the officers of Carnegie-Mellon's Chemical Engineering Graduate Student Association (ChEGSA). Arrangements for the symposium began with a call for papers. Prospective speakers were required to turn in the titles of their talks. It was at this point that the organizers realized that they were on to something. The response from students and faculty was overwhelming. Twenty-seven students responded positively, with 29 papers to present. This was twice the number that had been anticipated.

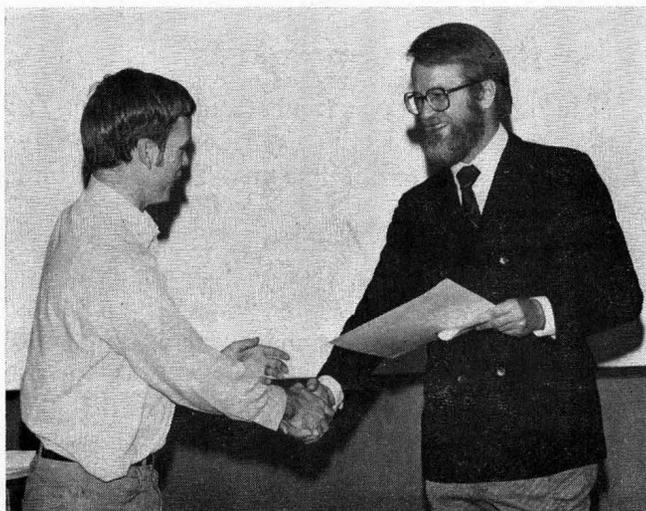
One month before the symposium, speakers submitted abstracts of their talks. The abstracts were collected in a booklet, along with the agenda of talks. Copies of the booklet were distributed to all faculty members and graduate students in CMU Chemical Engineering, and also to the heads of the departments in the School of Engineering. Each student was given 20 minutes to talk, with 5 additional minutes for questions. Topics ranged from separation of polymer wastes to synthesis of heat exchange networks. Other interesting topics were

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trace metal levels in Pittsburgh air (there's more than just a trace), and the velocity of blood flow in a rabbit's ear. Interesting discussions started during the symposium, and are continuing.

As an incentive for the students, a prize was awarded for the best paper. It consisted of an expense paid trip to the next AIChE convention, to deliver the winning paper, and a check for \$100 from Tomlinson Fort. The judging committee was made up of 5 faculty members, headed by Dr. Robert Rothfus, the senior member of the department. Speakers were judged on content, presentation, and a written copy of the talk.

After much deliberation, the judging committee chose Jerry Westermann-Clark as the prize winner. The title of his talk was "Coion Exclusion Potential in Charged Membranes." Jerry entered



... and receiving his award and the congratulations of Professor Fort.

CMU in September, 1976, with a B.S. from the University of Pennsylvania. He has a Masters Degree from Carnegie-Mellon and his Ph.D. in September, 1980. His work was supervised by Dr. John Anderson. Jerry is now an Assistant Professor at the University of Florida.

The judges also named three runners up. They were Greg Townsend, for his talk "Pharmacokinetics of Adriamycin in Normal and Neoplastic Tissues" with Dr. Rakesh Jain supervising; Lewis Grimes, with a talk entitled "The Synthesis and Evaluation of Networks of Heat Exchangers that Feature the Minimum Number of Units," supervised by Dr. Arthur Westerberg; and Michael Reilly for his talk "Ambient Trace Metal Levels in Pittsburgh Air," supervised by Dr. Eric Suu-berg. □

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**PRAIRIE DOG APPENDIX\***

R. L. KABEL  
 Pennsylvania State University  
 University Park, PA 16802

**SOLUTION:**

We see that the wind velocity increases as a logarithmic function of the height above the earth's surface. Because of the higher velocity at 2.5 m than at 0.5 m there will be a lower pressure at the top of the tube than at the bottom. This pressure difference will induce an upward flow in the tube.

A Reynolds Number can be calculated for flow through the tube:

$$Re = \frac{D\langle v \rangle \rho}{\mu} = \frac{0.01\text{m} (1 \text{ ms}^{-1}) (1.2 \text{ kg m}^{-3})}{1.8(10^{-5} \text{ kg m}^{-1} \text{ s}^{-1})} = 667$$

which indicates laminar flow.

Thus the Hagen-Poiseuille equation can be used to find the pressure drop. Eq. 2.3-19 Bird, et. al. (or the Prairie Dog problem) gives

$$Q = \frac{\pi \Delta p R^4}{8\mu L} \quad \text{or} \quad \Delta p = \frac{Q8\mu L}{\pi R^4}$$

$$Q = \langle v \rangle A = \langle v \rangle \pi R^2$$

$$= 1 \text{ ms}^{-1} (\pi) (0.005^2 \text{ m}^2) = 7.85(10^{-5} \text{ m}^3 \text{ s}^{-1})$$

$$\mu = 1.8(10^{-5} \text{ kg m}^{-1} \text{ s}^{-1})$$

$$L = 2 \text{ m}$$

$$R = 0.005 \text{ m}$$

Substituting, we obtain

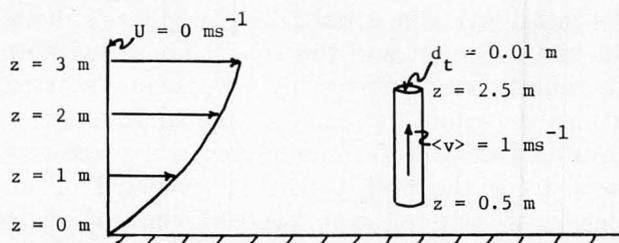
$$\Delta p = 11.52 \text{ kg m}^{-1} \text{ s}^{-2}$$

This pressure drop can be related to horizontal wind velocity by the Bernoulli equation:

$$\Delta \left( \frac{1}{2} \frac{\langle v^3 \rangle}{\langle v \rangle} + \hat{\phi} \right) + \int_{p_1}^{p_2} \frac{1}{\rho} dp + \hat{W} + \hat{E}_v = 0$$

Neglecting friction and work,  $\hat{E}_v$  and  $\hat{W}$  are zero. If the air can be assumed to be incompressible under these conditions,  $\rho$  is constant and

\*The problem statement was presented in *CEE* Vol. 14, No. 4 (Fall 1980).



