

CHE

chemical engineering education

VOLUME VIII

NUMBER 2

SPRING 1974

CHEMICAL ENGINEERING DIVISION OF AMERICAN SOCIETY FOR ENGINEERING EDUCATION

The Changing Role of the Chemical Engineer

N. A. COPELAND

Introducing Behavioral Science into a ChE Lab

E. R. HAERING & J. B. MARTIN

Teaching Undergrad Mass & Energy Balances

D. WOODS, G. BENNETT, G. HOWARD, M. GLUCKMAN

Perturbation Techniques & Analog Computing

J. F. PAUL

Comments on Gibbs' Equation

A. H. LARSEN & C. J. PINGS

An Inexpensive Time Bomb

N. DE NEVERS

CACHE Computer Problem

R. S. KIRK

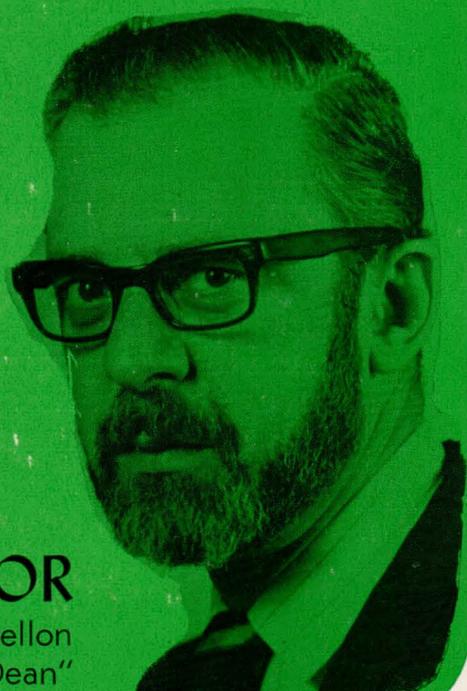
A Foreign Study Program

D. L. ULRICHSON & M. A. LARSON

ChE at MICHIGAN STATE

HERB TOOR

of Carnegie-Mellon
"The Professor's Dean"





Find out if the chemistry's right.

At Du Pont, the best chemistry is people chemistry.

Anything can be achieved if you have the right people and they talk to each other.

So we look at you as much as at your grades.

We look for compatibility as much as talent.

And that goes for engineers and chemists as well as business students.

If you want to find out what fields

have openings, what states you can work in and more, meet with the Du Pont recruiter when he comes to your campus.

Or if you've already graduated and have experience, write Du Pont direct, Room N-13400, Wilmington, Del. 19898.

And as you know by now, we're equally interested in women and men of any color.

The chemistry is what counts.



An Equal Opportunity Employer M/F

EDITORIAL AND BUSINESS ADDRESS

Department of Chemical Engineering
University of Florida
Gainesville, Florida 32611

Editor: *Ray Fahien*

Associate Editor: *Mack Tyner*

Business Manager: *R. B. Bennett*
(904) 392-0881

Editorial and Business Assistant: *Bonnie Neelands*
(904) 392-0861

Publications Board and Regional Advertising Representatives:

SOUTH: *Charles Littlejohn*
Chairman of Publications Board
Clemson University

Homer F. Johnson
University of Tennessee

Vincent W. Uhl
University of Virginia

CENTRAL: *Leslie E. Lahti*
University of Toledo

Camden A. Coberly
University of Wisconsin

WEST: *William H. Corcoran*
California Institute of Technology

George F. Meenaghan
Texas Tech University

SOUTHWEST: *J. R. Crump*
University of Houston

James R. Couper
University of Arkansas

EAST: *G. Michael Howard*
University of Connecticut

Leon Lapidus
Princeton University

Thomas W. Weber
State University of New York

NORTH: *J. J. Martin*
University of Michigan

Julius L. Jackson
Wayne State University

Edward B. Stuart
University of Pittsburgh

NORTHWEST: *R. W. Moulton*
University of Washington

Charles E. Wicks
Oregon State University

PUBLISHERS REPRESENTATIVE
D. R. Coughanour
Drexel University

UNIVERSITY REPRESENTATIVE
Stuart W. Churchill
University of Pennsylvania

LIBRARY REPRESENTATIVES
UNIVERSITIES: *John E. Myers*
University of California, Santa Barbara

SPRING 1974

Chemical Engineering Education

VOLUME VIII

NUMBER 2

SPRING 1974

FEATURES

74 Introducing Behavioral Science
Into An Engineering Laboratory
E. R. Haering and M. A. Larson

82 Teaching Undergraduate
Mass and Energy Balances
*D. Woods, G. Bennett, G. Howard
M. Gluckman*

DEPARTMENTS

56 The Educator
Herb Toor of Carnegie-Mellon

58 Departments of Chemical Engineering
Michigan State

66 Views and Opinions
The Changing Role of the Chemical
Engineer, *N. A. Copeland*

78 International
A Foreign Study Program
D. L. Ulrichson and M. A. Larson

98 Laboratory
An Inexpensive Time Bomb
N. de Nevers

70 Classroom
Comments on Gibbs' Equation: The
Condition for Chemical Equilibrium in
Open Systems, *A. H. Larsen and C. J. Pings*

94 Application of Perturbation Techniques
To Analog Computing, *J. F. Paul*

90 Problems for Teachers
CACHE Computer Problem

102 Book Review

CHEMICAL ENGINEERING EDUCATION is published quarterly by the Chemical Engineering Division, American Society for Engineering Education. The publication is edited at the Chemical Engineering Department, University of Florida. Second-class postage is paid at Gainesville, Florida, and at DeLeon Springs, Florida. Correspondence regarding editorial matter, circulation and changes of address should be addressed to the Editor at Gainesville, Florida 32611. Advertising rates and information are available from the advertising representatives. Plates and other advertising material may be sent directly to the printer: E. O. Painter Printing Co., P. O. Box 877, DeLeon Springs, Florida 32028. Subscription rate U.S., Canada, and Mexico is \$10 per year, \$6 per year mailed to members of AIChE and of the ChE Division of ASEE, and \$4 per year to ChE faculty in bulk mailing. Write for prices on individual back copies. Copyright © 1974. Chemical Engineering Division of American Society for Engineering Education, Ray Fahien, Editor. The statements and opinions expressed in this periodical are those of the writers and not necessarily those of the ChE Division of the ASEE which body assumes no responsibility for them. Defective copies replaced if notified within 120 days.

The International Organization for Standardization has assigned the code US ISSN 0009-2479 for the identification of this periodical.

Summer Program on Modeling and Optimization

Sir:

A special summer program will be held July 29 through August 7, 1974 on the topic "New Developments in Modeling, Simulation and Optimization of Chemical Processes" at Massachusetts Institute of Technology.

This special summer program will present basic principles necessary to understand and apply new techniques for computer-aided design and control of industrial-scale chemical processes. Topics to be covered include steady-state process simulation, process optimization, dynamic modeling and simulation of chemical processes, computer-aided process synthesis, and comprehensive problem-oriented computing systems for chemical process design. Participants will use M.I.T. computing facilities for solution of case-study problems. Please contact:

Director of the Summer Session

M. I. T., Room E19-356

Cambridge, Massachusetts 02139.

Lawrence B. Evans

Massachusetts Institute of
Technology**CACHE
COMPUTER
PROBLEMS**

CHEMICAL ENGINEERING EDUCATION, in cooperation with the CACHE (Computer Aides to Chemical Engineering Education) committee, is initiating the publication of proven computer-based homework problems as a regular feature of this journal.

Instructions for submission of problems precede the first of these articles which appears on page 90 of this issue.

***Parsons is a Good Place to Work!***

There is no limit to the opportunities offered by Parsons—high salaries, good benefits, advancement, professional freedom—and a work environment unequalled anywhere.

Parsons is expanding its operations. Our new world headquarters will be completed in the summer of 1974. This \$20 million, 400,000 square-foot facility was designed specifically for our business. It is located in a suburban area near the Rose Bowl in Pasadena, California, close to some of the country's famous universities in case you want to further your academic career—with Parsons' tuition aid plan.

Parsons is one of the leaders in the engineering design and construction of petroleum refineries, metallurgical plants and chemical plants. We have prepared a booklet describing the advantages of working for Parsons—for your copy of "Parsons is a Good Place to Work," write to Personnel Manager,

The Ralph M. Parsons Company

ENGINEERS / CONSTRUCTORS

617 West Seventh Street,
Los Angeles, Ca. 90017

AN EQUAL OPPORTUNITY EMPLOYER

PRENTICE-HALL

Help your students explore the latest contributions to chemical engineering.

Electrochemical Systems

by John S. Newman, University of California, Berkeley

NEW—a unified framework for the analysis of problems in electrochemical systems. Introduces the beginning student to the development, design, and operation of electrochemical syntheses, processes, energy conversion and storage devices, and corrosion.

1973, 440 pp., \$18.95

Optimization and Design

by Mordecai Avriel, Israeli Institute of Technology, Marcel Rijckaert, and Douglass Wilde, University of Connecticut

Integrates a collection of advanced survey articles, examples, and discussions of the impact of optimization theory on engineering design. Focuses appropriate parts of optimization theory on the peculiarities of engineering design in an attempt to revolutionize design methods.

1973, 528 pp., \$18.95

Polymer Materials Science

by J. Schultz, University of Delaware

Suitable for graduate level, this new text explores polymeric materials for students whose interest centers on the properties of the final, solid polymer. Aids in understanding the correlations between structure and bulk properties and in considering how processing conditions might affect such properties.

January 1974, approx. 496 pp., \$19.95

Basic Principles and Calculations in Chemical Engineering, Third Edition 1974

by David Himmelblau, University of Texas, Austin

Basic introduction to chemical engineering that includes material balances, energy balances, and the basic principles of physical chemistry encountered later in chemical engineering design, analysis, and control.

1974, approx. 544 pp., \$15.95

Process Synthesis

by Dale Rudd, University of Wisconsin; Gary Powers, M.I.T.; and Jeffrey Sirola, Tennessee Eastman Co.

An introductory undergraduate level book that deals with synthesis of processes — combines synthesis methods with material and energy balancing to form a new introduction to engineering.

1973, 320 pp., \$15.95

Chemical Kinetics and Reactor Design

by A. R. Cooper, and G. V. Jeffreys, both of the University of Aston, Birmingham

Sound basis of chemical reactor concepts, this text features liberal graphical representation of the results of illustrative calculations of real systems within the book.

1973, 400 pp., \$18.95

Modeling Crystal Growth Rates From Solution

by Makota Ohara, Yoshitomi Pharmaceutical Industries, Ltd., and Robert Reid, M.I.T.

Provides a critical analysis and evaluation of theories which purport to predict crystal growth rates of solutes from solution.

1973, 288 pp., \$19.95

Mathematical Methods in Chemical Engineering Volume III: Process Modeling, Estimation, and Identification

by John Seinfeld, California Institute of Technology and Leon Lapidus, Princeton University

A comprehensive self-contained treatment of the mathematical techniques of process modeling that emphasizes probability theory, stochastic processes and parameter estimation relating to systems identification.

1974, approx. 544 pp., \$19.95

The Elements of Chemical Kinetics and Reactor Calculations: A Self-Paced Approach

by H. Scott Gogler, University of Michigan

Offering a different teaching approach to learning chemical reaction engineering, this text provides an excellent way to bring graduate students from varying backgrounds in reaction kinetics up to a common level

1974, approx. 448 pp., \$21.00

Thermodynamics and Its Applications in Chemical Engineering

by Michel Modell and Robert Reid, both of M.I.T.

Provides advanced treatment of chemical engineering thermodynamics with an emphasis on the application of fundamental concepts to solve practical problems.

1974, approx. 528 pp., \$18.95

For more information write: Robert Jordan, Dept. J-915, Prentice-Hall, Englewood Cliffs, New Jersey 07632

The Professor's Dean

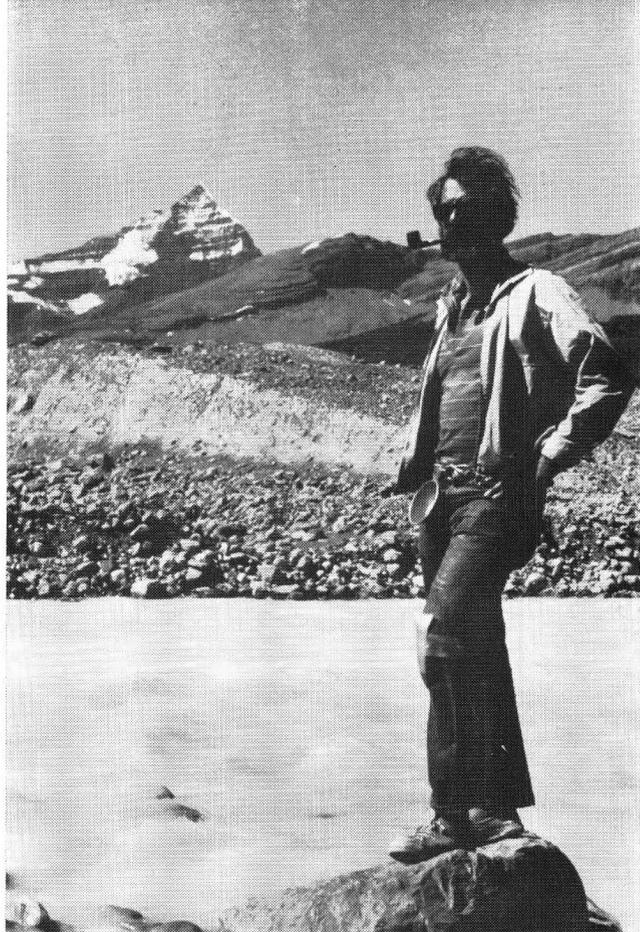
Herb Toor

OF CARNEGIE-MELLON

THE ChE DEPARTMENT FACULTY
Carnegie-Mellon University
Pittsburgh, Pa. 15213

Herb Toor, a former chemical engineer, is now Dean of Carnegie Institute of Technology, the engineering arm of Carnegie-Mellon University. He is a very good dean. He provides a plethora of new ideas, only a few good, but all are stimulating. He is very tolerant of initial mistakes, which makes us try that much harder. Herb has effectively focused the college's new efforts, particularly in scientific design and engineering in public affairs, and has sharply pruned inefficient programs. At the same time, he is a professor's dean because he talks in four-letter words that professors understand—words like “dumb”, “good”, and “cash”. These aren't the only words; one faculty wife suggested he should be the “Professor of Anglo-Saxon”.

How Herb got this way isn't clear. His academic record is usual the mixed bag. Born in Philadelphia, he was an undergraduate at Drexel, where he partially supported himself by repairing pinball machines. He went to Northwestern for his doctorate, where he worked on heat transfer under Professor Leon Stutzman, now at the University of Connecticut. Because he had no job on graduation, he followed his wife to England on her post-doctoral fellowship. While there, he worked for Monsanto. He came to Carnegie in 1953; and, except for a year in India as a UNESCO scholar, he has been here since. He became associate professor in 1957, professor in 1961, department head in 1965, and Dean of Engineering in 1969. These dates are approximate because Herb's file was accidentally burned, apparently a case of spontaneous combustion.



Herb has effectively focused the college's new efforts.

One's first impression when seeing Herb lecture is that he must always be surrounded by a small black cloud. Herb starts an hour's lecture with two cigars; he then switches to his pipe; and, he finishes the class by bumming cigarettes from the students. During the lectures, Herb changes the notation in his equations. He does this without a hint, and rotates the symbols so that what was once flux becomes the concentration, and what was once the concentration becomes the flux. He fills all of the blackboards; then goes back to write over everything with a series of arrows and other mnemonics. At the end of the lecture, all the boards look like extremely intricate oriental rugs woven by drunken Arabs.

These eccentricities are coupled with a lucid physical insight into the problems being discussed. Herb has a very strong feel for what is actually happening. He easily makes approximations which make almost anyone else blanch, but then quickly returns to show that these approximations are, in fact, justified. He is a master at constructing and using homework or class exercises with a keen sense of balance between analytical techniques and the real physical nature of the problem. In short, he teaches judgment on when to use a sophis-

ticated technique or model, and when and how to make a simple guess sufficient for the purposes at hand.

Herb's research is also characterized by these rapid, incisive approximations based on physical insight. The mathematical level of his work is not particularly great, and his experimental work can be incomplete and abortive. At the same time, the research is excellent because it undertakes important problems and solves their limiting cases of behavior. Herb started with studies of mass transfer, then generalized these studies to multi-component systems, climbed almost immediately to problems of turbulent mixing, and extended these to the study of fog. In all these efforts, new physical insight is the basic foundation; and, in all these cases, he discovered most of the important effects involved.

The work on fog is a good example of this insight. This problem was originally connected with cooling tower design. Fog formation involves coupled heat and mass transfer, but because fog forms in air, the Prandtl and Schmidt numbers are about equal. As a result, the continuity and energy equations have the same form and can be uncoupled and solved. In this way, one can predict when and where fog forms to a surprising degree of accuracy.

This willingness to make approximations in research has something of a social parallel in the parties which Herb gave for the entire department when he was department head. At these parties, he was once famous for singing Slovenian Christmas carols with Larry Canjar. The parties are symbolized by Artillery Punch. The recipe for this is given in Table I. The effect of even a small glass of this punch is immediate. New students disappear after only one deep breath of the vapor. One graduate student drove her husband and three others home only to find on arrival all asleep in the back seat with their arms around each other. She had no way to unload them.

Since Herb is Dean, he is no longer quite as

Herb's research is also characterized by these rapid, incisive approximations based on insight . . . the research is excellent because it undertakes important problems and solves their limiting cases of behavior.