**FIGURE 1**

$$\int_{p_1}^{p_2} \frac{dp}{\rho} = \frac{p_2 - p_1}{\rho}$$

The potential energy difference  $\Delta \hat{\phi}$  between points is negligible and for turbulent flow of air,  $\langle v^3 \rangle / \langle v \rangle \cong \langle v \rangle^2$ , and

$$\langle v_2 \rangle^2 - \langle v_1 \rangle^2 = \frac{2(p_1 - p_2)}{\rho}$$

Taking point (1) at the bottom and point (2) at the top, both terms are positive. Thus we have one equation and two unknowns. The logarithmic velocity profile

$$\frac{U(z)}{U_*} = \frac{1}{k} \ln \frac{z}{z_0} \quad \text{or} \quad U(z) = \frac{U_*}{0.4} \ln \left[ \frac{z}{0.04} \right]$$

provides two more equations but only one more unknown,  $U_*$ . Since  $U$  in the log velocity profile and  $\langle v \rangle$  in the Bernoulli equation are the same thing (i.e. the horizontal wind velocity) we can combine these equations.

$$\langle v_2 \rangle = \frac{U_*}{0.4} \ln \left[ \frac{2.5}{0.04} \right] = 10.34 U_*$$

$$\langle v_1 \rangle = \frac{U_*}{0.4} \ln \left[ \frac{0.5}{0.04} \right] = 6.31 U_*$$

$$(10.34 U_*)^2 - (6.31 U_*)^2 = \frac{2(p_1 - p_2)}{\rho}$$

$$67.10 U_*^2 = \frac{2(11.52 \text{ kg m}^{-1} \text{ s}^{-2})}{1.2 \text{ kg m}^{-3}}$$

$$= 19.20 \text{ m}^2 \text{ s}^{-2}$$

$$U_* = \sqrt{\frac{19.20}{67.10}} = 0.535 \text{ ms}^{-1}$$

This value of  $U_*$  can now be used in the velocity profile to get velocity at 3 m.

$$U(z) = \frac{U_*}{k} \ln \frac{z}{0.04} = \frac{0.535}{0.4} \ln \frac{3}{0.04}$$

$$= 5.77 \text{ ms}^{-1}$$

□



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## TEACHING MARKET ANALYSIS

J. T. RYAN

University of Alberta  
Alberta, Edmonton, Canada

BRETT HAUGRUD

Sherritt Gordon Mines  
Fort Saskatchewan, Alberta, Canada

**M**ARKETING OF CHEMICAL PRODUCTS is a subject which is almost completely ignored in a chemical engineer's university education. This omission is unfortunate since marketing is usually the crucial constraint on the commercial viability of many projects. In spite of its obvious importance, market analysis is not taught to undergraduates; the undergraduate is not trained to

**TABLE I**  
**Capital Costs<sup>(1)</sup>**

	ALBERTA	GULF COAST
Capacity	1000 T/D 720 mm lb/yr	2000 T/D 1440 mm lb/yr
Direct Fixed Cost (excluding working capital)	66 mm \$Can	80 mm \$US
Debt <sup>(2)</sup>	20.5 mm \$Can	25 mm \$US
Equity	45.5 mm \$Can	55 mm \$US
Interest rate on debt	Canadian prime + 1½% <sup>(3)</sup>	US prime + 1%
Term on debt	15 years	15 years
Yearly debt charge <sup>(4)</sup>	\$2.2 mm \$Can	\$3.1 mm \$US
Interest rate on equity	Canadian prime + 4%	US prime + 3%
Term on equity	15 years	15 years
Yearly charge: equity recovery, return on invest- ment <sup>(5)</sup>	5.6 mm \$Can	7.65 mm \$US
Total Yearly Capital Charges on D.F.C.	7.8 mm \$Can	10.75 mm \$US
Unit Capital Charges on D.F.C.	1.09 ¢Can/lb	0.747 ¢US/lb

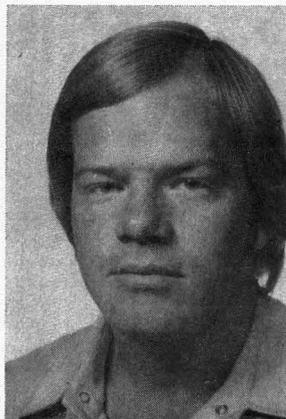
(1) Unless stated otherwise, costs are expressed in the currency of the home country.

(2) Debt-equity ratio of 0.45.

(3) Canadian prime interest rate = 8½%, U.S. prime interest rate = 8%.

(4) Both debt and equity charges taken as uniform payment retirement.

(5) Working capital and salvage neglected.



**Brett Haugrud** graduated from the University of Alberta with a B.Sc. in Chemical Engineering in 1973 and a MSc in Chemical Engineering from the same school in 1978. He worked for several years as an engineer in the Research Department of a Canadian Potash Company before accepting his present position as process engineer for Sherritt Gordon Mines, Fort Saskatchewan, Alberta. (L)

**Jim Ryan** received his Ph.D. from the University of Missouri (Columbia) in 1966. He has taught at the University of Alberta since that time. Primary teaching duties include the senior design project, undergraduate fluid mechanics and introductory thermodynamics. He serves as a consultant to the petroleum industry, mainly in the area of pipeline design and explosions. Occasionally serves as a writer and researcher for CBC-TV and Radio. (R)

analyze a market problem even in a rudimentary fashion. The neglect of the marketing process by the students' professors is understandable since their training emphasizes the scientific aspects of the chemical production process, such as research, development and design. From an academic's view, the estimation of a market size and its location is regarded as a black art best left to someone else.

This paper presents a technique which hopefully transforms market estimation from a black art into a dark gray one. Its objective is a quantitative means of estimating a potential market area at a given time for an undifferentiated chemical. An undifferentiated product is one which does not have any unique property that can be attributed to its manufacturer. The manufacturer cannot claim that his product is better than his competitor's since both products are identical within normal engineering specifications. Methanol, fertilizer-grade ammonia and polymer-grade ethylene are examples of undifferentiated products, while almost anything that is advertised as unique

or better is a differentiated product. Consequently, the major factor which will govern the sale of this type of chemical is its price, not its quality.

The potential market area for an undifferentiated chemical, produced by a given plant, is defined as that region where the delivered cost of the chemical is equal to or less than other competing producers. The delivered cost of a chemical commodity to a customer is the sum of the production costs, transportation charges, tariffs and currency exchange. The last two expenses are applicable only if the commodity is traded internationally. Rather than analyzing the position of all potential competitors for a market, the technique of estimating a market area can be illustrated more simply by considering only two competitors.

As an example, assume that two hypothetical methanol producers, one located in southern Alberta and the other on the Texas Gulf Coast, are

in competition with each other. In recognition of historical precedence, the capacity of the Canadian plant is taken initially as one half that of the Gulf Coast plant. Table I gives the illustrative capital costs and financial charges for each of the two plants. The financial arrangements are simplified in order to make the presentation of the results concise. Unit prices of inputs and associated unit manufacturing costs are shown in Table II. The cost figures in both tables are given in the currency of the home country.

Until recently, the plant gate cost of Gulf Coast methanol was significantly below that of methanol produced in Alberta. In fact, at one time the cost of methanol delivered from the Gulf Coast to Alberta was less than the plant gate cost of Alberta methanol. That situation was due primarily to the economics of scale typical of the American plants and the generally low level of natural gas prices. As is obvious from Table II,

**TABLE II**  
**Manufacturing Costs**

	ALBERTA		GULF COAST	
Capacity	720 mm lb/yr 1000 T/D		1440 mm lb/yr 2000 T/D	
Direct Fixed Capital	54 mm \$Can		80 mm \$US	
Working Capital	4.9 mm \$Can		5.8 mm \$US	
<b>VARIABLE COSTS</b>		<b>Unit Cost</b>		<b>Unit Cost</b>
		<b>¢Can/lb</b>		<b>¢US/lb</b>
Natural Gas as Feedstock and Fuel (32 mm Btu/ton)	\$1.25/mm Btu	2.05	\$1.95/mm Btu	3.28
Power	3¢/KW-hr	.02	3.5¢/KW-hr	.02
Catalyst		.15		.15
Water, misc.		.03		.03
		<u>2.25</u>		<u>3.48</u>
<b>FIXED COSTS</b>				
Labour & Admin.—80 people	\$22,000/yr	.244	\$20,000	.111
Maintenance & Local Taxes	5% of DFC	.375		.278
Sales	2% of Plant Gate Cost	.078		.09
		<u>.69</u>		<u>.479</u>
<b>CAPITAL COSTS</b>				
Unit debt on D.F.C.		.307		.215
Unit equity on DFC		.779		.531
Interest on W.C.		.03		.036
		<u>1.11</u>		<u>.782</u>
	<b>SUMMARY</b>			
Variable Costs		2.25		3.48
Fixed Costs		.69		.48
Capital Costs		1.11		.78
		<u>4.05</u>		<u>4.74</u>

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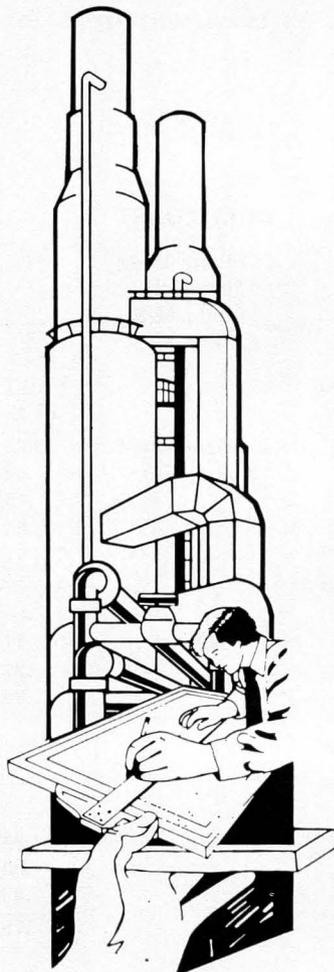
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**The potential market area for an undifferentiated chemical, produced by a given plant, is defined as that region where the delivered cost of the chemical is equal to or less than other competing producers.**

the situation is now reversed. The plant gate cost of Alberta methanol is below that of the Gulf Coast even though there is a considerable size advantage in favour of the American plant. The reason for the reversal is that the Alberta plant now has a large advantage in natural gas prices. It should be noted these are new gas prices (as of January, 1978) and do not apply to older plants which have long term contracts at lower natural gas prices or to plants that can blend the old and new gas prices.