TABLE I
Toor's Artillery Punch

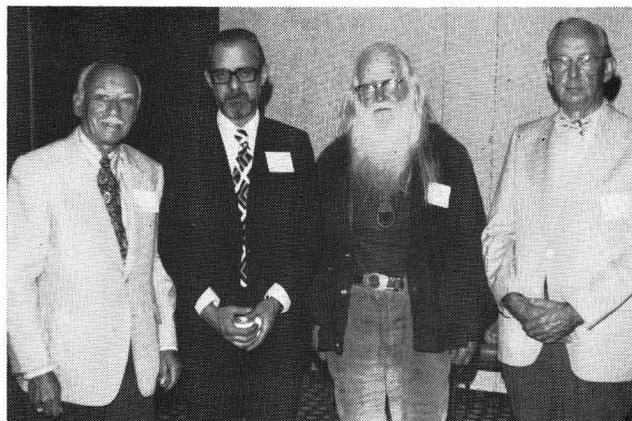
Combine:

- 1 bottle—Bourbon
- 1 bottle—Brandy
- 1 bottle—Burgundy
- 1 bottle—Sherry
- 1 bottle—Soda Water

Add:

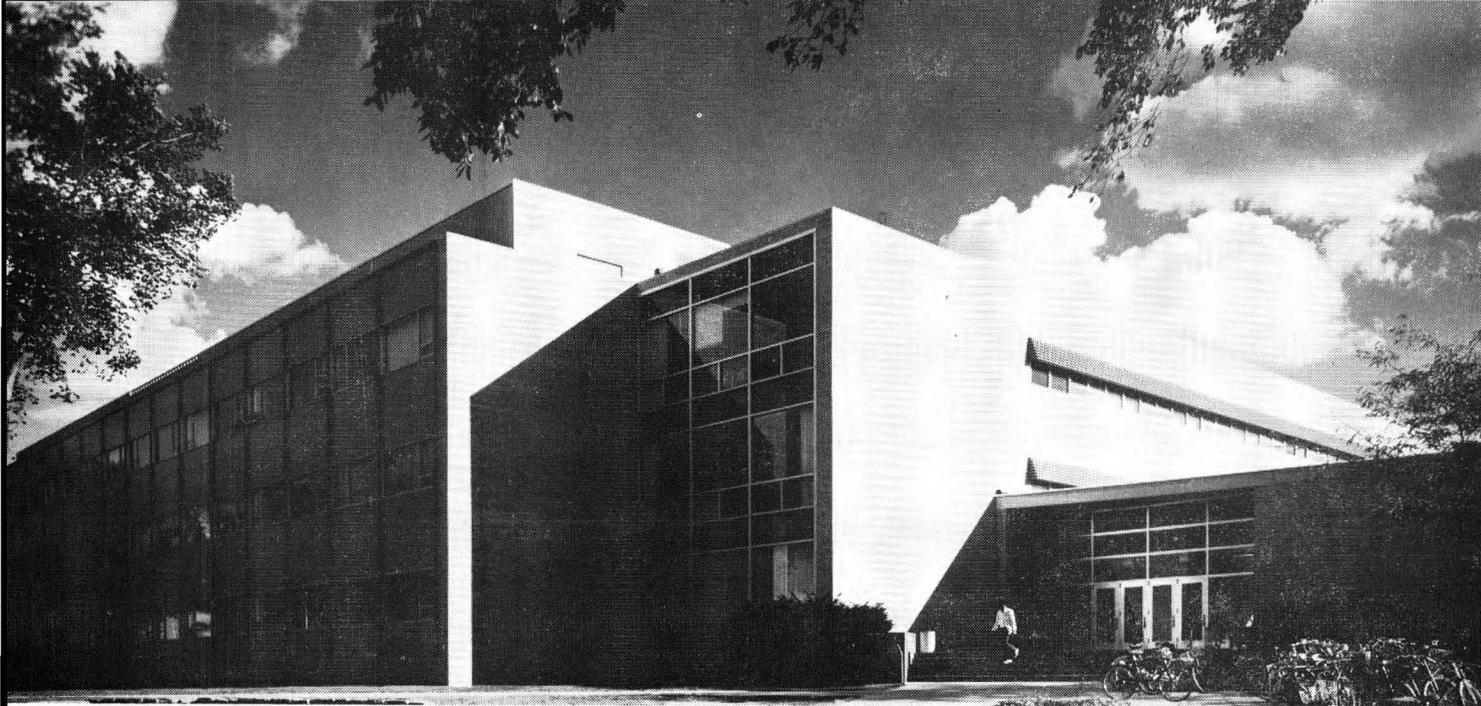
- Juice of 6 Lemons
- 1/2 cup Sugar

human as he once was. He does still come out with an occasional eccentricity. For example, he once attended a luncheon meeting wearing a somewhat unusual costume: jeans, with holes in the knees; sneakers, with holes in the toes; and a green and blue shirt with one hole neatly circumscribing his navel. After this experience, he took a trip to Brooks Brothers, walked in, and said he wanted to buy a suit that would make him look like a banker. After the salesman stopped laughing, they did sell him the suit.



Since Herb is Dean, he is no longer as human.

We have enjoyed working with Herb because this same honesty in buying a suit extends throughout his professional association. He is exceptionally good at avoiding win-lose arguments, so that it's increasingly hard to take a stand without his agreeing with the most sensible part of what you're saying. He does have very strong opinions which sometimes require "subjective logic", which means shouting that you are right and everyone else is a goddamn fool. As a department, we all regret not seeing more of Herb's honesty, his objectivity, and his insight. We all look forward to the day when he stops fooling around at that dean's job and returns to something more reasonable—like being a professor in chemical engineering. □



ChE department

MICHIGAN STATE

M. H. CHETRICK and FRAN MURRAY
Michigan State University
East Lansing, Michigan 48823

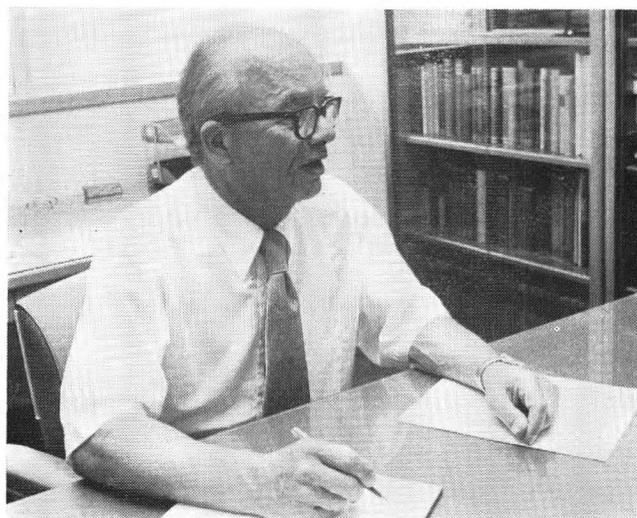
CHEMICAL ENGINEERING HAS been taught at Michigan State University for more than 60 years. The first course offerings were described in the 1912-13 catalog, although a department was not formally established until 1931. Engineering instruction at Michigan State University actually dates back to 1885, when at the then Agricultural College of the State of Michigan—the name of the institution has been changed five times—a mechanical engineering program was offered. In 1892 a civil engineering program was established, followed by one in electrical engineering in 1896.

In its 1912 course offerings, the Chemistry Department included engineering electives for seniors, and in the following year “engineering chemistry” became one of four “group” options for juniors and seniors. The first class of four graduated with a B.S. in this option in 1914.

Over a period of time the chemistry courses were expanded, and in 1930 the department became “Chemistry and Chemical Engineering.” A separate chemical engineering department was

established in 1931, with Professor Harry S. Reed transferring from the Chemistry Department to head the Chemical Engineering Department. Transferring with him were Professor Henry Publow, who succeeded Professor Reed as department head in 1935, and two graduate students.

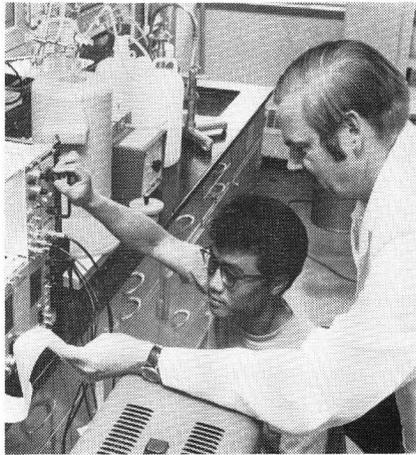
Professor C. C. Dewitt became head of the department in 1940, and in the following year the



Dr. M. H. Chetrick, Chairman of the department.

department was renamed Department of Chemical and Metallurgical Engineering. At this same time, approval was granted to offer the Ph.D. degree in chemical engineering.

In 1950, the department was split into two separate departments, the Department of Chemical Engineering and the Department of Metal-



Dr. Donald K. Anderson and doctoral candidate do biomedical research on transport of ions out of muscle cells.

lurgical Engineering, with Professor Dewitt remaining as head of Chemical Engineering. Professor C. Fred Gurnham succeeded Professor Dewitt as Department Chairman in 1952 and served in this capacity until 1961. The present Chairman is Professor M. H. Chetrick who assumed this position in 1963 when he first came to Michigan State University.

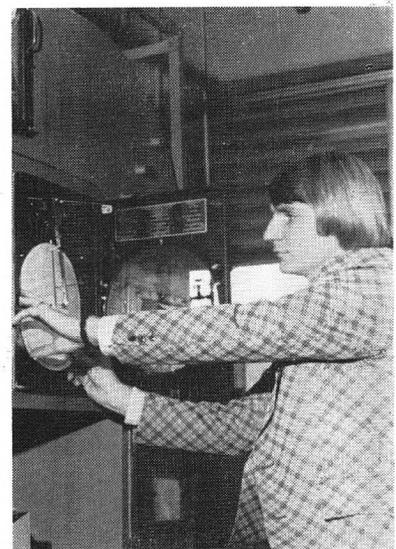
INNOVATION MARKS CHANGES

INNOVATION HAS marked the successive changes and growth in the department since its beginning. The major innovations came during the past 10 years with the miniaturization of laboratory equipment, with several major overhauls of the curriculum, and with the reduction of credit hours required for a B.S. degree (from 212 to 180 quarter hours). Present evidence indicates that these pioneering steps have been in the right direction, resulting in more knowledgeable graduates.

The miniaturization of laboratory equipment came in 1963 when the department was moving from older quarters to the new Engineering Building which houses all the departments of the Col-

lege of Engineering. This move presented an excellent opportunity to objectively reevaluate laboratory instruction as the cost and time for designing and installing a new miniaturized laboratory would be no greater than that involved in disassembling, moving, and reassembling the large equipment from the older quarters. The decision was made to switch to miniaturized laboratory units in the interest of improved instruction, more optimum use of students' time, and better utilization of laboratory space. The smaller sized equipment also could be readily adopted for operation under direct digital computer control, and several such experiments were developed by Professor G. A. Coulman. Extensive use of glass equipment was made in order that students could see what was occurring in their experiments. It is of interest to note that several well known chemical companies in Michigan sent representatives to examine the new miniaturized laboratory at MSU and then proceeded to install similar equipment in their R & D laboratories.

The reduction in the credits required for graduation occurred in 1964 and attracted national attention as well as a great deal of skepticism. It appeared at times that the only support



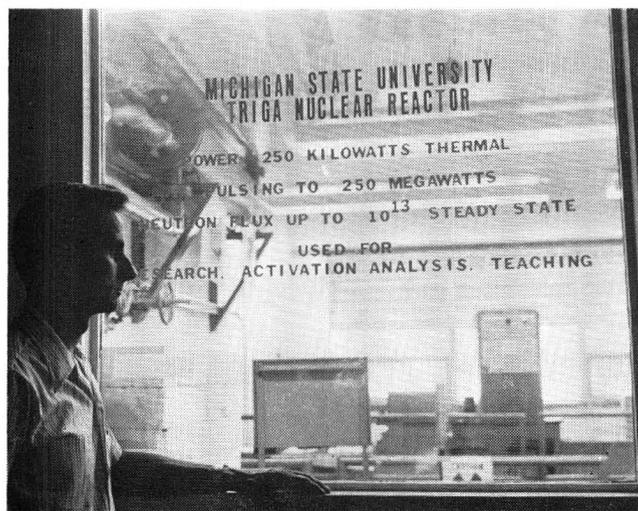
Dr. Paul M. Schierholz operating an experimental drier.

which the department had for this action was from the other departments in the College of Engineering at MSU who also reduced their requirements from 212 to 180 quarter hours. The value of greater concentration permitted by the reduction of required credits has proved itself many times. The current graduates have much more

depth and understanding of chemical engineering. As an example, since 1967 and continuing each year since then, MSU chemical engineering seniors have won first, second, or third place or honorable mention in the Student Contest Problem sponsored annually by the AIChE.

The last major revision in the undergraduate curriculum became effective in Fall, 1973. The purpose of this change was to make the curriculum more flexible and to provide better accommodations for transfer students who have always represented a large fraction of the chemical engineering graduates from MSU.

In the new curriculum, a student may elect the conventional program of study, which includes twenty hours of electives, or pursue a "coordinated elective" program by including up to 32 hours of electives in an approved area peripheral to chemical engineering. If a coordinated elective plan exceeds twenty hours, a student may take up to an additional twelve hours of electives by waiving certain optional courses in the senior year.



Dr. Bruce W. Wilkinson by the nuclear reactor.

COORDINATED ELECTIVE PROGRAMS

Examples of coordinated elective programs include:

1. Biomedical Engineering

In the past few years, Chemical Engineers have become increasingly interested in the application of chemical engineering fundamentals to the solution of problems which are biological or medical in nature. Examples of these are the

artificial heart, lung and kidney machines. As a result, the Chemical Engineering Department has available a biomedical minor, available at the student's option, which will provide background in physiology and biomedical engineering. The recommended courses listed below may be substituted for electives and for selected courses in the curriculum.

ANT	316	General Anatomy	3
PSL	331	Human Physiology	4
PSL	332	Human Physiology	4
*BME	411	Electric Theory Nerves	4
*BME	424	Materials in Biomedical Engineering	3
*BME	431	Biological Transport Mechanisms	4
*BME	481	Tissue Biomechanics	3
			25

*BME designates a biomedical engineering course.

2. Chemical Systems Science

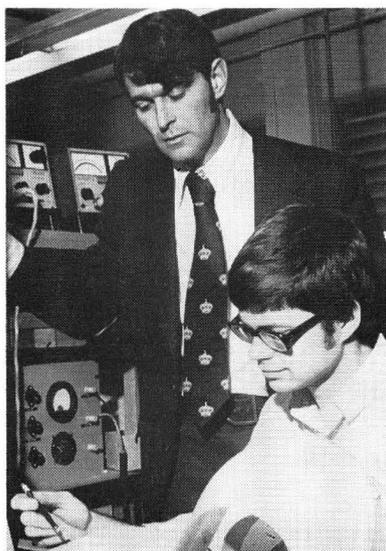
This option can be structured to provide in-depth knowledge for automatic control of industrial processes as well as the application of computers to real-time supervision and optimization. This selected group may be enhanced by alternatives available.

EE	311	Fundamentals of Systems Modeling	3
EE	312	Analysis of Linear Systems	3
EE	313	Analysis of Large Scale Systems	3
EE	415	Control Systems	3
EE	416	Control System Design	3
CHE/SYS	465	Process Optimization Methods	3
CPS	300	Computer Programming	3
CPS	311	Assembly Language & Machine Organization	4
CPS	312	Generative Coding and Information Structures	4

29

3. Environmental/Ecological Engineering

The interface of industry and the environment becomes critical as man assumes a dominant influence on the quality of his life. The opportunity to know and relate to the natural environment will provide the chemical engineer with the foundation needed to effectively meet the present and future challenges. Many courses exist, of which a selected few are shown, that will lead to appropriate knowledge



Dr. Martin C. Hawley directing a graduate student in research on coal gasification.

for acceptably working at the interface.

LBC	140	Biology I	3
LBC	141	Biology II	3
ZOL	389	Animal Ecology	4
ZOL	404	Biological and Ecological Concepts for Engineers and Mathematicians	3
BOT	450	Ecology	4
MPH	444	Environmental Microbiology	3
FW/ZOL	476	Limnology (Ecology of Lakes and Streams)	3
CE	483	Environmental Engineering II—Water Pollution Control	4
CE	487	Environmental Engineering IV—Water and Waste Water Analysis	4
BCH	401	Basic Biochemistry	5
			<hr/> 36

(Students may select up to 32 hours)

4. Nuclear Engineering

Nuclear engineering includes the application of fission and fission processes to the generation of energy. In addition, the application of by-product radioisotopes to the study of various engineering processes is also investigated. Many of the physical principles are similar to chemical engineering processes and the theories involved are directly transferable from chemical to nuclear engineering. Courses which can form a nuclear engineering option include:

PHY	364	Introduction to Modern Physics I	3
PHY	365	Introduction to Modern Physics II	3
PHY	498	Introduction to Nuclear Physics	3
PHY/CEM	430	Introduction to Radioisotope Techniques	3
CHE	821	Theory of Nuclear Reactors	3
CHE	825	Radioisotope Engineering	3
CEM	830	Nuclear and Radiochemistry	3
CHE	460	Special Problems (Nuclear Reactor Laboratory)	3-6

24-27

5. Polymer Science and Engineering

The rapidly expanding field of polymer science and engineering is an excellent option for students interested in the synthetic polymer industry. It is also becoming clear that understanding of the molecular properties of synthetic polymers is an aid in the study of the behavior of some important materials occurring in nature, including the proteins, nucleic acids, and other constituents of living organisms. An understanding of these materials and their function in the living cell is a hopeful pathway of advancement in biology. Therefore, in addition to the polymer science courses listed below several of the basic Biochemistry courses would provide a useful combination for those interested in Macromolecular Science and Biochemistry.

CEM	462	Theoretical Chemistry II—(Statistical Mechanics)	3
CHE	446	Polymerization	3
CHE	442	Polymer Science and Engineering	3
CHE	847	Physical Chemistry of Macromolecules	3
CHE	848	Rheology and Macromolecular Fluid Mechanics	3
CHE	460	Special Problems (Theoretical or Experimental Independent Study of Polymer Science)	3-6

18-21

Each year since 1967, MSU seniors have won 1st, 2nd, 3rd place or honorable mention in the AIChE Student Contest Program.

6. Chemistry

It is possible for chemical engineering students to pursue an in-depth interest in chemistry. The regular chemical engineering program includes 33 credit hours in chemistry which is nearly equal to the requirement for chemistry majors. Additional courses from the following list may be taken under the coordinated elective option. The student may also choose to develop a hybrid coordinated elective program by selecting a few courses from this list and courses in mathematics, physics, etc.

CEM	355	Organic Chemistry Laboratory	2
CEM	356	Organic Chemistry Laboratory	2
CEM	372	Analytical-Physical Chemistry Laboratory I	2
CEM	373	Analytical-Physical Chemistry Laboratory II	2
CEM	411	Systematic Inorganic Chemistry	4
CEM	430	Intro. to Radioactivity and Radioisotope Techniques	3
CEM	446	Polymerization	3
CEM	462	Theoretical Chemistry II	3
CEM	471	Analytical-Physical Chemistry Laboratory III	2
CEM	472	Analytical-Physical Chemistry Laboratory IV	2
CEM	473	Analytical-Physical Chemistry Laboratory V	2
CEM	484	Modern Physical Chemistry	3
CEM	492	Chemical Spectroscopy	3
CEM	499	Seminar on Chemical Physics	1

7. Mathematics

Chemical engineers with special talent and background in mathematics are frequently sought out by their colleagues and employers to solve the difficult problems for which their expertise qualifies them. The three programs listed below are aimed at: I. Giving the student a strong foundation in advanced mathematics. II. Combining this with special computer capability. III. Giving the student as strong a program of mathematics as a math major takes.

I. Coordinated elective in mathematics

MTH	334	Theory of Matrices	4
MTH	421	Vector and Tensor Analysis	4
MTH	424	Advanced Calculus	4
MTH	451	Numerical Analysis I	4

16

in addition to MTH 215 and CHE/MTH 381

II. Coordinated electives in math and computer

MTH	334	Theory of Matrices	4
MTH	421	Vector and Tensor Analysis	4
MTH	424	Advanced Calculus	4
MTH	451	Numerical Analysis I	4
CPS	300	Computer Programming	3
CPS	311	Assembly Language and Machine Organization	4

23

in addition to MTH 215 and CHE/MTH 381

III. Coordinated electives with math major equivalent

MTH	334	Theory of Matrices	4
MTH	421	Vector and Tensor Analysis	4
MTH	424	Advanced Calculus	4
MTH	425	Advanced Calculus	3
MTH	451	Numerical Analysis I	4
MTH	452	Numerical Analysis II	4
STT	351	or STT 441	4

27

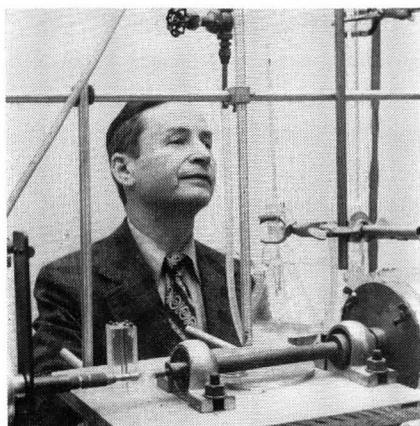
in addition to MTH 215 or CHE/MTH 381

8. Business/Economics

Students interested in the business aspects of the chemical process industries, such as production management, may combine a strong chemical engineering capability with knowledge and expertise in business and economics. These students may develop a coordinated elective program in business and economics from the following list of courses. Other courses such as computer science may be also coordinated with this type of program.