To estimate the delivered cost at any point, the transportation costs, tariffs and currency exchanges must be added to the average plant gate production costs. The effect of these factors can be illustrated in a simple example. Suppose the two plants attempt to sell methanol in the San Francisco area. The Gulf Coast producer can transport methanol by ship through the Panama Canal while the Canadian producer is restricted to more expensive rail transportation. In addition the American producer will not have to pay a tariff while the Alberta plant must. All of these factors favour the American plant and tend to erode the plant gate cost advantage enjoyed by the Canadian plant. On the other hand, the devaluation of the Canadian dollar relative to the U.S. dollar in effect lowers the plant gate cost of Alberta methanol by about 10%. Table III summarizes all of these effects and shows that the U. S. producer is able to deliver methanol into San Francisco more cheaply than his Canadian competitor. As a consequence, San Francisco is regarded as a potential market area for the U. S. producer.

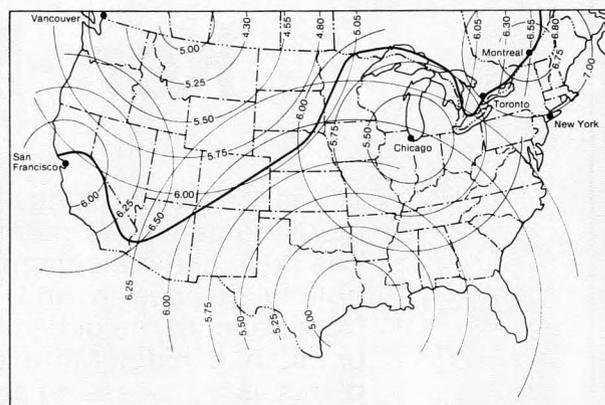
**TABLE III**

**Cost of Methanol Delivered to San Francisco**

	ALBERTA	GULF COAST
Plant Gate Cost	4.05 ¢Can/lb (3.65) ¢US/lb	4.74
Rail to San Francisco 1,324 miles at 2¢/ton-mile	1.32 ¢US/lb	—
Ship to San Francisco 4000 at .5¢/ton-mile	—	1.0¢
Tariff—7.6 ¢/US gal	1.15 ¢US/lb	—
Delivered cost	6.12 ¢US/lb	5.74 ¢US/lb

The technique used to calculate the delivered costs of the two competitors in the San Francisco area can be generalized to any point of sale. The results of this generalization are best presented on a map as a series of curves of constant delivered costs. These lines will be circles with their centers located at each plant. When a commodity shipment encounters an international border, the "iso-cost" lines will have a discontinuity as a result of tariffs and exchange rates. In general, the magnitude of the discontinuities will not be the same for both competitors.

A further complication arises where there is a possibility of change in mode of transportation. For instance, to market methanol in the U.S. Midwest, the Gulf Coast producer might ship his product via barge to Chicago, then distribute from Chicago either by rail or by truck. The base cost in Chicago would then be the Gulf Coast plant gate cost plus the barge charges to Chicago. Local Midwest costs would be the Chicago cost plus rail or



**FIGURE 1. Iso-Cost Lines and Market Line for Base Case.**

truck transportation charges to the market area. Consequently, the iso-cost lines in the Midwest are again circles, but their origin is at Chicago instead of the plant site. In addition to Chicago, San Francisco and Montreal were chosen as distribution centers.

The technical exercise is to construct the lines of constant cost for each distribution center. A set of these curves is shown in Figure 1. Each of them is labelled with the delivered cost in the currency of the consuming country. These circles are idealizations since the railroads do not run in straight lines. The actual iso-cost lines would be severely distorted, particularly in the west. At this stage of the analysis, this is viewed as a second order effect and is neglected. The potential market

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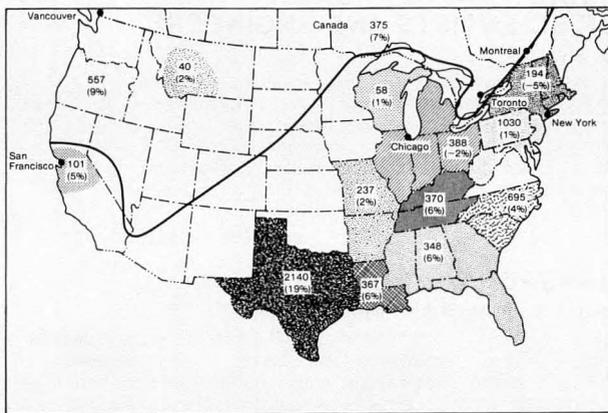
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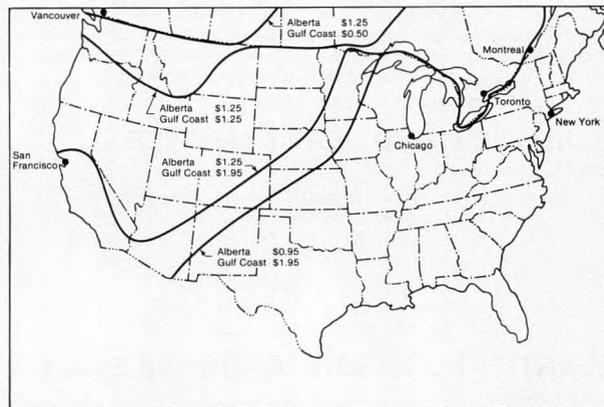
**FIGURE 2. Approximate Yearly Consumption and Growth Rate of Methanol by Region.**

area for each competitor is found by drawing a line connecting the intersections of the lines of equal constant costs. This, the market line, is also shown in Figure 1. The market area for Alberta methanol is north of the line and the Gulf Coast market is to the south.

As can be seen from the figure, Alberta's market area is all of Canada west of Quebec City and a large portion of the northwest and west central United States. The Gulf Coast producer has a lower delivered cost everywhere else. Once the geographical areas which represent potential markets for the two competitors are established, the objective is to locate customers within those areas. Figure 2 shows the approximate demand for methanol by region. The upper number is the 1977 capacity of chemical plants which use methanol as a chemical feedstock, expressed in mm lb/yr. Below this number is one in parentheses which is the six year net growth in demand for feedstock methanol. The data used to construct this figure were taken from the Chemical Economics Handbook [2] and include only specific plants listed in that publication. These values are somewhat low because they do not take into account demand for methanol as a solvent, gas line antifreeze, etc. Since a large fraction of methanol is used in manufacturing resins for plywood and other wood products, the markets are concentrated in those regions which have a significant harvestable forest. The pacific northwest and southeastern states are examples of this concentration.

By superimposing the market line on the consumption patterns, it is possible to compare the production of the two plants with the requirements of customers potentially available to each. It is clear from Table 2 that the price paid for

natural gas is the most significant component of methanol manufacturing costs. The base case natural gas prices were taken as the prevailing new gas prices (1978). Actual prices could be significantly different if old gas was under contract. A number of cases were studied to show the effect of gas prices on the market line. The cases examined are designated on Figure 3 as one through four with line 2 being the base case. When the Alberta producer has a price advantage of \$1.00/mm Btu, the change in the market size is fairly small. The only new market penetrated is San Francisco where about 100 mm lb/yr are consumed. Case 3 occurs when both competitors have the same natural gas costs. The Gulf Coast producer can now capture most of the Pacific northwest market as well as the eastern Canadian market. This situation would force the Alberta producer to operate at less than full capacity, further improving the position of the U. S. competitor. Since a small change in any economic or technical variable could cause a large change in market size, competition in the PNW would be intense. Price discounting by both parties would be a definite possibility. Finally, if the Gulf Coast operator enjoys old prices and the Alberta producer pays new gas prices, the Texas plant would capture all of the PNW. The Alberta producer would be left with only the three western Canadian provinces, whose total market is less than his breakeven production rate. The problem is



**FIGURE 3. Effect of Natural Gas Price on Market Area.**

solved since he must then shut down if actually operating or decide not to build a new plant.

Operating under the base case conditions, the Gulf Coast producer has access to a market of approximately 6000 mm lb/yr, while the Alberta manufacturer has a maximum market of 970 mm

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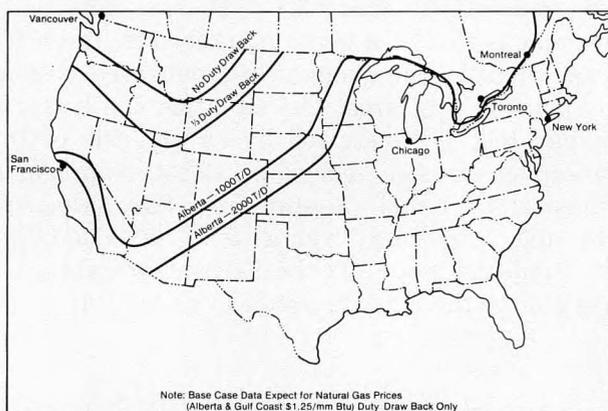
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lb/yr. With the indicated growth rates, these markets will have expanded to 7050 and 1220 mm lbs/yr respectively during the three years taken for planning and construction. To operate at full capacity, the new American producer must capture 20% of the market available to him, whereas the equivalent number for the Alberta plant is 60%. The potential market available to the Alberta producer at start-up is about twice the capacity specified in the base case, i.e. 1000 T/D. As a first step, he might consider doubling the plant capacity to 2000 T/D in order to capture the entire base case market area plus any other market that becomes available as a result of the economics of scale. Figure 4 shows the market



**FIGURE 4. Effect of Plant Size and Duty Draw Back on Market Area.**

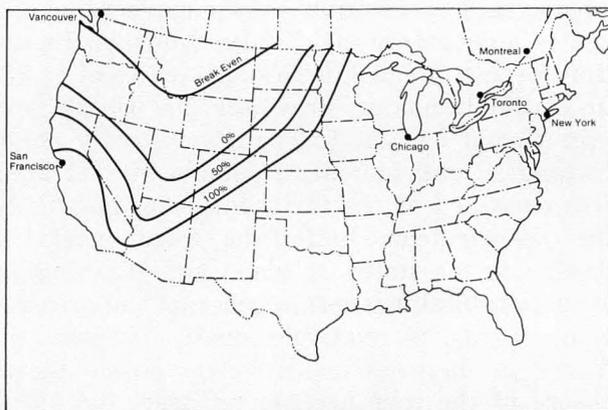
lines for the 1000 and 2000 T/D plants. All other factors were held constant. The interesting feature of the increase in plant size is that, in spite of the reduced unit cost of methanol, not one more major customer was added to the Alberta market. The only effect of the increase was to add sufficient capacity to satisfy the demand of the customers that a 1000 T/D plant could not. It is obvious that the next plant size that should be tried is about 1200 T/D. However, this is too precise a refinement in view of the potential effects of changes in other variables.

On occasion, a commodity is imported into a country, processed, then exported in a different form. When this occurs, the duty or tariff originally imposed on the imported good is forgiven. This is called a duty drawback. In the PNW up to one-third of imported methanol is exported in the form of resin. In effect, the cost of the Alberta produced methanol is reduced by an amount equal to the duty drawback, which improves the competitive position of Alberta methanol in a con-

tested area. The sensitivity of the market line to a change in duty drawback is also shown on Figure 4 for the case of equal natural gas prices of \$1.25/mm Btu. With no duty drawback, the Alberta producer should be able to capture virtually all of Washington and half of the Idaho market area. With one-third of the tariff forgiven, he will be able to penetrate one-half of the Oregon market in addition to the states of Idaho and Washington. The incremental increase in geographical area due to the change is relatively small; however, the amount of increased sales should be significant because of the concentration of users located in the area. It should be noted that the line representing the one-third duty drawback is misleading. The line is for drawback based on the average, whereas in reality the drawback is specific for only those plants which exported the processed methanol.