EC	210	Fundamentals of Economics	4
EC	318	Money, Credit and Banking	4
EC	320	Macroeconomics I	3
EC	321	Macroeconomics II	3
EC	324	Microeconomics I	3
EC	325	Microeconomics II	3
EC	426	Introductory Mathematical Economics	3
EC	427	International Trade and Finance	5
EC	434	Comparative Economic Systems	4
EC	470	Monetary Theory	3
MGT	300	Production Management	4
MGT	306	Analysis of Processes and Systems	4
MGT	310	Fundamental of Personnel Administration	4
AFA	201	Principles of Accounting I	5
AFA	202	Principles of Accounting II	5

Students may select 20 to 32 credits in any combination of the above courses, or may select



Dr. Carl M. Cooper at a glass distillation column.

other approved courses in the school of business. In addition to the above, other programs may be developed by students, subject to department approval.

ENROLLMENT AND HONORS

DESPITE A DOWNWARD national trend of enrollment in chemical engineering and other branches of engineering, the number of graduates in MSU's chemical engineering department has continued to climb modestly. During the past four years, the number of degrees granted to graduates were:

Degrees Granted	Academic Year			
	1969-70	1970-71	1971-72	1972-73
B.S.	30	32	33	39
M.S.	3	8	8	9
Ph.D.	1	1	3	3

Women majoring in chemical engineering at MSU make up almost 20% of the total enrollment in the upper undergraduate classes.

STUDENT HONORS

To a large extent, the quality of an educational program can be judged by the caliber of its graduates. Perhaps the greatest satisfaction to the faculty of a department in a university is the honors received by its students for outstanding performances. This not only recognizes the outstanding students but also reflects very favorably on the educational program and training they received in the department.

Among the honors received by chemical engineering students at MSU, their performance in the annual AIChE Student Contest Problem must

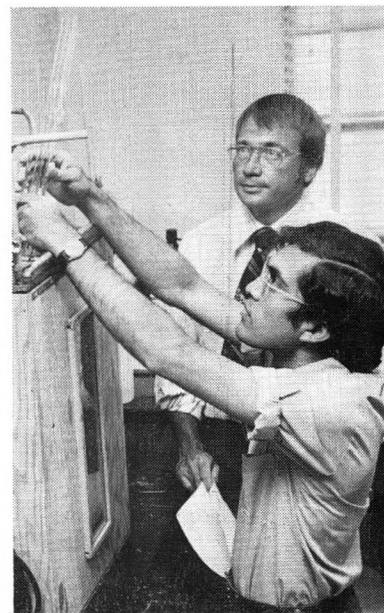
be ranked among the most outstanding. The past six year record of MSU prize winners in this competition is as follows:

- 1968 Third Prize—Carl L. English
- 1969 First Prize—Jerome L. Trumbley
- Second Prize—Jon A. Branson
- 1970 Honorable Mention—Steven R. Auvil
- 1971 First Prize—Allen G. Croff
- 1972 Third Prize—Timothy O. Bender
- 1973 Third Prize—Michael J. Murry

The MSU entries in this competition during the past six years have been coordinated by Professor M. C. Hawley who also teaches the design course in which the Student Contest Problem is worked.

PROFESSIONAL ACTIVITIES

The department faculty have been very active in professional organizations, especially in the ChE Division of ASEE. Two of its faculty members were elected to serve as Chairman of the



Dr. Robert F. Blanks and doctoral candidate work on polymer research.

Division, Professor M. H. Chetrick in 1958-59 and Professor D. K. Anderson in 1971-72. In addition both served as secretary-treasurer and vice chairman during the years directly preceding their terms as chairman. Professor Chetrick also was the Division's representative on the general council (predecessor to the present Board of Directors) from 1961-62.

If a coordinated elective plan exceeds twenty hours, a student may take up to an additional twelve hours of electives by waiving optional courses in the senior year.

Professor M. C. Hawley was program chairman of the Division for the 1973 Annual Meeting and served with other faculty members of the department on various committees of this organization.

THE FACULTY AND RESEARCH PROGRAM

THE GRADUATE PROGRAM has grown over the past 10 years from a small one with a few masters candidates to one with approximately 30 graduate students. During this period, research funding from outside sources has grown to a point where grants and contracts provide financial support for most of the graduate students as well as for its faculty.

Research interests within the department are quite varied. In addition to research programs in such traditional areas as distillation, thermodynamics, and kinetics, there are supported research programs on mass transport in blood vessel walls, use of high temperature plasmas to produce chemicals from coal, and gas separation in high speed centrifuges.

There is considerable interdisciplinary research involving members of the department with other departments of MSU. There currently are research programs jointly conducted with the departments of chemistry, physiology, biochemistry, mechanical engineering, electrical engineering and systems science.

The increased number of graduate students has also permitted the development of more graduate courses, especially in specialty areas such as polymer engineering, nuclear engineering, and optimization methods.

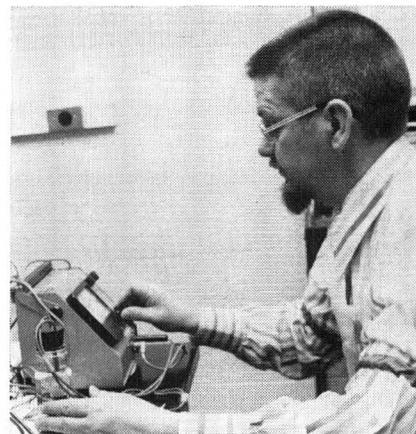
The present faculty consists of eight full time members with a wide variety of professional background as well as teaching and research interests. A summary of the individual faculty and their research activities is as follows:

D. K. Anderson has been on the faculty since 1960 and is currently a professor in the department. He also holds the rank of professor of physiology and is engaged in several joint research projects between the Departments of Chemical Engineering and Physiology. He is chairman of a College of Engineering committee on biomedical engineering. He was one of ten MSU faculty members who received a Distinguished Faculty Award in 1973. Research interests

include biomedical engineering, cardiovascular physiology and transport phenomena.

R. F. Blanks came to MSU in 1969 from Union Carbide Chemicals and Plastics where he was a research scientist. His research areas are in thermodynamics and rheology of polymer systems. He is an associate professor in chemical engineering.

M. H. Chetrick has served as professor and chairman of the department since coming to MSU in 1963 from the University of Louisville. Also taught at the University of North Dakota. Previous industrial experience was with Shell Oil, Monsanto, and Battelle Memorial Institute. Also served as a consultant for many years with the U.S. Bureau of Mines on coal gasification. Current research interests are in kinetics, reaction engineering, and synthetic fuels.



Dr. George A. Coulman using research equipment.

C. M. Cooper a member of the faculty since 1948, he was previously employed with Phillips Petroleum and Vulcan-Cincinnati. He is presently a professor in the department. His research activities are in thermodynamics and phase equilibria, modeling of transport processes, and distillation.

G. A. Coulman came to MSU in 1964 from University of Waterloo (Canada). Also previously employed with Dow Corning and American Metal Products. Currently an associate professor, he is active in research in process systems theory, process dynamics and control, applied chemical engineering mathematics, and environmental systems.

M. C. Hawley has been on the faculty since 1964 and is presently an associate professor of chemical engineering. Serves as a consultant to industry in areas of economics, new business ventures, and computer simulations. Active research areas include porous media transport, kinetics and reaction engineering, and synthetic fuels.

P. M. Schierholz the newest faculty member, he joined the department late in 1973 as assistant professor. Previous industrial experience with duPont. Research interests in crystallization, water treatment, and chemical process simulation.

B. W. Wilkinson joined the department in 1965 after industrial work with Dow Chemical. He was responsible for the planning of the University Triga Reactor and has been the supervisor of this nuclear reactor since it became operational in 1969. Research interests are in the area of radiation engineering, radioisotope engineering, nuclear reactor theory, and environmental engineering. □



We're looking for people who are looking for the good life.

The good life involves a lot of the things we've always taken for granted. Like the availability of enough food to feed an ever-growing population. A cure for disease. Thick forests. A clean environment. And the time to relax and enjoy it all. Except now we're going to have to stop looking at life through a tunnel and find ways to protect all forms of it—from our homes to the farthest corner of the earth. Because life is fragile. And its protection is a major concern at Dow. So we're looking for people with scientific, engineering, manufacturing and marketing backgrounds who'll direct their precious talents, enthusiasm and ideas to the development of Dow products and systems for the good life. And we'll provide a dignified, motivational environment to work and grow. If you or someone you know loves life and wants to live it wisely, get in touch with us. Recruiting and College Relations, P.O. Box 1713, Midland, Michigan 48640.

*Trademark of The Dow Chemical Company
Dow is an equal opportunity employer—male/female



DOW CHEMICAL U.S.A.

THE CHANGING ROLE OF THE CHEMICAL ENGINEER*

N. A. COPELAND

*E.I. du Pont de Nemours & Co.
Wilmington, DE 19898*

CHEMICAL ENGINEERING TO ME is a peculiarly American institution. I was first reminded of this many years ago when I was studying in Switzerland. I observed that there were no chemical engineering textbooks by European authors. Walker, Lewis and McAdams, and Badger and McCabe were the standard references, and they were available only in English. Also, at that time there were as yet no departments of chemical engineering in the European universities as we had already known them in this country for many years.

In recent years, as I have had occasion to become somewhat familiar with the chemical industry in Europe, I have been struck with the different role of the chemical engineer over there as compared to this country. For example, I find it interesting that the heads of several of the leading engineering firms engaged in the design of chemical plants in Europe are not engineers but chemists. Likewise, I have observed that, at least in the German chemical industry, people with chemical engineering backgrounds are not found in positions of high authority—much in contrast to the situation in this country. I recall two or three years ago that the president of one of the largest chemical companies in Europe was quoted in *C. & E. News* as saying that he did not hold chemical engineers in very high esteem. He said that he could get more done with one chemist and two technicians than he could with one chemist and one chemical engineer.

I have concluded that chemical engineering in the United States is a more prestigious profession than elsewhere and that we, perhaps better than others, have learned the value of bridging the gap

between chemistry on one hand, and engineering on the other, for the benefit of the chemical industry.

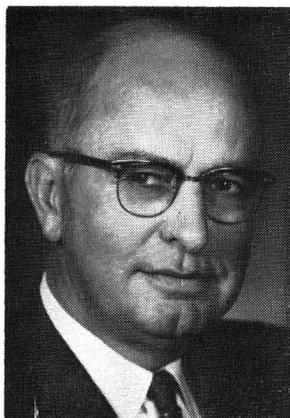
Certainly the chemical engineer has played a vital role in the American chemical industry for many years. I propose to talk about how I think that role is being changed by what is going on in the industry and by forces outside the industry which impinge on the profession.

CHANGES IN THE CHEMICAL INDUSTRY

THE CHEMICAL INDUSTRY has always been a changing industry, which makes it an interesting place to work, but it seems that the rate of change is now faster than ever before. In fact, it is probably changing at a rate faster than any other high technology industry with the exception of electronics. The industry has become large-volume, investment-sensitive, highly-competitive and more prone to rapid obsolescence. Competition to a large degree is the result of high profit margins of a few years ago which attracted newcomers to the industry, especially the oil companies who forward integrated into petrochemical products. We suffer from overcapacity at times, and profit margins are not what they used to be. The year '72, it should be noted, was the best year for some time and '73 to date looks even better. Further progress will depend heavily upon the performance of the chemical engineer and, as I will attempt to show, the engineer will be more important than ever.

The role of research in the chemical industry is changing. There has been considerable discussion in the literature about how our industry's research is not as productive as it once was. This is a highly debatable point and, of course, depends upon definitions of productivity. In any event it is certainly true that research is more competitive than ever, partly because there are more highly capable research organizations around than there were a few years ago. It is be-

*Presented to Delaware Valley Section AIChE, April 11, 1973.



Norman Copeland is a senior vice president, member of the Executive Committee, and a director of the du Pont Company. Prior to those assignments he was chief engineer of the company, one of the largest private engineering organizations in the world. He is a graduate of MIT and the University of Delaware (PhD '49) and is a member of the Visiting Committees of MIT (ME), Lehigh (ChE) and Delaware (Research Foundation).

coming more difficult to come up with a new product on which a completely exclusive patent position can be obtained and with which we can proceed, with less than optimum technology to exploit the market with a comfortable margin. Then too, the nature of research is changing in the chemical industry. It is moving in the direction of support for existing products or variations of them. There are fewer examples in recent years of a chemical company researching itself into large, completely new proprietary areas in the manner, say, of nylon, which is probably the all-time classic.

We have certainly learned that invention and discovery cannot be bought merely by massive application of dollars and platoons of Ph.D.'s. Nevertheless, the rewards for good research, in my view, are as great as ever. It is just a tougher game than it used to be.

As a consequence of the foregoing considerations, it seems to me that the competitive position of a chemical company in the future is likely to depend less on patent positions and more on technology. I am certainly not underrating the value of a good patent position; I am saying that such a position is harder to get nowadays. Also for many important products of our industry, basic patents have expired.

To me this state of affairs means that the engineer, especially the chemical engineer, has a more important role to play.

LARGER SCALE OF OPERATION

AS THE INDUSTRY BECOMES more competitive and as more products approach commodity status, scale of operation becomes increasingly important. Exploiting this advantage of scale to a large extent depends upon the chemical engineer. We continue to build larger and larger single-line plants, for example, in methanol, polyvinyl acetate, textile fibers, DMT, etc. and I see the trend continuing. Scale-up factors seem to be getting larger each year, calling for increasing sophistication on the part of the chemical engineer. Our engineers recently extrapolated a very complex process from a 1 lb-per-hour mini-plant to a 150MM lb-per-year commercial plant. After a certain number of headaches, the plant is now operating at capacity. A great deal of time and money was saved by this approach as compared to carrying the product through a pilot plant. I should point out that this particular case involved an intermediate for internal use, so that market development was not involved.

The development and design of large single-line plants inherently require superior engineering. Continuity is critical; the malfunction of a single piece of equipment can shut down millions of dollars of investment. Since plant utility or time on line is so important and is the multiple of the individual utilities of a large number of equipment items, highly sophisticated techniques have been developed to predict during the design stage overall plant utility for various equipment configurations and to select the arrangement giving the best trade-off between down-time and investment.

In addition to our scale of operation getting larger, our processes are becoming more complex. This increasing complexity augments the need for better, more sophisticated engineering. The chemical engineer must not only comprehend basic relationships but very complicated interactions as well. This situation is particularly evident in process control which, in many of our processes, ex-

... invention and discovery cannot be bought merely by massive applications of dollars and platoons of Ph.D.'s . . . Nevertheless, the rewards for good research . . . are as great as ever. It's just a tougher game.

ceeds the ability of human operators to handle directly. As a consequence, the industry is moving to computer control which is developing rapidly and has already attained an astounding level of development. Process control has become a profession in its own right. The use of computers requires more quantitative knowledge of the effects of process variables and their interactions than was previously necessary. The chemical engineer must provide this knowledge and it takes an especially good engineer to do it adequately.

As our technology becomes increasingly complex, more specialized knowledge in-depth is required for optimization of plant design. The chemical engineer is becoming more dependent on other engineering specialties. Our modern chemical plants are developed and designed by teams of engineering specialists.

There are, it seems to me, some important consequences of increased specialization and the growing importance of technology vs. patent position. Specialization is possible only in a fairly large engineering organization. Certainly outside assistance can and should be brought in when appropriate but this can present problems when we are dealing with proprietary technology. Technology can best be kept proprietary if the engineering is done in-house. Hence it seems to me that a competitive advantage in some types of large-scale chemical manufacture will accrue to those companies large enough to support their

We continue to build larger single-line plants . . . whose development and design inherently require superior engineering.

own specialized engineering organization. This does not necessarily apply to the manufacture of true commodity chemicals where the technology can be readily purchased, along with turn-key plants supplied by highly competent contractors.

ENVIRONMENTAL AND ENERGY CRISES

PREVIOUSLY, I REFERRED TO forces outside the chemical industry which impinge on the practice of chemical engineering. One of the most potent of these is the drive to clean up the environment. In the chemical industry much of

this task falls in the domain of the chemical engineer. There are certainly thousands of chemical engineers engaged in finding ways of cleaning up existing effluents to streams and rivers and exhausts to the atmosphere from existing plants. In some cases, they have been able to do this on a breakeven or a profit basis by recovery of valuable materials, recycling, etc. But this is getting more difficult all the time and, as regulations have become tighter, engineers are endeavoring to come up with solutions imposing the least economic penalty on the operation. Many ingenious solutions to many difficult problems have already been found. At the same time there are cases where there is simply no way out and the operation must be closed. As you are aware, the stated goal of existing legislation is zero stream pollution by 1983. Strictly interpreted, of course, this means that industrial effluents by then must be composed of nothing but pure water. Now we as chemical engineers know that such a goal is impossible without limitless supply of energy for free, and even then we would transfer much of the environmental problem to the solids waste and air pollution areas. It is not my purpose to discuss the wisdom of existing environmental legislation. I know that some legislators fully realize that absolute zero pollution is unattainable. But (politics aside) they feel that setting such a goal will push us to the limit of technical feasibility and perhaps inspire us to do things we didn't think possible.

In addition to the impact on the chemical engineer of the task of cleaning up existing operations, environmental considerations are strongly affecting his activities in the design and the development of new processes. He must now take environmental problems into account every step of the way. The process development is not finished until environmental problems have been satisfactorily dealt with, and obviously his choice of processes is greatly affected.

Another outside force which will have an increasingly profound effect on the chemical industry, and hence the chemical engineer, is the energy shortage. This shortage is already with us and will be getting far worse. The problems of the environment and the energy shortage are closely related and eventually priorities will have to be set—just how and by whom is not clear. Unfortunately, in our free society these kinds of problems tend to be neglected until a crisis develops. We have been hearing about the environmental crisis

Continuity is critical . . . our processes are becoming more complex . . . as a consequence, the industry is moving to computer control.

for sometime. Now the energy crisis is getting the attention of the public. There appears to be a growing awareness that the two crises cannot be solved independently. Environmental regulations have forced the substitution of oil and gas, already in short supply, for coal, which we have in abundance. Furthermore, present and future auto emissions controls are resulting in much less efficient automobile engines. This in turn means greater demand for oil. Environmental concerns have blocked exploitation of Alaskan oil as well as drastically slowed up adoption of nuclear power plants. We will be forced to import larger amounts of crude oil from the Middle East which will result in untenable foreign trade deficits.

All of this has a great bearing on the chemical industry, not only in regard to energy to run our industry but, of even greater importance, on the cost and availability of hydrocarbon feed stocks upon which the industry basically depends and for which there are no substitutes.

The energy shortage is already having considerable influence on how we do our chemical engineering. Energy consumption is becoming a much more important factor in process development and design. Increasing attention is being given to heat and energy recovery in the design of new plants. We used to install energy recovery systems if they showed a return on investment at current energy costs. Now we feel that energy recovery should be installed on a breakeven basis since costs can go only one way and that is up. Rising energy costs are also making it appropriate to restudy existing plants for opportunities for energy conservation. We are already doing this, and what we have found in several instances is that in order to make *significant* savings in energy, we must make *significant* changes in our processes. This poses a real challenge to the ingenuity of our chemical engineers.

COMPUTERS IN THE PROFESSION

I PREVIOUSLY MENTIONED computers for process control. No discussion of changes in the practice of chemical engineering, or engineering in general for that matter, would be complete

without a few words about the effect of computers and computer systems on the profession. The computer has certainly increased engineering productivity many-fold and has enabled us to solve problems that we couldn't tackle previously. We have become so accustomed to the power of the computer that it is hard to visualize how we would function without it. It has removed much of the old drudgery from our work. I can remember hours and hours of slide rule work until I was bleary-eyed making a trial-and-error plate-to-plate distillation calculation; then to find that I had made some stupid mathematical error early in the calculation.

I am impressed with the impact that the computer is having on the design function. Our engineers have available to them well over a hundred programs of various size and complexity, covering just about all phases of design activity. Computer-balanced flow sheets are becoming standard for most major projects. Computer-made piping diagrams are becoming commonplace. Here again computers are relieving the engineers of drudgery. More important, they are providing him with greater flexibility and unprecedented speed to optimize designs.

One area where we should be able to use computers to a larger extent is in energy conservation. There are computer programs to make overall plant steam and water balances, but I get the impression that they are not used very much and that they are cumbersome and expensive. It seems to me that we have more opportunities in this field. The computer's influence on our work has already been revolutionary and the process is still going on.

Now, I have dwelt on the use of computers to a large extent, and in most instances I have commented on some interrelationship between the computer and the engineer. The computer is not lessening the role of the chemical engineer. Far from it; it is upgrading his role.

CONCLUSION

I have tried to suggest from my point of view how changes within the chemical industry and an increasing number of outside forces are changing the role of the chemical engineer. The need for chemical engineers with the basic ability to define and solve problems is greater than ever. Today's chemical engineer has a lot more knowledge and resources to draw on; but his problems are becoming a lot more difficult too. Change and challenge have always made chemical engineering interesting. It looks as though it is going to continue that way. □

COMMENTS ON GIBBS' EQUATION:

The Condition For Chemical Equilibrium In Open Systems*

A. H. LARSEN† AND C. J. PINGS

California Institute of Technology
Pasadena, California 91109

The first law of thermodynamics establishes the existence of the internal energy E , a state function, for a closed system. Assume that E exists and is a state function for open systems also. Define q to be the heat transferred to the system due to a temperature gradient, and w to be the work done by the system in addition to that required to introduce or remove material at the boundary. Neglecting kinetic and potential energy changes, the first law for an open system becomes

$$dE = \delta q - \delta w + \sum_{k=1}^s \bar{H}_k^{(e)} dn_k^{(e)}, \quad (1)$$

where δ is a variation operator used to indicate that q and w are not state variables, but are path-dependent functions instead, and where $\bar{H}_k^{(e)}$ is the partial molal enthalpy of species k (of s species present) entering or leaving the system, and includes the work required to transfer material across the boundary. If the only work done by the system is expansion work, it follows that

$$\delta w + \delta D_v = PdV, \quad (2)$$

where δD_v is the differential of viscous dissipation of energy. Here dD_v/dt , i.e. the time derivative, is the same quantity as denoted by E_v by Bird *et al.* [1].

For an open system, the second law of thermodynamics may be written

$$TdS = \delta q + TdS_{irr}^{(i)} + TdS^{(e)}, \quad (3)$$

*Supported in part by the Directorate of Chemical Sciences, Air Force Office of Scientific Research, under Grant AFOSR-68-1382.

†Present Address: Management Information and Systems Department, Monsanto Company, 800 North Lindbergh Boulevard, St. Louis, Missouri 63166.

where $dS_{irr}^{(i)}$ and $dS^{(e)}$ are internal and external contributions to the differential change in the entropy of the system, due to irreversible chemical reaction and viscous dissipation, and to material entering or leaving under different conditions than in the system. Assuming that a state function S , established for closed systems, also exists for open systems, dS is a perfect differential. The internal entropy generation term $dS_{irr}^{(i)}$ must be positive.

In an open system, the differential extent $d\xi$ of a single chemical reaction is defined by

$$dn_k = \nu_k d\xi + dn_k^{(e)}, \quad (4)$$

where dn_k is the differential change in the number of moles of species k crossing the boundary of the system. Write

$$TdS_{irr}^{(i)} = Ad\xi + \delta D_v, \quad (5)$$

where A is called the affinity of the reaction. In the absence of viscous dissipation, eq. (5) is essentially a defining relationship for the affinity A .

Define *chemical equilibrium* by the vanishing of the chemical reaction part of $dS_{irr}^{(i)}$, independent of the existence of irreversibilities introduced by viscous dissipation or by material entering or leaving the system. Then

$$Ad\xi = 0 \quad [\text{eq}], \quad (6)$$

where [eq] indicates constraint to paths of chemical equilibrium. Since the variation $d\xi$ is arbitrary, the necessary and sufficient condition for chemical equilibrium becomes

$$A = 0 \quad [\text{eq}], \quad (7)$$

which means that the driving force for the reaction is zero. If $A \neq 0$ even though no reaction occurs ($d\xi = 0$), the system is not at stable equilibrium. For example, a mixture of hydrogen and oxygen at room temperature does not react at any measurable rate, but may be made to do so by

introducing a spark or a suitable catalyst, such as spongy platinum. The spontaneous reaction is highly irreversible, showing that $dS_{\text{irr}}^{(i)}$ is positive or, from Eq. (5), that $A \neq 0$. The unreactive mixture is not at true chemical equilibrium, but its state has been termed "false equilibrium" [2] or "metastable equilibrium" [3].

Substituting Eqs. (1), (2), (3), and (5) into the differential of Gibbs energy,

$$dG = dE + PdV + VdP - TdS - SdT, \quad (8)$$

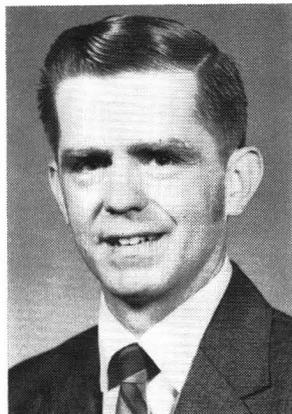
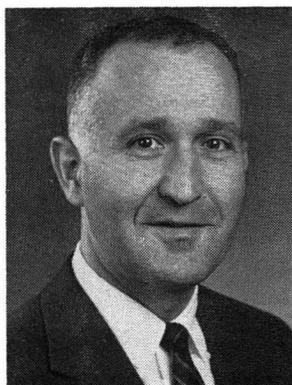
we obtain

$$dG = -SdT + VdP - Ad\xi + \sum_{k=1}^s \bar{H}_k^{(e)} dn_k^{(e)} - TdS^{(e)}, \quad (9)$$

which may be considered as a form of Gibbs' equation for open systems in the absence of external force fields [2]. Since $ds^{(e)}$ depends on material crossing the boundary, and vanishes for $dn_k^{(e)} = 0$ ($k = 1, 2, \dots, s$), we have immediately

$$A = - \left(\frac{\partial G}{\partial \xi} \right)_{T,P,n^{(e)}}, \quad (10)$$

where the subscript $n^{(e)}$ indicates that the differentiation is performed under the constraint of no



Cornelius J. Pings is Professor of Chemical Engineering, Dean of Graduate Studies, and Vice Provost at Caltech, from which he received his B.S., M.S., and Ph.D. degrees. He serves currently as Chairman of the Redevelopment Agency for the City of Pasadena. For his research efforts in applied chemical thermodynamics and the physics and chemistry of liquids, he has received awards from ASEE and AIChE.

A. H. Larsen is an engineering specialist in the Corporate Engineering Department of Monsanto Company, where he is responsible for physical properties service and for development and application of process simulation technology. He earned B.S.Ch.E. and B.A. degrees from the University of Utah and a Ph.D. degree in Chemical Engineering from the California Institute of Technology.

A general condition of chemical equilibrium for open systems is derived . . . with the condition of chemical equilibrium defined in Eq. 6, a restriction to constant temperature and pressure is unnecessary.

material crossing the boundary. Hence the affinity of a chemical reaction in an open system is the same as that in a closed system. Considering the Gibbs energy G to be a function of temperature, pressure, and the numbers of moles of all species present, Eq. (10) becomes

$$A = - \sum_{k=1}^s \left(\frac{\partial G}{\partial n_k} \right)_{T,P,n_1} \left(\frac{\partial n_k}{\partial \xi} \right)_{T,P,n^{(e)}} = - \sum_{k=1}^s \nu_k \mu_k \quad (11)$$

with the use of Eq. (4). The chemical potential μ_k of species k is defined by

$$\mu_k = \left(\frac{\partial G}{\partial n_k} \right)_{T,P,n_1}, \quad (12)$$

where the subscript n_1 means that the number of moles of each species except species k is held constant. Invoking the principle of microscopic reversibility (Tolman) [4], each reaction in a multiple-reaction system at chemical equilibrium must be independently in equilibrium. Therefore, from Eqs. (7) and (11), it follows that

$$\sum_{k=1}^s \nu_{ik} \mu_k = 0 \quad (i = 1, 2, \dots, r) \text{ [eq],} \quad (13)$$

which is the condition of chemical equilibrium, valid for open systems.

Using a different derivation, a number of authors, including Hougen [5], Lewis and Randall, [6], Moore [7], Van Ness [8], Aris [9], Waser [10], and Luder [11], imply that Eq. (13), or its equivalent, holds as the condition for chemical equilibrium only at constant temperature and pressure, and fail to indicate its generality. From the above development, with the condition of chemical equilibrium defined by Eq. (6), a restriction to constant temperature and pressure or to any other set of constraints is unnecessary. Since the chemical potentials are intensive variables, they possess a value at every point in a system;

hence, chemical equilibrium exists at any point for which Eq. (13) holds. In fact, Eq. (13) is valid as the condition of chemical equilibrium for *arbitrary* thermal and mechanical variations in an open system.

Further information can now be obtained regarding the nature of $dS^{(e)}$, the contribution to dS due to material crossing the boundary. The usual form of Gibbs' equation for open systems (Prigogine and Defay [2]) is

$$dG = -SdT + VdP + \sum_{k=1}^s \mu_k dn_k \quad (14)$$

Equating two expressions for dG , from Eqs. (9) and (14), we have

$$\sum_{k=1}^s \mu_k dn_k = -Ad\xi + \sum_{k=1}^s \bar{H}_k^{(e)} dn_k^{(e)} - TdS^{(e)} \quad (15)$$

Substitution from Eqs. (4) and (11) results in

$$TdS^{(e)} = \sum_{k=1}^s [\bar{H}_k^{(e)} - \mu_k] dn_k^{(e)} \quad (16)$$

Now

$$\mu_k = \bar{H}_k - T\bar{S}_k, \quad (17)$$

and

$$\mu_k^{(e)} = \bar{H}_k^{(e)} - T^{(e)}\bar{S}_k^{(e)} \quad (18)$$

where $\mu_k^{(e)}$ and $\bar{S}_k^{(e)}$ are the chemical potential and partial molal entropy, respectively, of species k crossing the boundary, and $T^{(e)}$ is the temperature of the material crossing the boundary. Hence, Eq. (16) becomes

$$TdS^{(e)} = T \sum_{k=1}^s \bar{S}_k dn_k^{(e)} + \sum_{k=1}^s [\bar{H}_k^{(e)} - \bar{H}_k] dn_k^{(e)} \quad (19)$$

$$= T^{(e)} \sum_{k=1}^s \bar{S}_k^{(e)} dn_k^{(e)} + \sum_{k=1}^s [\mu_k^{(e)} - \mu_k] dn_k^{(e)}.$$

Therefore $dS^{(e)}$ includes a term to account for the differences between either partial molal enthalpies or chemical potentials of the species crossing the boundary and those in the system, depending on whether the partial molal entropy terms are described in terms of properties of the system or of properties of the material crossing the boundary.

REFERENCES

1. Bird, Robert B., William E. Stewart, and Edwin N. Lightfoot, "Transport Phenomena," Wiley, New York

(1960), p. 214.

2. Prigogine, I., and R. Defay, "Chemical Thermodynamics," trans. by D. H. Everett, Wiley, New York (1954).
3. Hatsopoulos, George N., and Joseph H. Keenan, "Principles of General Thermodynamics," Wiley, New York (1965), p. 416.
4. Tolman, Robert C., "The Principles of Statistical Mechanics," Oxford University Press, London (1938), p. 163.
5. Hougen, Olaf A., Kenneth M. Watson, and Roland A. Ragatz, "Chemical Process Principles," 2nd ed., Part II, Wiley, New York (1959), p. 982.
6. Lewis, Gilbert N., and Merle Randall, "Thermodynamics," 2nd ed., revised by Kenneth S. Pitzer and Leo Brewer, McGraw-Hill, New York (1962), pp. 143, 173.
7. Moore, William J., "Physical Chemistry," 3rd ed., Prentice-Hall, Englewood Cliffs, N. J. (1962), p. 171.
8. Van Ness, Hendrick C., "Classical Thermodynamics of Non-Electrolyte Solutions," Macmillan, New York, (1964), p. 117.
9. Aris, Rutherford B., "Introduction to the Analysis of Chemical Reactors," Prentice-Hall, Englewood Cliffs, N. J. (1965), p. 41.
10. Waser, Jurg, "Basic Chemical Thermodynamics," Benjamin, New York (1966), p. 160.
11. Luder, William F., "A Different Approach to Thermodynamics," Reinhold, New York (1967), p. 62.

Nomenclature

- A = Affinity of a chemical reaction
 D_v = Viscous dissipation of energy
 E = Total internal energy
 G = Total Gibbs energy, $H - TS$
 H = Total enthalpy
 n_k = Number of moles of species k
 P = Pressure
 q = Heat transferred to the system due to a temperature gradient
 S = Total entropy
 s = Number of species in the system
 T = Absolute temperature
 V = Total volume
 w = Work done by the system

Greek Symbols

- δ = Variation operator
 μ_k = Chemical potential of species k
 ν_{ik} = Stoichiometric coefficients of species k in reaction i
 ξ = Extent of chemical reaction

Superscripts and Subscripts

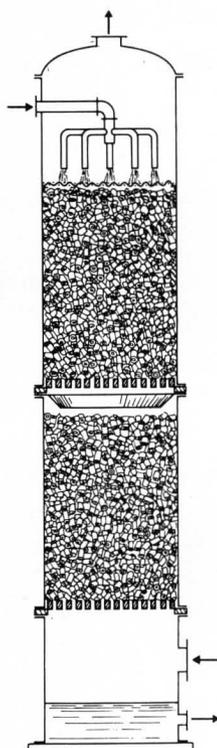
- = Partial molal quantity
 (e) = Material crossing the boundary
 (i) = Material in the system
 i = Chemical reaction
 irr = Irreversible process
 k = Species of material
 $n^{(e)}$ = Differentiation performed under constraint of no material crossing the boundary

Proceedings of

***THE WORKSHOP ON THE UNDERGRADUATE
CHEMICAL ENGINEERING LABORATORY***

Edited by A. J. Perna and H. S. Fogler

This volume from the 1972 ASEE Summer School for Chemical Engineering Faculty contains



- Copies of papers presented by the Conference on a wide variety of topics (e.g. computer aided, bench scale, and pilot plant experiments; roles and philosophies of the various laboratories).
- Selected experiments from over twenty universities on instrumentation, control transport processes, chemical kinetics and unit operations.
- Summary of the survey of industry and chemical engineering departments on current status, philosophies, and expected trends in Chemical Engineering laboratories.

This volume can be ordered by sending a check of \$10.00 payable to the Department of Chemical Engineering, University of Michigan to:

H. S. Fogler, Workshop Coordinator
Department of Chemical Engineering
University of Michigan
Ann Arbor, Michigan 48104

Funds collected from the sale of the Proceedings (above printing costs) will be applied to the next Chemical Engineering Summer School.

INTRODUCING BEHAVIORAL SCIENCE INTO AN ENGINEERING LABORATORY

E. R. HAERING and J. B. MARTIN
Ohio State University
Columbus, Ohio 43210

THE SUCCESSFUL PRACTICE of engineering requires not only technical competence, but also skill in working with people. A laboratory course that includes working in groups offers an opportunity to develop these interpersonal skills along with the practical applications of technical knowledge.

The Chemical Engineering Operations Laboratory at Ohio State University is such a course. The laboratory is offered during the Summer quarter between the third and fourth years. The students have completed such chemical engineering courses as Process Calculations, Thermodynamics, Transport Phenomena and a Unit Operations theory course. The laboratory is designed to be the fundamental laboratory course in chemical engineering operations. Laboratory investigations of the operating characteristics and efficiencies of such chemical engineering equipment as distillation, filtration, drying, evaporation, liquid-liquid extraction and heat transfer equipment are conducted by the students. Typically the students, working in groups of five or six, spend three days on each problem with one day devoted to defining the problem and deciding upon the data required, one day of experimental work and one day of data reduction. At the completion of an experiment, the group submits a complete technical report concerning their findings.

Each group is led by a student foreman who is responsible for seeing that a particular problem is solved. The foremanship is rotated among all members of the group during the course. The squad foreman's duties include:

- determining exact nature of the problem to be studied.
- leading the squad in the development of the plan of attack to be used in solving the problem.
- organizing and supervising the laboratory and calculation efforts of the squad.
- guiding the preparation of the final report.

In short, the squad foreman is given the opportunity to act as a typical technical group leader and is presented with responsibilities that emphasize his managerial role. This aspect of the course has been expanded by the introduction of cognitive and experiential learning from the behavioral sciences.

SETTING OBJECTIVES

WE SET AS OBJECTIVES for this portion of the course:

1) to develop an awareness that there is a body of knowledge about how organizations can become more effective, 2) to develop an appreciation of participative management, 3) to establish a conceptual framework for further learning about organizations, 4) to provide an understanding of what is meant by experiential learning, 5) to increase skill in giving and receiving positive feedback, 6) to help each student to appreciate his own strengths.

Objectives 1 and 3, and to some extent 2, represent an intellectual kind of learning. Since our objectives were limited ones, requiring little depth of understanding, we decided to impart this information by lecture and discussion. Two one-hour lectures were presented; one on managerial styles and one on organization development.

A quick check with the students indicated practically no knowledge of management theory. A few students acknowledged a slight acquaintance with Maslow's hierarchy of needs, but the names of other behavioral scientists elicited practically no response. The first lecture was, therefore, a survey of management and motivation theory. The subjects covered, though superficially, were:

- Scientific Management (Frederick Taylor)
- Human Relations Approach (Hawthorn Experiments)
- Theory X and Theory Y (Douglas McGregor)
- Hierarchy of Needs (Abraham Maslow)
- Two Factor Theory of Motivation (Frederick Herzberg)
- Texas Instruments (Scott Myers)
- Managerial Grid (Blake and Moulton)

The second lecture defined organization development as planned change for organizational improvement based on behavioral science. Typical

steps in introducing organization development into a system: **education, team building, inter-group problem solving** and **organizational redesign** were described. To give some meaning to the steps, examples of activities associated with each step were discussed.

We felt the other objectives required experiential learning. Each squad met separately for approximately 3 hours with Dr. Martin. After responding to any questions generated by the lectures, he led the squad in an abbreviated team-building exercise. Each squad was asked to produce a list of the abilities or characteristics of individuals that contributed to effective squad performance in this laboratory course. These lists ranged from 12 to 37 items. Included were abilities for performing particular aspects of the work such as operator skills in the laboratory, writing ability, graphical ability, computer skills, mechanical skills, manual skills, and technical knowledge. Also listed were more personal characteristics such as willingness to work hard, willingness to sacrifice, dependability, ability to get



Edwin R. Haering is an Associate Professor of Chemical Engineering at The Ohio State University. He is a native of Ohio and received his B.Ch.E., M.S., and Ph.D. degrees at Ohio State. He is teaching in the areas of chemical engineering operations, chemical kinetics, reactor design and process design. His major research interests are adsorption, heterogeneous catalysis and chemical reactor design and analysis. (LEFT ABOVE)



J. B. Martin, Adjunct Associate Professor of Chemical Engineering, The Ohio State University, has spent his entire professional career within research and development at The Procter & Gamble Company, Cincinnati, Ohio. He received a BS in Chemical Engineering from Auburn University, (1943); MS (1947) and PhD (1949) degrees from The Ohio State University. He has been honored by the College of Engineering of The Ohio State University as a Distinguished Alumnus. Dr. Martin is a member of the Chemical Engineering Division of ASEE, was a Director of AIChE (1968-70), and is Past President of the Engineering Society of Cincinnati. He is a registered Professional Engineer in Ohio. (RIGHT ABOVE)

along with people, and ability to organize. There were also more specific items, including the ability to communicate with a particular teaching assistant.