So far it has been assumed that the determination of the market size was undertaken so that both potential competitors can make the capital investment decision of whether to build a plant or not. A more interesting situation occurs when one of the plants is already in production, while the decision to construct the other has yet to be made. For the sake of argument, suppose the Texas plant exists and that the Alberta plant has yet to be built. The Alberta plant must use the average cost of production which includes return on equity to determine its market. On the other hand, the Gulf producer makes his decisions based on the marginal cost of production.

In the short term, the existing plant can sell its production at a cost equal to the variable production cost or breakeven. In the midterm, the producer can sell at a price which includes all manufacturing and debt repayment costs, but excludes equity capital recovery or return on equity. Operating for an extended period under this condition will have adverse effects on either the value of the company's stock or the plant liquidation value. Figure 5 shows the market lines for the Texas plant selling its product under several pricing options. The Alberta producer is assumed to have full equity recovery and return. On this figure, four market lines are shown. The three most southern lines are parametric in the fraction of original anticipated return and recapture of equity. The line designated as 100% corresponds to the original base case and that line marked as 0% is the case where only production and debt costs are met. Finally, the market area outlined



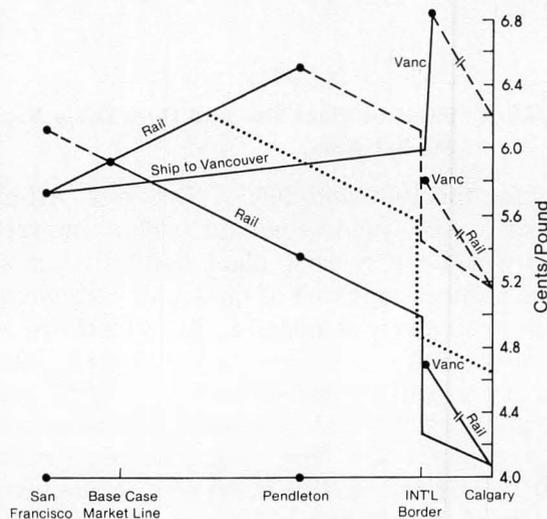
**FIGURE 5. Effect on Percent Capital Recovery for Gulf Coast Plant on Western Market Area.**

by the breakeven line is the situation where only the variable costs of production are achieved. In the last case there is no allowance made for equity or debt repayment. By selling its product at the marginal cost of production, the northernmost line, the Gulf Coast producer is able to capture most of the PNW market. However, this situation can only be a short-lived phenomenon, since this market is equal to about one-third of the Texas plant's production. Usually, selling at the margin is resorted to when a small fraction of the plant's capacity is under-utilized. In the long run, the Alberta producer does not need to worry about this single competitor capturing a large share of the PNW methanol market. This is certainly not the case if a large number of U. S. producers are operating at less than their capacity. The market line in Eastern Canada was shown only for the base case. The Gulf Coast producer selling into Eastern Canada at breakeven or at the margin would be in violation of Canadian dumping laws, so these lines were not drawn. Dumping occurs when a company sells internationally at a price below its domestic price.

Thus far, the analysis has been used to find the respective market areas for two competitors under a variety of conditions using the concept of delivered cost as the sole criterion. By interpreting the technique in a slightly different manner, the two competitor price can be estimated. Here, a two competitor price at a given point is defined as the higher of the two delivered costs at that point. The concept of this price is best illustrated by a simple example. Suppose the two methanol producers are attempting to sell methanol to hypothetical customers in Pendleton, Washington and Vancouver, B.C. As shown on Figure 6, the cost of Gulf Coast produced methanol in Pendleton is

6.5 U.S.  $\phi$ /lb, whereas the Alberta plant cost delivered at the same point is 5.34 U.S.  $\phi$ /lb. Given that there are no other suppliers, the Alberta producer can charge slightly less than 6.5 U.S.  $\phi$ /lb and still capture the Pendleton market.

By subtracting transportation, tariff and currency conversions from the Pendleton price, the FOB plant gate price of methanol in Calgary is approximately 5.2 Can.  $\phi$ /lb. This is shown on the figure as a dashed line. Since the plant gate cost was only 4.05 Can.  $\phi$ /lb, the sales into Pendleton will yield a profit of 1.15 Can.  $\phi$ /lb in addition to the required profit embedded in the cost calculation. On the other hand, the American plant can set the price in San Francisco at the Alberta delivered cost of about 6.1 U.S.  $\phi$ /lb. The basic principle is that in a given market area, the price is set equal to the competitor's delivered cost at any point in that area. The situation can be more complicated, as illustrated by an analysis of the Vancouver market. The Gulf Coast plant could transport methanol via ship from San Francisco and land it in Vancouver at 6.8 Can.  $\phi$ /lb. This delivered cost would fix the FOB plant gate price available to the Alberta producer at 6.2 Can.  $\phi$ /lb.



**FIGURE 6. Two Competitor Pricing in PNW.**

However, the Canadian plant might then be violating American anti-dumping laws by selling to the U.S. at 5.2 Can.  $\phi$ /lb FOB plant gate and in the Canadian market at 6.2 Can.  $\phi$ /lb. Because the PNW market size is much larger than that in Vancouver, the delivered price of methanol in Vancouver should be set at 5.8 Can.  $\phi$ /lb instead of the 6.8 Can.  $\phi$ /lb calculated in the absence of anti-dumping laws. Oddly enough, the U.S. anti-dumping law has had the effect of lowering the price to

the Canadian methanol consumer while benefitting neither the American methanol producer nor American consumers.