FEEDBACK: STRENGTH AND WEAKNESS

EACH squad member then selected from the list two or three (depending on the length of the list) items which represented the greatest strength for each other member of the squad. We decided to emphasize strength because: 1) we doubted that in the short time available we could develop sufficient candor to insure a meaningful discussion of weaknesses, 2) there would be insufficient time available to deal with the feelings generated by negative feedback, 3) we wanted to give practice in giving and receiving positive feedback, because the emphasis on feedback is so often negative.

The choices were displayed so that the information as to who said what about whom was shared within the squad. Each member was then asked to elaborate on his opinions and to cite examples of the behaviors that led to his choices. One of the eight squads chose to repeat this portion of the exercise with regard to weaknesses.

The students participated actively in the exercise. While the information shared tended to be somewhat superficial, it was felt that there were useful exchanges in each squad.

We asked the students for short critiques of this insertion into the laboratory. Their reactions were quite favorable and they recommended a similar program for next year. The lectures were seen as interesting, pertinent, and helpful. The response to the team building sessions was more mixed. About half the class were, to some degree, dissatisfied with these experiences. In general, those who expected an improvement in the performance of the squad were disappointed. A number pointed out, quite correctly, that real improvement could not be achieved without dealing with deficiencies. In retrospect, we see that we could have been more explicit about the limitations on the exercise. There seemed to be satisfaction with the exercise as a learning experience, although several students would have preferred to have used the time for computation and report writing.

We have concluded that this addition to the course is well worthwhile, and hope to continue this exposure to the behavioral sciences in engineering education. □

McGRAW-HILL IS

PRINCIPLES OF NON-NEWTONIAN FLUID MECHANICS

G. ASTARITA, University of Naples and G. MARRUCCI, University of Palermo. 1974, 304 pages (tent.), \$19.50 (tent.)

An accessible yet rigorous treatment of non-newtonian fluid mechanics is provided in this advanced text. Modern continuum mechanics and rheology are presented and developed up to the solution of cases of fluid mechanics problems, particularly for polymeric materials. Along with a consideration of nonlinear thermodynamics, the book offers a critical review and classification of a large number of constitutive equations.

THE INTERPRETATION AND USE OF RATE DATA: The Rate Concept

STUART W. CHURCHILL, University of Pennsylvania. 1974, 512 pages (tent.), \$19.50. Solutions Manual

Here is a completely new treatment of rate processes in which a generalized structure is used, greatly simplifying the number of concepts needed to study bulk transfer, momentum transfer, heat transfer and chemical reactions. Emphasis is on the relationship between design and uncertainties in measurement, and these concepts are reinforced with over 300 problems based on raw experimental data from the literature.

A McGraw-Hill/Scripta Book

INTRODUCTION TO METALLURGICAL THERMODYNAMICS

DAVID R. GASKELL, University of Pennsylvania. 1973, 550 pages, \$19.50

Treating in depth the thermodynamics of high temperature systems encountered in metallurgy, this book demonstrates the thermodynamic method through an extensive illustration program, using as examples real systems which have been carefully selected to illustrate the principles involved. The text introduces basic laws and necessary thermodynamic functions and makes applications that are numerous and thoughtful.

A McGraw-Hill/Scripta Book

MOMENTUM, HEAT AND MASS TRANSFER, Second Edition

C. O. BENNETT, University of Connecticut, Storrs and J. E. MYERS, University of California, Santa Barbara. 1974, 752 pages, \$17.95. Solutions Manual

Combining a rigorous approach to fundamentals with an extended treatment of practical problems, this revision treats principles of transport phenomena as applied to simple geometries and then extends the discussion to analyze practical areas such as flow in pipes and equipment, filtration, heat exchangers and evaporators, gas absorption, liquid-liquid extraction and distillation.

SOLIDIFICATION PROCESSING

MERTON C. FLEMINGS, Massachusetts Institute of Technology. 1974, 335 pages, \$19.50. A Solutions Manual will be available

Here is the only significant book in the field in ten years. Building on the foundations of heat flow, mass transport and interface kinetics, the author presents the fundamentals and relates them to practice. Among the processes considered are crystal growing, shape casting, ingot casting, growth of composites and splat cooling.

ENVIRONMENTAL SYSTEMS ENGINEERING

LINVIL G. RICH, Clemson University. 1973, 448 pages, \$16.50. Solutions Manual

In this quantitative introduction to the subject, Professor Rich uses a systems approach, in which the focus is on the system as a whole and how the components interact. Although water environment is considered in greatest detail, also included are air pollution and its control, solid waste management and radiological health. The mathematics of systems analysis and computer solutions is used extensively.

McGraw-Hill Book Company

AN OPEN BOOK

COMPUTER-AIDED HEAT TRANSFER ANALYSIS

J. ALAN ADAMS and DAVID F. ROGERS, both of the United States Naval Academy. 1973, 480 pages, \$17.00

A balanced approach between theory and analysis/application of that theory is presented for all three modes of heat transfer. A thorough development of the methods for formulating mathematical models in terms of non-dimensional parameters is stressed. Well documented, interactive computer programs, written in the BASIC programming language, are an integral part of the text.

APPLIED STATISTICAL MECHANICS: Thermodynamic and Transport Properties of Fluids

THOMAS M. REED and KEITH E. GUBBINS, both of the University of Florida. 1973, 510 pages, \$18.50

With emphasis on applications, this text introduces the various ways in which statistical thermodynamics and kinetic theory can be applied to systems of chemical and engineering interest. Presented is a fundamental, up-to-date treatment of statistical-mechanics with primary interest focused on molecular theory as a basis for correlating and predicting physical properties of gases and liquids.

CHEMICAL ENGINEERING KINETICS, Second Edition

J. M. SMITH, University of California, Davis. 1970, 544 pages, \$16.50

By developing principles of kinetics and reactor design and applying them to actual chemical reactors, this text acquaints students with the tools necessary to design new chemical reactors and predict the performance of existing ones. Emphasis is placed on real reactions using experimental rather than hypothetical data.

PROCESS MODELING, SIMULATION, AND CONTROL FOR CHEMICAL ENGINEERS

WILLIAM L. LUYBEN, Lehigh University. 1973, 558 pages, \$18.50. Solutions Manual available from the author

Professor Luyben has devoted his book to presenting only useful, state-of-the-art, applications-oriented tools and techniques most helpful for understanding and solving practical dynamics and control problems in chemical engineering systems. Written for the undergraduate student, this text offers a unified, integrated treatment of mathematical modeling, computer simulation, and process control.

HEAT TRANSFER, Third Edition

JACK P. HOLMAN, Southern Methodist University. 1972, 480 pages, \$13.50. Solutions Manual. Five cassette tapes with accompanying student workbook also available. Audio Tapes, \$35.00; Workbook, \$2.50

A brief and concise treatment of *all* phases of heat transfer, featuring in this edition a set of review questions at the end of each chapter, additional problems, use of SI units, increased emphasis on numerical methods in the chapters on conduction, and expanded discussion of techniques applicable to computer solution, additional empirical relations for free convection, and a new chapter on environmental problems.

MASS TRANSFER OPERATIONS, Second Edition

ROBERT E. TREYBAL, New York University. 1968, 688 pages, \$17.50

The basic approach of this revised text, which treats the major subjects in categories of gas-liquid, liquid-liquid and fluid-solid contact, has been retained as has its application of modern theories and data to practical design of equipment. A major addition to the book includes material on multi-component gas absorption and distillation.

Prices subject to change without notice.

1221 Avenue of the Americas, New York, N.Y. 10020

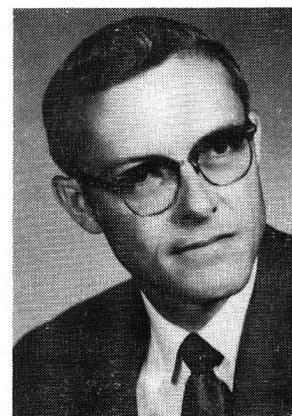


A FOREIGN STUDY PROGRAM IN CHEMICAL ENGINEERING

D. L. ULRICHSON and M. A. LARSON
Iowa State University
Ames, Iowa 50010

IN 1971-72, THE CHEMICAL engineering faculty at Iowa State University (ISU) began giving careful consideration to the development of a foreign study program. Because of the increasing frequency with which our graduates found employment overseas and because of a need for more international contacts between technically trained people, it seemed that such study would add an important new dimension to our degree program. At the time this was under consideration, Professor M. A. Larson was on sabbatical leave at the University College London (UCL). From this advantageous position he was able to work directly with the faculty at University College (primarily Dr. John Garside) in developing the idea. The program that was developed with UCL was approved by ISU in 1973 and the first group went to London in June 1973. This group, under the direction of Professor D. L. Ulrichson, consisted of 14 students: one senior, ten juniors and three sophomores.

It was extremely fortunate that unique personal contact existed between UCL and Iowa State because UCL was ideally suited for such a program. The University College was founded in 1826 and has grown to considerable academic prominence. It was the first University in England to offer degrees to persons who were not members of the Church. The ChE department is one of the most highly regarded in England and its faculty includes some very distinguished members of the chemical engineering profession. Professor P. N. Rowe, head of the department, and Professor J. W. Mullin are extremely active in leadership positions in the Institute of Chemical Engineers.



Maurice A. Larson is Professor of Chemical Engineering at Iowa State University. His technical areas of specialty include crystallization and fertilizer technology. He teaches courses in Process Control and Dynamics and Process Design. In professional activities he has been active in the ASEE, in the AIChE where he has had several local section offices and in the ACS. He is currently Secretary-Treasurer of the Division of Fertilizer and Soil Chemistry. (Left above)

Dean L. Ulrichson was educated at the University of Nebraska (B.Sc. '62), University of Illinois (M.Sc. '63) and Iowa State University (Ph.D. '70). He has had five years of industrial experience with the DuPont Company and has been engaged in teaching and research in the Chemical Engineering and Computer Science Departments at Iowa State University since 1970. His research interests are in process modelling and simulation and energy engineering with particular emphasis on the hydrogen economy. He has been faculty advisor of the AIChE Student Chapter and received an Outstanding Counselor Award in 1973. (Right above)

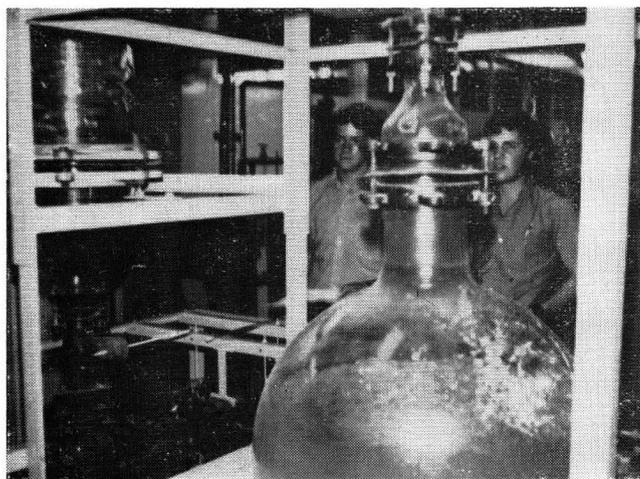
UCL is located near the center of London and within easy walking distance of the British Museum and the University of London Library at Senate House. The London Transport's bus and subway system also provides convenient access to the Parliament Buildings, Buckingham Palace, the theatre and shopping districts. The cultural and academic environment that London and Univer-

sity College could offer made it a natural for a meaningful foreign study experience.

PROGRAM GOALS

THERE WERE FIVE BASIC goals which seemed both realistic and desirable for the program: (1) provide an opportunity to study chemical engineering design and research problems as they exist in a different country; (2) provide individual contact with persons of another culture who are engaged in the practice of the same profession; (3) provide an opportunity to learn more about the impact of the expanded European Economic Community on the objectives and economics of chemical manufacturing in the U.S. and on the foreign operations of prospective employers; (4) provide an opportunity to work in the metric measurement system and learn about the problems which U.S. industries must soon face when they convert to the metric system; (5) provide an opportunity for individual travel in England and other countries both during and after the program.

With these objectives as a framework, a program was developed which provided for: (1) visits to chemical manufacturing plants in the U.S. before departure; (2) two weeks of lectures, laboratories, and study periods at University College London; (3) a one week tour through southwest England and Wales with visits at University College Swansea in Wales and British manufacturing plants; (4) two more weeks of study, lectures, and laboratories at UCL; (5) residence accommodations provided in dormitories where students of other nationalities and backgrounds were also



Heat transfer experiment in UCL lab.

Because of a need for more international contacts between technically trained people, it seemed that such a study program would add an important new dimension to our degree program.

staying; (6) air travel to and from London by youth fare rather than charter so each student could plan visits to other countries and return to the U.S. when he desired; and (7) 12 credits which applied toward the B.Sc. degree in chemical engineering at ISU. The total cost of the program including passport, transportation, fees, room and board was estimated at \$966 for each student.

IMPLEMENTATION

DURING THE SPRING QUARTER of 1973, the participating students attended an orientation program which provided travel information and the nucleus for required reports on the history and economy of the United Kingdom. Details such as travel arrangements, passport and vaccination requirements and possible optional tours to be arranged in England were also discussed.

There were 24 lectures, all given by the UCL staff, during the four weeks of classes. The lecture topics included University of London history, the metric system and preferred numbers, the development of the British and U.S. chemical industry and the impact of the European Economic Community on these industries, and discussion of several of the more prominent research projects at UCL. The students were offered 22 different laboratory experiments from which they were to choose and complete 8 experiments in 16 laboratory sessions. The laboratory experiments offered were quite varied and generally unstructured. Students were encouraged not to perform a specific set of runs in a given experiment but to investigate that aspect of the experiment which most interested them. Reports were required on each experiment and evaluation of these reports was the basis for 4 of the 12 credits awarded for satisfactory completion of the program. The balance of the credits was based on a series of reports on the lecture topics and selected industrial visits.

The other dimension of the program which made the program quite exciting was the frequent breaks from the classroom-laboratory routine. The

evening of the first day of classes the students were introduced to a uniquely British institution, the sherry party. The sherry party was held in a UCL conference room and the students and UCL staff had an opportunity to get acquainted while sampling sherry, pretzels, potato chips and nuts. A wine and cheese party, with many delightful varieties of cheese, was held during the third week of classes and a dinner party with a preceding social hour closed the program on the last day of classes. Other breaks during the program consisted of visits to the chemical engineering department of Imperial College in London, the Science Museum and Gordon's Distillery. All of the industrial visits in the U.K. were most impressive because of the extremely gracious hospitality.

. . . the British way of life . . . is a slower paced life, with less emphasis on materialism and much more emphasis on the impressive history and time honored traditions.

The evenings and weekends were free for the students, and they took advantage of the many attractions available in London and the vicinity. The tennis matches at Wimbledon were popular as was the Shakespearean Theatre-in-the-Round in Regents Park. The many theatres and movies were not neglected and even the pubs (bars) were occasionally visited.

After the first two weeks in London, a week long tour to Wales via charter bus was scheduled. The bus route took us through Stonehenge, a huge stone monument of 15th century B.C. origin, and Bath where the Romans built swimming pool type baths over warm springs in the 1st to 4th centuries A.D. These baths were only discovered and excavated during the 19th century. Our headquarters for the week were in a dormitory at University College Swansea. The first day was spent visiting the chemical engineering department at University College Swansea and the beaches along the Gower Coast. This area probably has the most beautiful coastline in all of England and many miles of lovely sand beaches. The water is a bit cold, however, for those used to the summer weather in Iowa. The next two days were spent visiting B.P. Chemicals Company and the British Steel Corporation's Strip Milling Division. Evening tours to the Black Mountains and local pubs were also organized. The return trip was sched-

uled through Stratford-on-Avon, the birthplace of William Shakespeare. Stratford was a bit too crowded with tourists to interest our group, but it is an interesting place to visit particularly if one can make arrangements early enough to see a play performed in the beautiful new theatre.

Two more weeks of lectures and laboratories in London then concluded the program on August 1. Several students were brave enough to rent cars and bicycles and venture into the surrounding countryside during this two week period. Old castles, some abandoned and some exquisitely preserved, abound for the interested tourist on such short trips. One point of particular interest is the Greenwich Observatory, only a few miles down the Thames from London.

At the conclusion of the program, each student planned to visit at least one other country. Scotland and France were the most popular spots, but hitch-hiking trips through Norway and bicycling trips through Germany were also planned. Although most of the students returned to the U.S. by August 15, two students traveled with backpacks and Eurail passes until September 1.

The total cost of the program was a few dollars less than the estimated cost of \$966. The average expense of entertainment and individual travel in and around London was about \$150 to \$200 per student. This did not include the cost of gifts for friends and relatives nor the cost of post-program traveling.

Probably the most important part of this program was simply the exposure to the British way of life. It is a slower paced life with less emphasis on materialism and much more emphasis on the impressive history and time honored traditions. Certainly it was an experience not soon to be forgotten. A similar program is planned for the summer of 1974.

A few quotes from student assessment are given below.

- "The values of the course lie within the labwork and class work to a small degree, but mainly in the lectures and plant tours. Valuable contacts and exposure to new topics in new ways are very good."

- "I have really enjoyed it over here plus I learned quite a lot. The teachers in the ChE department have been great just to talk to or when you have a problem with a lab they are always glad to help."

- "I think the program is very good, you learn a lot of things, including some chemical engineering."

- "As a learning experience the whole trip is hard to beat."

- "Good show old chap! Smashing idea." □



WE ENCOURAGE JOB HOPPING.

In fact at Sun Oil we've just adopted a new system that promotes it. • Internal Placement System.

- Here's how it works. Say you're in Production and you decide to take a crack at Marketing. Next opening in Marketing we'll tell you. You can apply and be considered. First. You have freedom to experiment and move around at Sun. You learn more and you learn faster.

- Why do we encourage job hopping? Because we happen to believe our most valuable corporate assets are our people. The more our people know, the stronger we are.
- Now—you want to know more? Ask your Placement Director when a Sun Oil recruiter will be on campus. Or write for a copy of our Career Guide. SUN OIL COMPANY, Human Resources Dept. CED. 1608 Walnut Street, Philadelphia, Pa. 19103.



An Equal Opportunity Employer M/F

TEACHING UNDERGRADUATE MASS AND ENERGY BALANCES-1972 +

DONALD R. WOODS
McMaster University
Hamilton, Canada. L8S 4L7.

GARY F. BENNETT
The University of Toledo
Toledo, Ohio 43606

G. MICHAEL HOWARD
University of Connecticut
Storrs, Conn. 06268

MICHAEL J. GLUCKMAN
The City College of New York
New York, N. Y. 10031

New needs, new challenges, new outlooks, new knowledge—these keep the engineering curriculum in a state of flux. The Education Projects and the Undergraduate Education subcommittees of the AIChE decided to bring together all those interested in the teaching of one particular subject to share experience, and to identify new trends and new needs.

A questionnaire was sent to all Chemical Engineering Departments in United States and Canada in June, 1972. Sessions were held at the New York AIChE meeting November 1972 and at the Vancouver meeting in August 1973. The response to the questionnaire was overwhelming and extremely interesting; the conference get-together was very well-received. We realize that studying a course out of the context of a complete program can be very misleading. The specific objectives, prerequisites, the other courses in the program and the staff and facilities available are unique to any program at one particular department. Nevertheless, despite these complications, it is useful to provide a snap shot view of the teaching of Undergraduate Mass and Energy Balance—1972 and some hints of future trends. We hope this is but a start of a series of critical summaries of the courses in our educational program. Mass and Energy balances is to many students their introduction to Chemical Engineering.

What are the characteristics of today's students? What are the content-objectives of the course? Is the lecture technique universally used? What do instructors believe are the major challenges? and What about the future?—these are some questions we try to answer.

THE CHARACTERISTICS OF THE STUDENTS

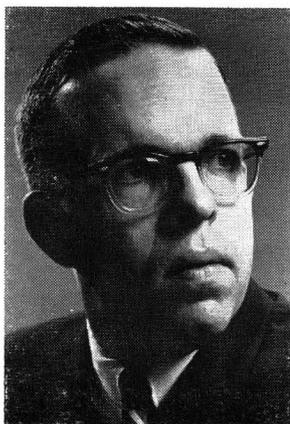
It is difficult, and perhaps even dangerous, to attempt to generalize about the nature of students in their sophomore year. However, we think that it is very useful to at least try to characterize the "consumers" to whom this course is presented. Some characteristics are:

- The majority of the courses they have taken have been in the sciences to broaden their knowledge of fundamental principles of physics, chemistry and mathematics.
- They are used to more or less memorizing "cook book" methods of solving problems.
- They are not used to open-ended problems, ill-defined problems requiring assumptions or problems where there are a number of "good" answers.
- They are not accustomed to the law of optimum sloppiness, or to doing "sloppy" order-of-magnitude calculations, or to the principle of successive approximation.
- They know very little about engineering hardware and about the chemical engineering profession but are very anxious to learn about these.
- In the early 1970's a prime concern is the relevancy of the material and of the profession. They are less willing to gain knowledge because we instructors say they need it. They want to, and almost demand, to be told why they are learning it and its potential application. They want to be "turned on".
- They believe they have well polished logical thinking and debating skills. Yet, for many these skills could be improved greatly.
- In particular for the traditional content in mass and energy balances, they believe that they know much of the material already.

Developing a single course to meet these diverse backgrounds, interests, and needs poses a challenge for even the most skilled teacher. A summary of these challenges is presented later.

CONTENT-OBJECTIVES

In general, the central themes of this course



Gary F. Bennett is a graduate of Queen's University and the University of Michigan (Ph.D.). He is head of the University of Toledo's Biochemical Engineering Laboratory and director of environmental programs for their adult and continuing education division. His honors include designation as "Outstanding Young ChE of the Year" and "ChE of the Year" by the Toledo Junior Chamber of Commerce. His teaching and research interests are in the areas of water pollution and biomedical engineering. (ABOVE LEFT)



D. R. Woods is Chairman of the Shared Teaching Experience subcommittee. He is presently developing a course to teach problem solving skills. His teaching interests are in process analysis, information management and cost analysis. The separation of oil-water systems and surface phenomena are his research interests. (ABOVE RIGHT)

are: developing problem solving ability, learning and applying the principles of conservation of mass, and learning and applying the principles of conservation of energy. Associated with these is the need for a set of units of measurement and a unit system, some basic laws about the behaviour of liquids and solids (physical and thermal properties and concepts), some mathematical skills, and some skill in communicating the results of engineering work. These associated needs can become a major focus of the course or they can be minimized to the extent that some of them are deleted entirely.

Other objectives usually include learning attitudes and manual skills. Bloom et al (1954) and Krathwohl et al (1964) classify the intellectual and attitudinal learning regions. Development of a professional attitude is considered to be important. Some professional concepts are listed in Table 1. The course tries to show what professionals do and to generate an appreciation of their role in society both now and in the future. This includes motivation of the students toward a professional career and the establishment of personal goals within the profession.

Some manual skills that some feel should be

Dr. Gluckman is an Assistant Professor in the Chemical Engineering Department at The City College of the City University of New York. Prior to joining The City College he worked for ten years as a Senior Process Design Engineer for the St. Regis Paper Company. Dr. Gluckman received the B.Ch.E. degree in 1958 from the University of Cape Town, South Africa, and a Ph.D. (Chemical Engineering) from the City University of New York in 1971. (NOT PICTURED)

G. Michael Howard is an Associate Professor of Chemical Engineering at the University of Connecticut. His main teaching interest recently has been the development of a general first course for all freshman engineers. He has taught courses in process dynamics and control, transfer operations, applied mathematics, and the ChE Laboratory. His research interests are in the general area of process modeling, simulation, and control. He holds degrees from Rochester, Yale, and Connecticut and has a variety of industrial experience.

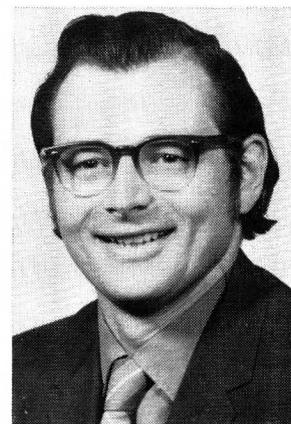


TABLE 1: Some Affective Domain Concepts Important to Chemical Engineers (levels 1 to 5)

USE OF ALL RESOURCES:

- What products and services are useful and needed by mankind?
- Does this represent the optimum long term use of natural resource resources?
- Sense of urgency of man's needs.
- Willingness to compromise theory with reality in satisfying man's needs.

VALUES OF HUMAN WORTH: plant safety, safe products, salary and job security, human relations and effect of present operations and products on future health of society.

ESTHETIC VALUES

MORAL AND ETHIC VALUES

- micro and macroscale
- employment (seeking and hiring and firing those working for you)
- environment
- use of natural resources
- use of intellectual human talent
- information
- honesty

INTERACTION WITH OTHER PROFESSIONALS

- Willingness to actively participate in professional organization.
- Loyalty to colleagues
- Confidence in one's own abilities
- Initiative to start programs on one's own maturity in outlook Reliability

learned include experimental techniques (such as ability to titrate, use a balance, make a thermocouple, to run equipment, to set up bench scale equipment) and skills in keypunching or patching together an analog computer.

The course is actually taught in many different ways as illustrated in Figure 1. These include integrated throughout the program with no course *per se*; as part of a thermodynamics course; with the emphasis on career guidance and professional responsibility, on stagewise processing, on solving several large case problems, on synthesis, on analysis or problem solving, on mathematical methods, techniques and/or simulation, on mass and energy balances, or on computer programming and systems. Most courses are mixtures of these approaches, and these are not mutually exclusive.

The textbooks and resources used are often indicative of the emphasis in the course. Texts that emphasize the conservation concepts include Anderson and Wenzel (1961), Himmelblau (1967), Hougen, Watson and Ragatz (1954), Ranz (1970), Schmidt and List (1962), Thatcher (1962), Tyner (1960) and Williams and Johnson (1971). Whitwell and Toner (1969) emphasize problem-solving. Henley and Bieber (1959), Henley and Rosen (1969), Blum (1971) and Dorf (1969) have a more mathematical bent. Meissner (1971), Shreve (1967), Stephenson (1966), Wendland (1971) and Thatcher (1962) are career and process oriented. Henley and Staffin (1963), King (1971) and Brian (1972) are used as texts by some to introduce processing equipment. The thermodynamics texts used are Balzhiser, Samuels and Eliassen (1971), Denbigh (1971), Smith and van Ness (1959), Sonntag and van Wylen (1971) and Wales (1970).

Over forty schools indicated that they were using Himmelblau's book. Whitwell and Toner, Schmidt and List, and Hougen, Watson and Ragatz were all used by more than five schools. More interesting is the fact that twenty five professors are using a very new book on their own notes in teaching this course.

Some outstanding new textbooks on the market that offer the opportunity to emphasize the areas illustrated in Fig. 1 are:

- Rudd, Powers, Sirola (1972) "Process Synthesis". Choice of cases exceptionally good; illustrates breadth of Chemical Engineering and the general universality of the principles they present. Identifies steps in synthesis as reaction path synthesis, material balancing and species

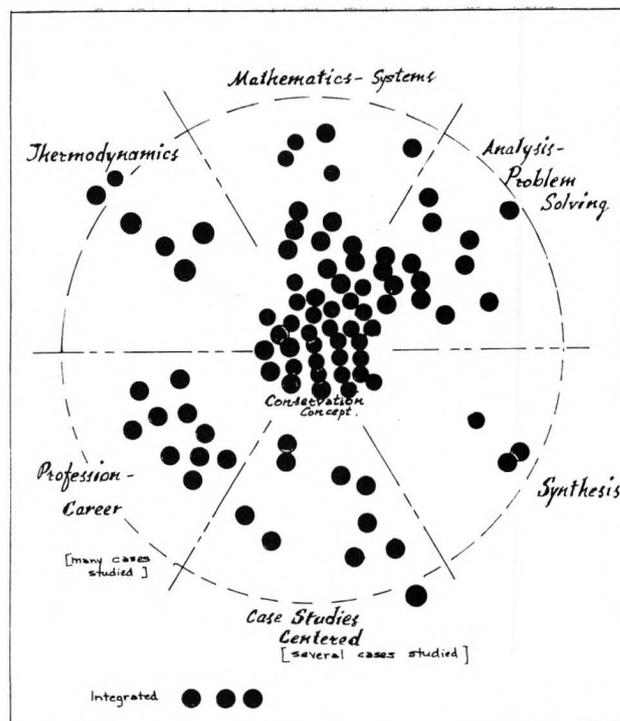


FIGURE 1—Classification of Approaches Taken. Central Region represents emphasis on mass and energy conservation concepts.

allocation, (review of separation technology) strategy for selecting separation task equipment, energy balances and task integration. Each step is abundantly illustrated via case examples from extremely diverse examples. Finally, two cases (fresh water from brine via freezing and detergents from petroleum) are discussed to illustrate synthesis as one large integrated operation.

- Russell and Denn (1970) "Introduction to Chemical Engineering Analysis". Formulation and problem solving are major themes. Introduces rate concepts. Interrelates experiments, modeling and application.
- Myers and Sieder (1972) "Chemical Process Logic". Systems approach with emphasis on mathematics, the use of the computer, solutions of sets of equations and the use of modular executive programs. Good review of mathematical techniques. Well organized and a good attempt to introduce ideas of process equipment.

While these may not suit one's particular objectives, they open up additional resources to us as instructors and provide exciting new trends for thought.

The case study approach attracts a number of professors. In this approach, an example of a process or a case problem is studied as a means of learning concepts through a "need-to-know" or in providing synthesis experience or to motivate the students via relevant problems that also illustrate professional responsibility. A wide variety of background case information is available; see Sherwood (1963); Bodman (1968); King (1971);

Smith (1967 ff). While the majority of these cases have been used for senior and graduate level design courses, nevertheless this provides background information that can be adapted to the second year purposes. (Seagrave's (1971) first four chapters provide interesting examples of mass and energy balances in biomedical applications.) Some cases used by Pappano at West Virginia in the mass and energy balance course and the corresponding objectives are:

Natural gas: alternative uses	To introduce "need-to-know" physical and chemical reaction material balances, conservation of resources and minimum cost criteria.
Reverse osmosis for plating wastes	
Cryogenic liquefaction of methane ethane	To introduce "need-to-know" ideal gas law, work in gas phase, first law and process trade off.
Gas storage	
Separation of a liquefied methane ethane mixture	To introduce "need-to-know" vapor pressure, Raoult's Law.

Rudd, Powers, and Siirola (1972) provide a fantastically broad spectrum of case examples and case problems to which anyone seeking to locate sparkling examples to intrigue freshmen or for examples in the mass and energy balance course is referred.

It is interesting to note the differences between Pappano and Rudd et al in the approach to offering synthesis experience. Pappano uses a number of cases each of which is solved applying all the steps in the synthesis. Rudd, Powers and Siirola (1972) illustrate each step. Later, they consider several cases in detail.

In general, the course is offered after 30 weeks of university training with about 45 hours of lecture time. Some schools use tutorial time only. The experimental laboratory has almost disappeared from the United States schools although the Canadian schools still seem to favor this experience.

THE LEARNING ENVIRONMENT

Traditionally the lecture mode has been used extensively in universities. For engineering, many experimental laboratories have been popular. For developing solving skill, traditionally we have required the students to work many problems for homework. However, with the availability of a variety of well written texts, movie films and film loops, slide-tape or cassettes, programmed texts and with the relatively small classes, many other options are available for us to use. The learning

environments can be classified as:

- Human-sender centered:** lecture, sender directed problem solving, some tutorial/discussion environments,
- Learner centered:** homework, games, student centered discussion, some tutorial/discussion environments,
- Mechanical-sender centered:** computer aided instruction, programmed texts, self-paced audio-visual or texts
- Object centered:** plant tours, experiments, demonstrations

Some learning environments are in between the centers. For example, the discussion, tutorial and recitation usually lie between the human sender center and the learner centered. The discussion is extremely flexible and can range from learner group discussion, guided learner group discussion, the guided problem-solving and guided synthesis to lecturer-directed discussion. Links exist between other centers where the professor is available as an extra resource to a programmed text. MacKenzie et al (1970) p. 32 point out that from a learner's viewpoint, what matters most is not the formal instruction he is given but the kind of learning resources to which he has access.

The variety of learning environment include lectures; demonstrations; student laboratories; individual or group homework problems; self-learning with textbook or printed notes, slide-tapes, films, TV tapes, programmed text, via computer simulations—interaction, and audio plus text; student-centered discussion; student-prepared lectures or reports; sender-directed problem solving or discussion; individual problems solved with discussion and games. Some indication of the mix of these environments is shown in Fig. 2 but this does not do justice to the wide variety of extremely interesting resources that are being used: plant tours oriented toward case projects,

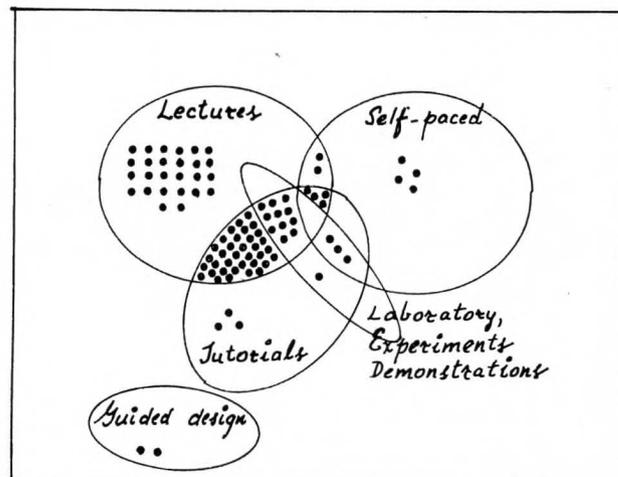


FIGURE 2—Learning Environment used by Respondents.

film loops, programmed texts [Wales (1970)], audio-visual packages and self-paced notes. Of particular interest is the sender-directed problem solving approach of Treybal at New York University and the guided design approach of Pappano. Many are getting away from the lecture and are using the time for discussion or group problem solving.

Self-paced programs have been developed by many in an attempt to overcome the motivational and boredom problems faced when all the class must proceed at the same pace. This has not been without its problems: the fantastic amount of time to prepare good material, the problem of getting the students to use the resources effectively, in particular to keep at the self-paced material. One particularly appealing approach is Pappano's working with the group as part of the team with the evaluation being performed by someone not associated with the course directly.

The sequencing and pacing varies greatly. Tulsa uses 10 of its 17 units on the background laws and equations; McGill uses 7 total units; Clarkson uses 13 units; Arkansas uses 22 units; and Cincinnati uses 15 units. The programs themselves range from the use of texts (such as Wales (1970)), to notes that identify the learning objectives, the rationale, the learning activities and the self-assessment task. MacKenzie et al (1970) suggest that the replacement of one learning environment by another is not ideal; it is better to offer two or more alternative learning environments and let the learner choose. It seems that most have elected to go all self-paced and the two alternatives are not offered. Cornell offers lecture or audio visual. It is interesting that the actual format of how the self-paced programs are run varies from school to school. Some still retain some lectures; some have lectures and tutorials; some have laboratories.

SUMMARY OF CHALLENGES

Three major challenges were voiced repeatedly:

- To provide sufficient drill so that problem-solving, and doing a mass and/or energy balance are second nature. The challenge is to get the students to appreciate the complexity of the problem yet keep each step simple so that they learn it readily. To further complicate matters there is a wide variation in our student's ability with this set of knowledge; perhaps wider than that in other courses. For some students, this is very easy; for others, it is extremely difficult.

- To motivate the students. This is related to the first challenge. However, we need the students to participate sincerely in the discussions, tutorials, in the self-paced programs. The students should be so interested that they are willing to extend themselves. The students want to be turned on. They seek relevancy.
- To develop self confidence maturity and professional attitudes.

Other challenges that can be specific to a particular school include:

- The preparation of new learning environments to better suit the needs of the students and the course objectives.
- The challenge of integrating, selecting and pacing the material: graphical, analytical and computer techniques; problem solving, properties, and conservation concepts; teach as separate course or integrate throughout the program.
- Finding good problems and cases.
- Having enough time available.

IDEAS FOR THE FUTURE

Besides the challenges listed in the preceding section some observations and ideas about the future concern the following topics:

- **Unit Systems.** There has been a lot of discussion about metrification (see for example Kroner (1972)). Only a few schools seem to have started to include the SI system. What should we be doing in view of the decision to adopt metric units in the near future?

- **Everyone discusses problem solving and developing a problem solving ability.** Yet the actual generalized strategy for problem-solving or even the strategy specific to solving mass and energy balances is not described clearly enough. One idea is to use Polya's generalized "four step" strategy of Define, Plan, Carry out the Plan, Look Back. Within this framework the substeps that offer a unique challenge to a specific type of problem could be discussed. This has been done for design and for plant improvement (see Figs. 4.3 and 4.4 in Crowe et al (1971) p. 76). A start on this for solving mass and energy problems is given in Table 3. Would it be profitable for us to spend more time elucidating the actual strategy for solving problems since this is such a major component of our program?

- **Many professors emphasize open-ended problems that require students to locate information for themselves.** Some have this as a part of their course now, or as part of other courses in the program. What emphasis should be placed on searching the literature in the Mass and Energy Balance course? Should we define a strategy for searching the literature? A suggested strategy is given in Table 4.

- **Engineers need to know something about cost estimation and the financial aspects of an enterprise.** Some introduce this as part of the course. Should we introduce more or is it too early in the program?

- **We believe it is important to develop a professional attitude.** How do we go about "teaching" it? What components of it should the students experience in the Mass and Energy Balance course?

- **There is a need to define the criteria used by engineers to make decisions.** These include technical feasibility,

TABLE 3: Generalized Strategy for Problem Solving

General	Specific to Mass & Energy Bal.
DEFINE:	
Identify need: accuracy & time available	
Specify criteria: technical, economic, financial, resources, social market ability, environment	
Identify system:	Draw a neat flow diagram. Identify boundaries or envelope. Classify type of operation (reaction-non-reaction; steady-state or transient; recycle?)
Identify system parameters:	Choose a basis, write stoichiometry. Identify unknowns, degrees of freedom Identify fundamental constraints
Collect information:	Cite source
PLAN:	
Develop models & set up equations	Identify subproblems, clearly state assumptions, Identify tie elements.
Decide on Solution Strategy	Use Method of Successive Approximation or not?
Select Mathematical Technique	
CARRY OUT:	
LOOK BACK:	
Check reasonableness Reiterate if necessary Communicate results	
DISCUSSION:	
Polya (1945) Thatcher (1962) Chapt 3 p. 57 to 68 Whitwell & Toner (1969) 38 p. 101 to 153 Andersen and Wenzel (1961) p. 174	Henley & Bieber (1959 Chpt. 3 p. 11 to 15 Tyner (1960) p. 3 Himmelblau (1967) p. 33 to 34 & thruout

economic, financial, environmental, socially accepted feasibility. How much of this should be in this course?