A word of caution is necessary to warn the reader that the actual price will probably not be equal to the one calculated above. Obviously the two competitor model is much too simple to be applicable in the commercial world. The extension of the technique to a multi-competitor one is straightforward in principle and a natural application for a computer simulation. However, even the more complicated model would probably not arrive at a realistic price because of the unavailability of accurate input data. The model would be useful in the commercial world in the hands of someone familiar with the industry. The technique has proven to be a very useful tool in showing students how the technical, economic and regulatory factors influence the potential markets for a chemical commodity. □

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2. Chemical Economics Handbook, Stanford Research Institute, Menlo Park, California, Vol. II, 1977.
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## AWARD LECTURE

### Kinetics of Coal Processing

Continued from page 18.

Reactant A diffuses through the product layer to the reaction surface where chemical change occurs. As reaction progresses, each pore of the particle has associated with it a growing reaction surface which initially corresponds to the inner surface of the pore. As the various reaction surfaces in the particle grow, it is inevitable that neighboring surfaces will intersect one another as the solid B separating them is consumed and replaced by the product Q.

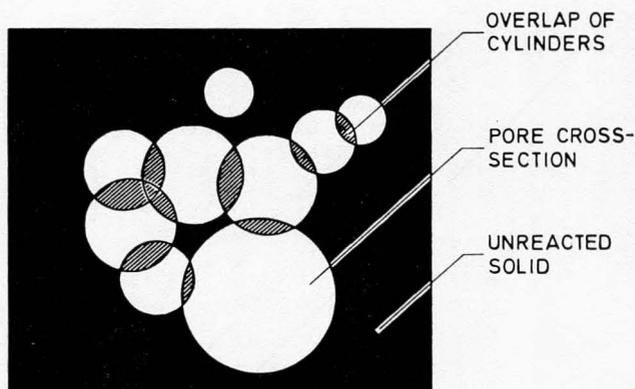
The growth of the total reaction surface may be followed in terms of the radial growth of a given set of overlapping cylinders, as shown in Figure 12. If the rate of reaction on the actual surface is proportional to the total surface area

$$\frac{S}{S_0} = \frac{1-X}{\left(1 - \frac{\tau}{\sigma}\right)^3} \sqrt{1 - \psi \ln \left[ \frac{1-X}{\left(1 - \frac{\tau}{\sigma}\right)^3} \right]} \quad (2)$$

and the conversion is

$$X = 1 - \left(1 - \frac{\tau}{\sigma}\right)^3 \exp \left[ -\tau \left(1 + \frac{\psi\tau}{4}\right) \right] \quad (3)$$

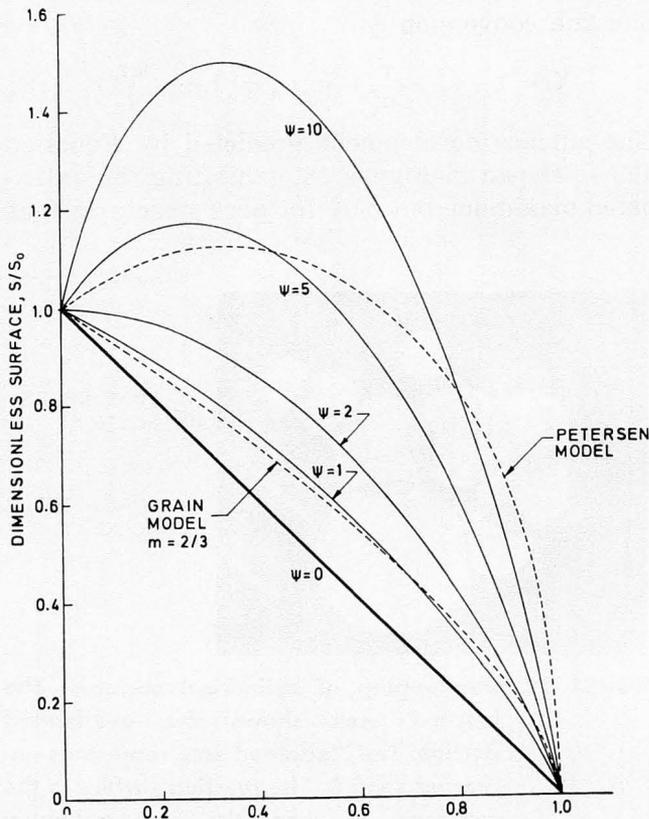
The surface development predicted by Equation (2) is shown in Figure 13, exhibiting the anticipated maximum, but only for pore structures that



**FIGURE 12.** Overlapping of cylindrical surfaces. The hatched area shows the overlapped portion. The blackened area represents unreacted solid B. The reaction surface is the interface between the nonoverlapped portion of the cylindrical surface and the unreacted solid. The product layer that is deposited as the reaction surface moves is not shown in this figure. (After Avrami).

provide  $\psi \geq 2$ . In this regard the model is more flexible than those based on an order of reaction or a grain model. The Petersen model (1957) can also describe either kind of behavior; but it makes no provision for further pore wall intersections and neglects the distribution of pore sizes. As an example of the use of the above technique, it is worthwhile to return to the data of Hashimoto et al. (1979) on the surface areas produced by steam activation of chars. As  $\sigma \rightarrow \infty$ , Equation (2) predicts a linear semilog relationship between the group  $[S/(1-X)]^2$  and  $(1-X)$ . This expectation is supported by the data within the limits of experimental error, as shown in Figure 14.

That the subject of coal processing is a complex matter with multiple branches is a commonplace. The emphasis of this paper has been to demonstrate that the newer techniques of experimentation and modeling can shed new light on the old fossil, if the broad problems of practice are dissected into manageable parts, each to be digested in its turn. □



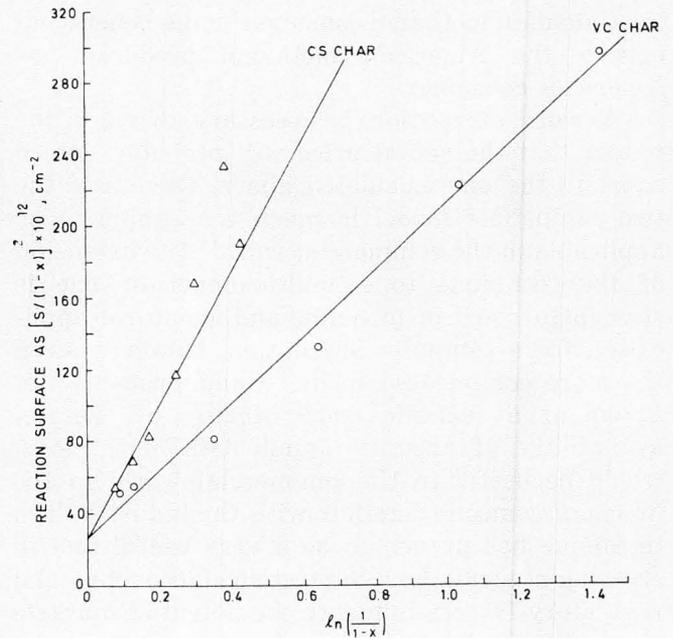
**FIGURE 13.** Development of the reaction surface with conversion according to the random pore model, compared with grain model for  $m = 2/3$  and Petersen model for  $\epsilon_0 = 0.26$ ,  $L_0 = 3.14 \times 10^6 \text{ cm/cm}^3$ ,  $S_0 = 2,425 \text{ cm}^2/\text{cm}^3$ .

#### NOTATION

$a, b$	=	stoichiometric coefficients
$C$	=	concentration of gaseous reactant A
$k_s$	=	rate constant for surface reaction
$L$	=	length of overlapped system
$n$	=	reaction order with respect to gas A
$p, q$	=	stoichiometric coefficients
$R_0$	=	initial particle radius
$S$	=	reaction surface area per unit volume
$S_0$	=	$S$ at $t = 0$
$t$	=	time
$X$	=	conversion

#### GREEK LETTERS

$\epsilon$	=	porosity
$\epsilon_0$	=	initial value of $\epsilon$
$\Psi$	=	$4\pi L_0(1 - \epsilon_0)/S_0^2$ , structural parameter
$\sigma$	=	$R_0 S_0 / (1 - \epsilon_0)$ , particle size parameter
$\tau$	=	$k_s C^n S_0 t / (1 - \epsilon_0)$ , dimensionless time



**FIGURE 14.** Correlation of the data of Hashimoto et al. (1979) with random pore model.

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## PROCESS CONTROL EDUCATION

Continued from page 34.

Then, if the field has not been able to respond in the way the critics had hoped, what explanation can be found?

Process control seems to have been unable to successfully compete for research and development funding with other fields, which have been able to be more convincing concerning return of investment, especially short term. Indeed, Shinnar [46] states that "the total expense of any major oil company on research in process control in any given year is less than for one major television commercial."

Changes can be expected, however. The increased emphasis on energy utilization will, as mentioned above, put increased demands on a less conservative and more tightly and carefully controlled operation of existing processes. One of the most efficient means to meet the increased cost of energy is and will be a more efficient energy utilization. Actually, one of the reasons for the receptivity of European industry to more sophisticated control approaches has been the high cost of energy in Europe. Now when the U.S.A. is experiencing higher energy costs—which will undoubtedly continue to climb—much more industrial interest in advanced control can be anticipated.

The rise of the energy costs will force process design in the same direction as process operation. The processes and plants will become more integrated, more sensitive, and more difficult to control. Thus, both from the design and the operational point of view more emphasis will have to be put on advanced control in the future.

Another circumstance which might have retarded the progress in process control research, is the structure of U.S. faculties. The American professor, be he assistant, associate or full, often has no other research assistance than his (graduate) students. And when students have learned enough to be fast and efficient workers they are ready to leave. This system is not very efficient in an applied field like process control, in which such a large amount of knowledge and technics from various fields have to be combined in every single non-trivial application. As expressed by Wallman et al. [10] in a LQG-application to the Foss chemical reactor: "It is undoubtedly evident from the account given here that the approach taken exacts a high price in engineering effort

and expertise. To recount, effort is required in process modeling, parameter estimation, variable reconstruction, and control system design. On top of all this rests an overhead in approximation and numerical methods."

The hierarchical European faculty system, in which research groups form naturally, almost by themselves, seems to be more efficient in this field. The difference may become larger in the future as the systems and problems to be treated are becoming more complex.

This organizational drawback in U.S. faculties is pronounced by the fact that most faculties have not gone in for process control whole-heartedly enough. One faculty member (the usual situation) is below the critical mass and no chain reaction, so important for creative work, is possible.

During the keynote address at the 1973 Joint Automatic Control Conference Richard Bellman, recently recipient of the IEEE Medal of Honor, the highest honor that can be given by the world's largest professional society, predicted that control science will be the most influential discipline for solving pressing national problems for the next two to three decades. Athans has agreed [2], "with no reservations whatsoever."

Even if Bellman and Athans turn out to be excessively optimistic, it is easy to agree with Athans when he continues: "Modern control science will continue to flourish with or without the support of the process control community."

It seems to me that the question of whether the chemical engineering community will be the one that bears the burden and wins the victories in chemical process control is still open. The potential is there, but so are the obstacles. □

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