- **The students should have some appreciation of processing equipment, how it works and what it looks like.** Rudd, Powers and Sirola (1972) handle this primarily via a glossary. Myers and Sieder (1972) discuss key equipment needed for the flow diagrams and processes they discuss in their book. Some use plant tours, others use experimental labs. Perhaps it would be worthwhile to discuss the importance and alternative approaches that could be used to discuss this.

- **There seem to be relatively few movie films available for this course.** Are the ones available useful? Should more be developed?

- **Finally, some are interested in learning more about good case studies.** Some are using them now, some are de-

scribed elsewhere (Walker and Delgass (1972)). Should we publish, like the AIChE case problems, a list and evaluation of cases useful for Mass and Energy Balances at the freshman-sophomore level?

SUMMARY

The content, learning environments, and student characteristics reported for a course "Introduction to Mass and Energy Balances" have been reviewed. The content centers around problem-solving and the conservation concepts with an introduction of the appropriate material on units and the properties of matter. The major learning activity is problem-solving as homework with lecturing being the primary learning environment. The students are not used to poorly defined problems or the use of order-of-magnitude calculations. They are searching for relevancy, especially in view of the image the chemical industry has concerning pollution and employment.

In general, a lot of exciting innovations are

TABLE 4: Generalized Strategy for Searching the Literature

General	Specific to Searching the Lit.
DEFINE:	
Identify need: accuracy & time available	clear statement of information needed
Specify criteria:	purpose, reader
Identify system:	where information sought fits in information resources available
Identify system parameters:	check in encyclopedias, dictionaries, thesauri for good definitions, for synonyms generate search statement.
PLAN:	
Decide on Solution Strategy:	successive approximation?
Develop search strategy	Identify "most" likely source of information (article, book, patent? person?) Select resources that will help locate source. Search by subject? by author.
CARRY OUT:	
LOOK BACK:	
Check reasonableness Iterate if necessary Communicate results	
DISCUSSION:	
Woods, Stone and Black (1969) Woods (1970)	

being tried: innovations in content, in motivation and in learning environment. The interesting trends in content are shifts toward case studies, design, problem solving and mathematics-systems. The challenge in motivating the students is met by careful choice of examples and pacing. The choice of learning environment is extremely important. Many are using self-paced environments. Some points for discussion are enumerated. □

Acknowledgement

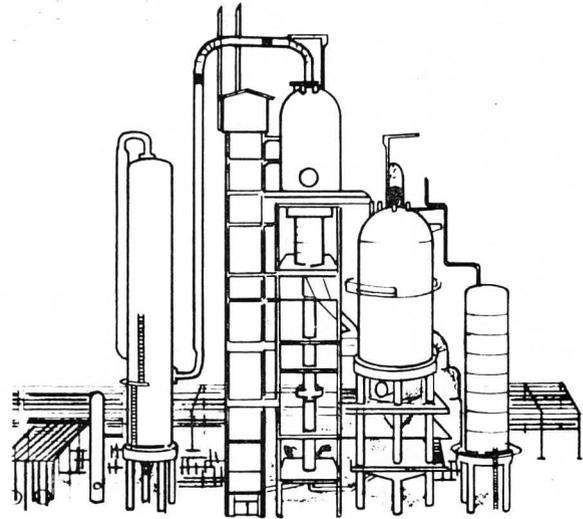
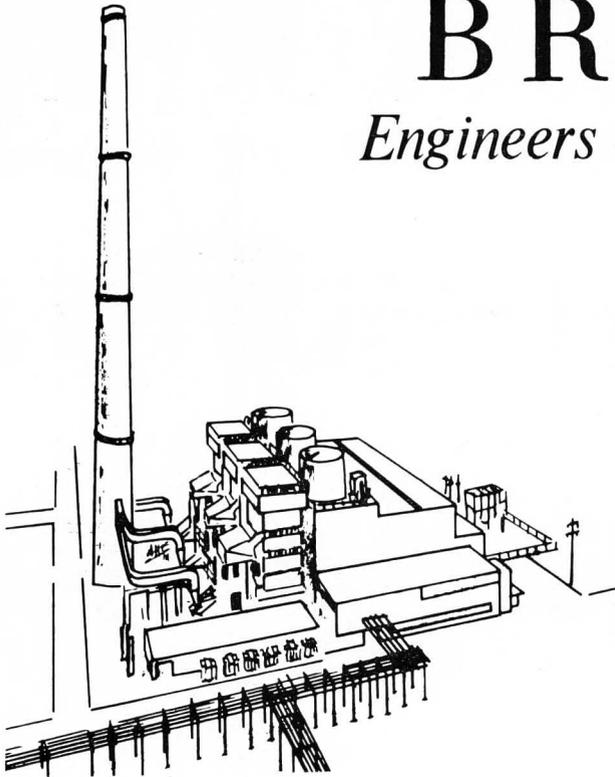
This article is a condensation of the original survey. More details can be obtained from D. R. Woods. This survey was made possible by the financial support of the Department of Chemical Engineering, McMaster University, Hamilton, Canada. We appreciate the assistance of Ms. Susan Anderson, Sheelagh Swords Courtney and Charlotte Traplin of that Department for their help in collecting and collating the information.

REFERENCES

- Anderson, L.B. and Wenzel, L.A. (1961) "Introduction to Chemical Engineering" McGraw-Hill, New York.
- Balzhiser, R., Samuels, and Eliassen, J.D. (1971), "Chemical Engineering Thermodynamics", Prentice-Hall.
- Bloom, B., et al (1954) "Taxonomy of Educational Objectives: Cognitive Domain", David McKay, New York.
- Blum, J.J., (1971), "Introduction to Analog Computation", Harcourt-Brace, Jovanovich Inc.
- Bodman, S.W., (1968) "The Industrial Practice of Chemical Process Engineering" The MIT Press.
- Brian, P.T.L. (1972) "Staged Cascades in Chemical Engineering", Prentice-Hall.
- Crowe, C.M. et al (1971) "Chemical Plant Simulation", Prentice-Hall.
- Denbigh, K.G. (1971) "The Principles of Chemical Equilibrium" 3rd ed. Cambridge, Cambridge.
- Dorf, R.C. (1969) "Matrix Algebra: A Programmed Introduction", Wiley.
- Henley, E.J. and Bieber, H. (1959) "Chemical Engineering Calculations: Mass and Energy Balances" McGraw-Hill, New York.
- Henley, E.J. and Rosen, E.M. (1969) "Material and Energy Balance Computations", Wiley, New York.
- Henley, E.J. and Staffin, H.K. (1963) "Stagewise Process Design", Wiley, New York.
- Himmelblau, D.M. (1967) "Basic Principles and Calculations in Chemical Engineering". 2nd ed. Prentice-Hall, Englewood Cliffs, New Jersey.
- Hougen, O.A., Watson, K.M. and R.A. Ragatz (1954) "Chemical Process Principles. Part I Material and Energy Balances" second edition, Wiley, New York.
- King, C. Judson (1971) "Separation Processes", McGraw-Hill and series of case studies in design and simulation, available from Dr. King, Dept. of Chemical Engineering, Univ. of California at Berkeley, Berkeley.
- Krathwohl, D., et al (1964). "Taxonomy of Educational Objectives: Affective Domain". David McKay, New York.
- Kroner, K.E. (1972). "Metrification—our Responsibility?". Engng. Education 63 1 p. 53.
- MacKenzie, Norman, Eraut, Michael and Jones, H.C. (1970). "Teaching and Learning: An introduction to new methods and resources in higher education". UNESCO and the International Association of Universities.
- Meissner, H.P. (1971) "Processes and Systems in Industrial Chemistry", Prentice-Hall.
- Myers, A.L. and Seider, W.D. (1972) "Chemical Process Logic", Univ. of Pennsylvania, Philadelphia, Penn.
- Polya, G. (1945) "How to Solve It", Princeton Univ. Press, Princeton, N.J.
- Ranz, W.E. (1970) "Describing Chemical Engineering Systems", McGraw-Hill.
- Rudd, D.F., Powers, G.J. and Sirola, J.J. (1972) "Process Synthesis", Prentice-Hall.
- Russell, F. and Denn, M. (1972) "Introduction to Chemical Engineering Analysis", Wiley, New York.
- Schmidt, A.X. and List, H.L. (1962) "Material and Energy Balances", Prentice-Hall.
- Seagrave, R.C. (1971) "Biomedical Applications of Heat and Mass Transfer", The Iowa State Univ. Press, Ames. Journal 50010.
- Sherwood, T.K. (1963) "A Course in Process Design", The MIT Press, Cambridge.
- Shreve, R.N. (1967) "Chemical Process Industries", 3rd ed. McGraw-Hill.
- Smith, Buford D. (1967 ff) Series of case studies in process design—simulation available from Dr. Smith, Dept. of Chemical Engineering, Washington Univ., St. Louis, Missouri.
- Smith, J.M. and van Ness, H.C. (1959) "Introduction to Chemical Engineering Thermodynamics", McGraw-Hill.
- Sonntag, R.E. and van Wylen, G.M. (1971) "Introduction to Thermodynamics: classic and statistical", Wiley.
- Stephenson, R.M. (1966) "Introduction to the Chemical Process Industries", Reinhold.
- Thatcher, C.M. (1962) "Fundamentals of Chemical Engineering", C.E. Merrill Books, Columbus, Ohio.
- Tyner, Mack (1960) "Process Engineering Calculations", The Ronald Press.
- Wales, C.E. (1970) "Programmed Thermodynamics", McGraw-Hill.
- Wendland, R.T. (1971) "Petrochemicals—the New World of Synthetics", Doubleday.
- Whitwell, J.C. and Toner, R.K. (1969) "Conservation of Mass and Energy", McGraw-Hill.
- Williams, E.T. and Johnson, R.C. (1971) "Stoichiometry for Chemical Engineers", McGraw-Hill.
- Woods, D.R., Stone, E. and Black, S.M. (1969) "Resources for Searching the Literature with examples in the field of Business-Economics". Chem. Eng. Dept., McMaster Univ., Hamilton, Canada.
- Woods, D.R., (1970) "Resources and Mechanics of Searching the Literature with examples for the Chemical Engineer" Chem. Eng. Dept., McMaster Univ., Hamilton, Canada.
- Walker, C.A. and Delgass, W.N. (1972) Chem. Eng. Ed. 6 No. 3 p. 124.

BRAUN

Engineers - Constructors



engineering for more energy requires new ideas - YOURS

With a background of 65 years of engineering for the process industries, C F Braun & Co occupies a unique ground-floor position in three of the newer energy fields — coal gasification, oil shale processing, and nuclear fuels. Our nuclear projects include plants for fuel fabrication, fuel reprocessing, and power generation. We are also engineering and will construct plants to convert coal and oil shale to clean commercial fuels.

You, as an engineer, recognize that your future job security and shortest route to promotion lie in areas of new industrial technology. You want individual recognition for your ideas. You want to be involved with new concepts. You want to work in a congenial

atmosphere with senior engineers who can help you advance rapidly in your career. You want to work in a company that provides the ideal environment for your professional growth. All of these, you will find at Braun.

The rapid growth of our engineering and construction work for the energy-conversion industries has opened many career positions in our Engineering Headquarters at Alhambra, California and in our Eastern Engineering Center at Murray Hill, New Jersey. For more information, please write to C F Braun & Co, Department K, Alhambra, California 91802 or Murray Hill, New Jersey 07974.



The following article introduces a new feature series by Chemical Engineering Education in cooperation with the CACHE (Computer Aides for Chemical Engineering Education) Committee. Proven computer-based homework problems suitable for undergraduate or first year graduate chemical engineering courses will be published on a regular basis.

The current problem, together with listings and documentation, is too long for full publication so the following article presents the problem and outlines the computer program developed to solve it. Complete documentation of the problem and program may be obtained for the cost of reproduction by writing the problem author.

Problems submitted for publication should be documented according to the published "Standards for CACHE Computer Programs" (September 1971). That document is available now through the CACHE representative in your department or from the CACHE Computer Problems Editor. Because of space limitations, problems should normally be limited to twelve pages total; either typed double-space pages or actual computer listings. A problem exceeding this limit will be considered. For such a problem

the article will have to be extracted from the complete problem description. The exact procedure to distribute the total documentation is evolving and may involve distribution at the cost of reproduction by the author, as we are doing with the current problem.

Before a problem is accepted for publication it will pass through the following review steps

- 1) selection from among all contributions an interesting problem by the CACHE Computer Problem Advisory Board
- 2) documentation review (with revisions if necessary) to guarantee adherence to the "Standards for CACHE Computer Programs".
- 3) program testing by running it on a minimum of three different computer systems.

It is hoped these problems will indeed be an aid in teaching computing and engineering to our students.

A. W. Westerberg
CCP Editor
U. of Florida
Gainesville, Fla. 32611

Non-Isothermal Tubular Reactor Program

R. S. KIRK

*University of Massachusetts
Amherst, Mass. 01002*

THIS COMPUTER PROGRAM is a numerical integration procedure for solving complex plug-flow reactor problems. The program will handle up to ten simultaneous reactions and ten different chemical compounds. The program is designed to handle a constant heat flux per unit area, but by proper choice of input data, isothermal or adiabatic (zero heat input) cases may be treated. With minor modification, the program has been used to calculate the heat flux, based on radiant heat transfer to the tubes with an internal film coefficient evaluated by the Dittus-Boelter equation.

The specific problem considered here is problem number 29, page 899, *Chemical Process Principles, Vol. III*, O. A. Hougen and K. M. Watson, John Wiley and Sons, Inc., New York, 1947. The discussion of the program refers specifically to this problem.

PROBLEM STATEMENT

IT IS DESIRED TO DESIGN a tubular heater and reactor for the pyrolysis of propane to produce a mixture of ethylene and propylene. Substantially pure propane is to be charged through a preheater which delivers it at a

temperature of 600°F and an absolute pressure not in excess of 60 lb per sq. in. to the inlet of the reactor-heater. In order to avoid secondary and reverse reactions the absolute pressure at the outlet of the reactor is maintained at 20 lb per sq in. The gases from the reactor are compressed and fractionated to recover the desired products and substantially pure propane which is recycled to the heater and reactor. The design is to be based on a total propane feed to the reactor of 7000 lb per hr and a conversion per pass of 80 per cent, corresponding to a net fresh charge of 5600 lb per hr.

A trial design is to be prepared on the basis of passing the entire heater and reactor charge in a single stream through a series of uniformly sized tubes each 30 feet long and connected together with 180° return bends. Each return bend has a volume equal to $3.1d^3$ where d is the inside diameter of the tube. The equivalent length of a return bend is 60 diameters of straight pipe, and the heated length of each tube is 28.0 feet. Tubes are available with inside diameters varying by $\frac{1}{2}$ -in. increments from 1 in. Since the maximum operating temperature permitted by the tube material is 1400°F, the heater will be designed to raise the charge to this temperature with a uniform heat input rate of 8000 Btu/(hr)(sq ft) based on the actually heated internal tube area. In order to obtain favorable heat-transfer conditions the tube diameter should be as small as possible without exceeding the allowable inlet pressure. In the

reactor section a constant temperature of 1400°F will be maintained by varying the heat-input rate.

It is required to determine the diameter and numbers of tubes for the specified service and also the temperature, pressure, conversion, product distribution, and heat-input-rate distribution curves throughout the heater and reactor, using the following kinetic data.

REACTION RATE DATA

r = rate of reaction, lb mole/(cu. ft.) (hr)

π = total pressure, atm.

$k = A \exp(-E/RT)$

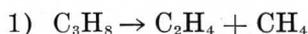
E = Cal./g-mole

T = temperature, °K

N = mole fraction

$K = \exp(-\Delta H^\circ/RT + \Delta S^\circ/R)$

Reaction



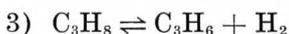
$$r = k\pi N_{C_3H_8} \quad \text{lb moles } C_3H_8$$

$$A = 3.0158 \times 10^{14}; E = 66500.$$



$$r = k\pi N_{C_3H_8} \quad \text{lb moles } C_3H_8$$

$$A = 3.6745 \times 10^{13}; E = 65000.$$



$$r = k\pi [N_{C_3H_8} - (N_{C_3H_6})(N_{H_2}) (\pi/K)]$$

$$A = 9.989 \times 10^{12}; E = 60000.$$

$$\Delta H^\circ = 30505.; \quad \Delta S^\circ = 32.85$$

(the values for ΔH° and ΔS° are at 1300°F; it may be assumed K does not vary with temperature)



$$r = k\pi [N_{C_3H_8} - (N_{C_2H_6})(N_{C_4H_{10}})/K]$$

$$A = 2.490 \times 10^{10}; E = 54000.$$

$K = 1.30$ (substantially independent of temperature)

METHOD OF SOLUTION

The material balance across a differential increment of a tubular (plug-flow) reactor is:

$$F dX = r dV_r$$

where

F = feed rate, mass units/hr.

X = moles of reactants converted/
unit mass of feed

r = reaction rate, lb moles/(hr)
(cu. ft.)

V_r = reactor volume, cu. ft.

The rate of reaction is a function of temperature, pressure and composition which vary along the length of the reactor, and which are all inter-related. There are four competing reactions and thus composition is a function of the four reactions rates. Thus:

$$r = r(T, \pi, X)$$

$$T = T(X)$$

$$\pi = \pi(X, T, \pi)$$

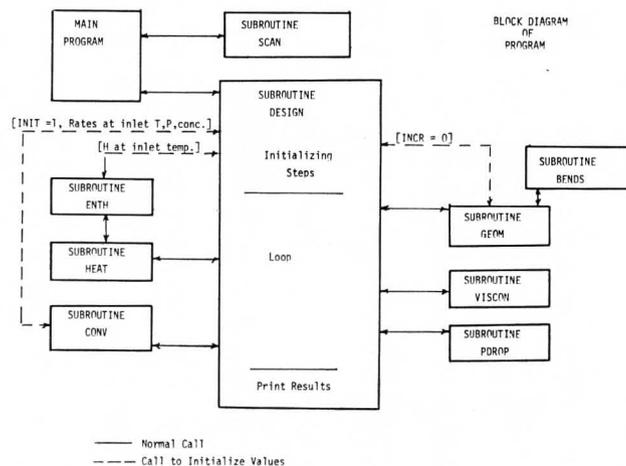
$$X = X(r)$$

Solution of this problem is a numerical integration of the four simultaneous material balance equations for the four reactions expressed in a difference form. The particular method of solution used in this program is based upon choosing a tube increment sufficiently small that the change in conversion can be calculated from the arithmetic average of the rates of reaction. That is:

$$\Delta X_i = \bar{r}_i \Delta V_r / F$$

where \bar{r}_i is the arithmetic average of the rates of reaction at the beginning and end of the increment for the i th reaction. Successive increments of volume ΔV_r are added until the total conversion, $\sum \Delta X$ of propane, reaches the desired level.

The detailed calculation procedure is described in the section *Subroutine DESIGN*.



Program Details

A discussion of each subroutine follows. Their inter-relationship is shown in the block diagram of the program. Subroutine DESIGN, the most important, is listed first, then the main program, and the other subroutines in alphabetical order.

Subroutine DESIGN

This subroutine is the executive subroutine,

providing the logic for the solution as well as initializing the variables and printing the results. Its operation is best described in tabular form. Reference is made to the various subroutines in the program. The letters A and B are affixed to each variable to designate respectively values at the beginning of an increment (known values, as TA) and values at the end of the increment (values to be calculated, as TB).

- 1) Convert feed data to lb. moles/hr and mole fraction
- 2) Initialize all variables for conditions at inlet to reactor
 - a) Establish heat transfer area, volume, and equivalent length for each tube increment and return bend (SUBROUTINES GEOM [INCR = 0] and BENDS).
 - b) Initialize enthalpy, HA (Subroutine ENTH)
 - c) Initialize rates of reaction, RA_i (Subroutine CONV [INIT = 1])
 - d) Set assumed conversions, $DDN_i = 0.0$
- 3) For each increment, establish area, volume and equivalent length. (SUBROUTINE GEOM [INCR])
- 4) Calculate heat input to increment and enthalpy at end of increment, HB. For assumed composition, calculate outlet temperature TB by Newton-Raphson secant procedure. (SUBROUTINES HEAT and ENTH). If exit temperature exceeds maximum value, TMAX, set $TB = TMAX$
- 5) Calculate viscosity of mixture at average temperature of increment (SUBROUTINE VISCON).
- 6) Calculate pressure drop across increment. (SUBROUTINE PDROP). If pressure falls below minimum set value; stop; print out results, and start over, using next size tube.
- 7) Calculate rates of reaction and conversion, DN_i for each reaction and compute changes in number of moles of each component. (SUBROUTINE CONV [INIT = 2])
- 8) Check if calculated conversions DN_i agree with assumed values, DDN_i within prescribed tolerance. If not, set $DDN_i = DN_i$, and repeat steps 3 through 8. If no convergent is obtained in 15 passes through loop (KRX), stop.
- 9) When satisfactory agreement between calculated and assigned conversions is obtained, proceed to next increment; store the results in array OUT if the end of a tube has been reached.

Calculate the changes in temperature, (e.g. $TDEL = TB - TA$), conversion, and composition of each component. Set the calculated values at end of this increment equal to the values at beginning of next increment. Set trial values of variables at end of next increment equal to values at beginning of increment plus changes in these variables occurring during this increment. For example:

$$\begin{aligned} (TA)_{n+1} &= (TB)_n \\ TDEL &= (TB)_n - (TA)_n; \\ \text{but if } (TB)_n &= (TA)_n, \text{ do not reset TDEL} \\ (TB)_{n+1} \text{ (trial)} &= (TA)_{n+1} + TDEL \end{aligned}$$

Return to Step 2 and proceed.

- 10) When conversion of key component (C_3H_8) reaches desired value, stop and print out results. Depending on input data, program will stop if a satisfactory solution is obtained, or will continue through a specified range of tube sizes.

The output array OUT has provision for 75 tubes; if more are needed, the program prints a warning and stops.

Main Program, REACT

The main program merely sets the logical unit numbers of the card reader (INP) and the printer (IOUT); then CALLs SCAN (to read in the data) and DESIGN (to perform the calculation).

Subroutine BENDS (FLBEND, VBEND, ABEND, DI)

This subroutine contains the constants for the return bends. For the specific problem listed, the following data is given:

Volume of return bend, $VBEND = 3.1 d_i^3$
 Equivalent length of straight pipe for pressure drop calculations, $FLBEND = 60 d_i$
 where d_i = internal diameter of tube, inches.
 $ABEND$ = heat transfer area of return bend.
 For specific problem given here, the return bends are not heated, thus $ABEND = 0$.

The constants in this subroutine must be changed by the user, if the return bends are heated, or if return bends with different volume and friction loss characteristics are used.

Subroutine CONV (PB, TB, VOL)

This subroutine calculates the rate of reaction, RB, for each reaction at the temperature TB, pressure PB, and assumed composition at the exit of the increment.

The conversion for each reaction is calculated from:

$$\begin{aligned} DN(K) &= 0.5 * (RA(K) + RB(K)) * VOL/FEED \\ DN(K) &= \text{conversion for the kth reaction, moles/mole feed} \\ RA(K) &= \text{rate at entrance of increment} \\ RB(K) &= \text{rate at exit if increment as calculated above} \\ VOL &= \text{volume of increment, cu. ft.} \\ FEED &= \text{feed rate, lb. moles/hr.} \end{aligned}$$

The number of moles of each component is then determined from the overall material balances.

The rate equations and material balances listed in this subroutine are for the four reactions given in the specific problem statement. For other problems, this subroutine must be rewritten.

Subroutine ENTH(HTOTAL, TEMP)

This subroutine calculates the enthalpy of the

reaction mixture at a temperature = TEMP (°R). Enthalpies are defined with respect to the elements at a base temperature of 77°F. Thus:

$$(H_i)_{77}^T = (\Delta H_{fi})_{77} + H_o^T - H_o^{77}$$

and $HTOTAL = \sum (XX_i) (WTMOL_i) (H_i)_{77}^T$,
Btu/lb. mole mixture

where: $(H_i)_{77}^T$ = enthalpy of component i at temperature T, above 77°F,
Btu/lb.

$(\Delta H_{fi})_{77}$ = heat of formation at 77°F,
Btu/lb.

H_o^T = enthalpy of component i at temperature T with respect to liquid at -200°F.

H_o^{77} = enthalpy of component i at 77°F with respect to liquid at -200°F.

XX_i = mole fraction of component

$WTMOL_i$ = molecular weight of component i

The total enthalpy change across the increment is:

$$\Delta H = (BMOLS * HB - AMOLS * HA) * FEED$$

where BMOLS and AMOLS are total moles/mole of feed.

Thus ΔH , as defined here, includes the heat of reaction as a function of temperature.

The peculiar set of base temperatures in the first equation is necessary to use the data in the *API Technical Data Book*—gaseous enthalpies based on liquid at -200°F and heats of formation at 77°F. The API book gives the following equation for H_o^T :

$$H_o^T = A(T/100) + B(T/100)^2 + C(T/100)^3 + D(100/T) + E$$

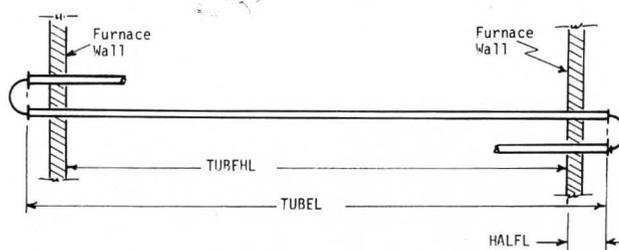
where A, B, C, D, E are constants for each component, Btu/lb., T = °R.

Any set of data may be used, as long as the enthalpies are referred to the elements. *The API Technical Data Book* provides a convenient set of data for an enthalpy equation, rather than a heat capacity equation.

Subroutine GEOM (INCR)

The initial call to GEOM [INCR = 0] triggers a call to BENDS to set the area, volume and length parameters for the return bends. Thereafter, this subroutine assigns to each specific increment the proper values of heat transfer area, volume, and equivalent length of straight pipe for pressure drop calculation.

The complexities of the subroutine are required to handle the case of furnace tubes whose ends and return bends are not heated and to allow the use of various sizes of increments in the integration. A diagram of the furnace is below:



The program identifies three different increments:

- 1) The normal increment—the entire portion of the increment is heated (if three or more increments per tube are used).
- 2) Cold increments—the increment at the beginning and end of each tube. The cold increments may include some heat transfer area if the increment size is greater than HALFL.
- 3) The return bends—in this problem the bends are cold and so ABEND (Subroutine BENDS) is set to zero. If the return bends are heated, ABEND should be set equal to the external surface area of the bend. Note that regardless of the number of increments used per tube, the return bend is treated separately.

For a furnace in which the whole tube is heated, the input data values of TUBEL and TUBEHL (see SCAN) should be identical.

Subroutine HEAT (HA, HB, TA, TB)

The enthalpy balance and exit temperature are calculated in this subroutine. The exit enthalpy is calculated by:

$$Q = FLUX * AREAX$$

$$HBD = (FEED * AMOLS * HA + Q) / (FEED * BMOLS)$$

Where

- Q = heat added, Btu/hr
 FLUX = specified flux
 AREAX = heat transfer area of increment (as set in GEOM)
 AMOLS = total moles entering/mole feed
 BMOLS = ditto for exit
 HA = enthalpy at beginning of increment, at temperature TA, Btu/lb mo'e of mixture
 HBRD = ditto at exit temperature TB; double precision
 FEED = feed rate, lb moles/hr.

The exit temperature TB is then calculated by a Newton-Raphson secant iteration based on TA

(Continued on page 102.)

APPLICATION OF PERTURBATION TECHNIQUES TO ANALOG COMPUTATIONS

JOSEPH F. PAUL
*California State University
Northridge, California 91324*

The object of this study is to investigate the use of perturbation techniques for determining the effect of small changes in parameters on the response of a system. Perturbation techniques have been applied to analog computation for many years (see references). However, an attempt will be made here to present a comprehensive tutorial development of the theory and then illustrate its use by applying it to a particular problem. The problem is studied in detail by first developing the perturbation equations and solving them on the analog computer, and then making an error analysis by solving the equations on the digital computer. A summary of the results is given at the end.

PERTURBATION EQUATIONS

THERE ARE TWO METHODS for developing the perturbation equations, both of which yield the same result. They are called the incremental method and the Taylor series expansion. The second method is considered here. If we expand the function $Z=f(x,y)$ in a Taylor series and neglect terms of second order and higher, we obtain:

$$f(x_0 + \Delta x, y_0 + \Delta y) = f(x_0, y_0) + \frac{\partial f}{\partial x} \Big|_{x_0, y_0} \Delta x + \frac{\partial f}{\partial y} \Big|_{x_0, y_0} \Delta y \quad (1)$$

For a particular example let $Z=XY$. Note that for this case:

$$\frac{\partial Z}{\partial X} \Big|_{x_0, y_0} = y_0; \quad \frac{\partial Z}{\partial Y} \Big|_{x_0, y_0} = x_0 \quad (2, 3)$$

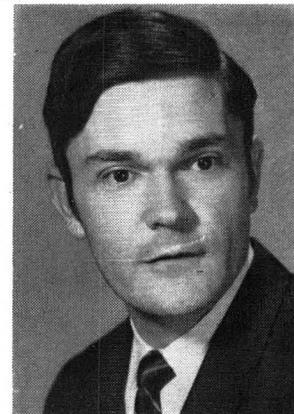
therefore:

$$z_0 + \Delta z = x_0 y_0 + y_0 \Delta x + x_0 \Delta y \quad (4)$$

where the error would be the sum of the higher order terms. Breaking equation (4) into two parts

$$z_0 = x_0 y_0; \quad \Delta z = y_0 \Delta x + x_0 \Delta y \quad (5, 6)$$

This is the same result which can be obtained by the incremental method.



Joseph F. Paul received his BS and MS degrees in ChE from Washington University and has obtained advanced study at University of Southern California. He formerly was employed by Electronic Associates, Inc., TRW Computer Co., and Monsanto Chemical Co. His areas of interest include applied mathematics, computer science, and process control.

INVESTIGATION

AN INVESTIGATION WAS MADE on a particular system which is described below. The object was to determine the response of the system to small changes in one of the parameters using perturbation techniques. First of all the perturbation equation was developed for the system using the incremental method. A study was then made using both the analog and digital computers.

For the first phase of the study both the nominal and perturbation equations were mechanized for the analog computer. A total of five runs were made utilizing increments of 1%, 2%, 3%, 4%, and 5% in the system parameter which was the mass flow rate of fluid in the system. Both the nominal and perturbed values of temperature were recorded on the X-Y plotter.

For the second phase, the system equations were programmed in Hytran Simulation Language, (HSL). This is a digital simulation language which permits the direct programming of

dynamic systems in block diagram format. The integration scheme employed was fourth order Runge-Kutta. First the nominal equation was solved to give the steady state temperature, and then the incremental temperature was obtained by solving the perturbation equation and also by perturbing the original equation and subtracting the nominal value from it. This last value was taken to be correct since it was computed from the original equation to eight significant figures, and compared to that obtained from the perturbation equation. The percent error was computed and compared to that predicted by evaluating the error term in the perturbation equation. These results are summarized later in a table.

PERTURBATION PROBLEM

A jacketed tank with constant level control is being heated by steam. How long will it take to reach its steady state temperature and what will it be? What is the effect of a small change in flow rate from the prescribed flow rate?

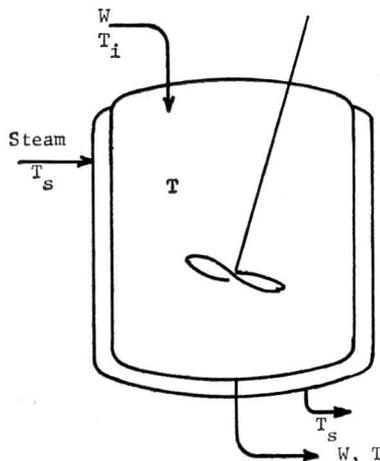


Figure 1

- A = area for heat transfer, ft²
- V = volume, ft³
- U = heat transfer coefficient, Btu/hr-F^o-ft²
- ρ = density in lbs/ft³
- C_p = specific heat in Btu/F^o-lb
- T_p = temperature of contents of vessel, F^o
- W = mass flow rate in lb/hr
- T_i = inlet temperature, F^o
- T_s = steam temperature, F^o

The overall equation of the process is

$$\frac{dT}{dt} = \left(\frac{UA}{\rho C_p V} \right) (T_s - T) - \left(\frac{W}{\rho V} \right) (T - T_i) \quad (7)$$

The flow rate W is perturbed such that $W = W_0$

+ ΔW and as a result, T changes by ΔT, i.e., $T = T_0 + \Delta T$ and

$$\frac{d(T_0 + \Delta T)}{dt} = \left(\frac{UA}{\rho C_p V} \right) (T_s - T_0 - \Delta T) - \left(\frac{W_0 + \Delta W}{\rho V} \right) (T_0 + \Delta T - T_i) \quad (8)$$

$$\frac{dT_0}{dt} + \frac{d\Delta T}{dt} = K_1 (T_s - T_0) - K_1 \Delta T - \frac{W_0 T_0 - W_0 T_i}{K_2} - \frac{W_0 \Delta T + \Delta W T_0}{K_2} + \frac{\Delta W T_i}{K_2} \quad (9)$$

where: $U = 150 \text{ Btu/F-hr-ft}^2$; $A = 7.5 \text{ ft}^2$; $\rho = 80 \text{ lb/ft}^3$;
 $C_p = 0.8 \text{ Btu/F-lb}$; $V = 100 \text{ ft}^3$; $K_1 = \frac{UA}{\rho C_p V} = 0.176 \text{ hr}^{-1}$;
 $K_2 = \rho V = 8,000 \text{ lb}$

Equation (9) can be thought of as the sum of the nominal values and the incremental values. It can be separated into two equations:

$$\frac{dT_0}{dt} = K_1 (T_s - T_0) - \frac{(W_0 T_0 - W_0 T_i)}{K_2} \quad (10)$$

$$\frac{d\Delta T}{dt} = -K_1 \Delta T - \frac{(W_0 \Delta T + \Delta W T_0)}{K_2} + \frac{\Delta W T_i}{K_2} \quad (11)$$

The same equations can be derived by the Taylor series expansion.

$$F = \frac{dT}{dt} = \left(\frac{UA}{\rho C_p V} \right) (T_s - T) - \frac{W}{\rho V} (T - T_i) \quad (12)$$

$$\left. \frac{\partial F}{\partial W} \right|_{T_0, W_0} = - \left(\frac{T_0 - T_i}{\rho V} \right); \quad \left. \frac{\partial F}{\partial T} \right|_{T_0, W_0} = - \frac{UA}{\rho C_p V} - \frac{W_0}{\rho V} \quad (13, 14)$$

The nominal equation becomes:

$$\frac{dT_0}{dt} = \left(\frac{UA}{\rho C_p V} \right) (T_s - T_0) - \frac{W_0}{\rho V} (T_0 - T_i) \quad (15)$$

and the incremental equation becomes:

$$\frac{d\Delta T}{dt} = - \left(\frac{T_0 - T_i}{\rho V} \right) \Delta W - \left(\frac{UA}{\rho C_p V} + \frac{W_0}{\rho V} \right) \Delta T \quad (16)$$

These equations agree exactly with equations (10) and (11) and thus verify the equivalency of the two methods.

TABLE 1. SCALED VARIABLES

VARIABLE	MAX	SCALE FACTOR	SCALED VARIABLE
T ₀	250	1/250	T ₀ /250
T _s	250	1/250	T _s /250
(T _s - T ₀)	250	1/250	(T _s - T ₀)/250
T _i	100	1/100	T _i /100
(T ₀ - T _i)	100	1/100	(T ₀ - T _i)/100
ΔT	1	1	ΔT

NOTE THAT ΔT IS SCALED TO A MAXIMUM OF ONE. ALTHOUGH THERE IS A FIVE PER CENT CHANGE IN THE PARAMETER ΔW, THERE IS LESS THAN ONE DEGREE CHANGE IN TEMPERATURE. THE PARAMETER ΔW DOES NOT HAVE TO BE SCALED SINCE IT DOES NOT APPEAR AS THE OUTPUT OF AN AMPLIFIER.

SCALED EQUATIONS

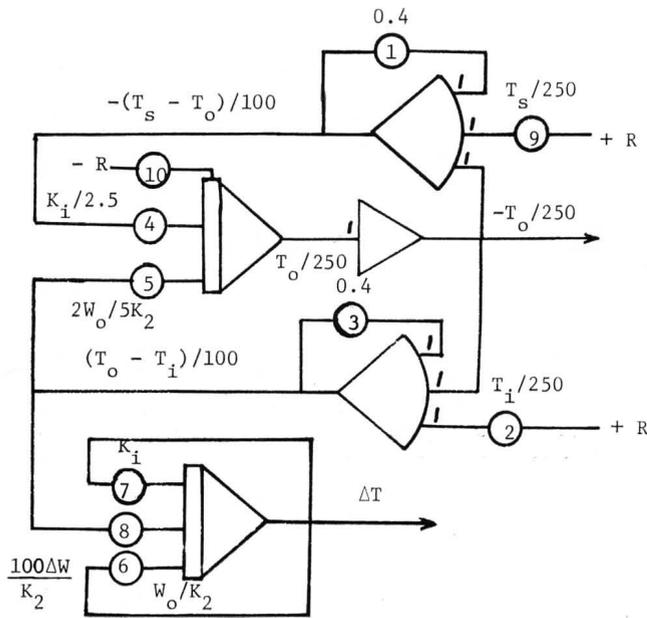
$$\frac{d\left(\frac{T_0}{250}\right)}{dt} = \frac{K_1}{2.5} \left(\frac{T_s}{100} - \frac{T_0}{100} \right) - \frac{W_0}{2.5K_2} \left(\frac{T_0}{100} - \frac{T_i}{100} \right) \quad (17)$$

$$\frac{d(\Delta T)}{dt} = -K_1 (\Delta T) - \frac{W_0}{K_2} (\Delta T) - \frac{100\Delta W}{K_2} \left(\frac{T_0 - T_i}{100} \right) \quad (18)$$

$$\left(\frac{T_s - T_0}{100}\right) = 2.5 \left(\frac{T_s}{250}\right) - 2.5 \left(\frac{T_0}{250}\right) \quad (19)$$

$$\left(\frac{T_0 - T_i}{100}\right) = 2.5 \left(\frac{T_0}{250}\right) - 2.5 \left(\frac{T_i}{250}\right) \quad (20)$$

Equations (17), (18), (19), and (20) are mechanized as depicted by Figure 2.



ANALOG DIAGRAM
Figure 2

In addition to the present problem, for an illustration of a non-linear set of equations let us put a valve on the inlet flow W still assuming an adequate level control at the outlet. Thus:

$$P_i - P_a = R_v W^2 = P_d \quad (21)$$

where P_i is upstream inlet pressure; P_a is atmospheric pressure; and R_v is resistance coefficient of the valve.

$$P_{do} + \Delta P_d = R_v (W_o + \Delta W)^2 = R_v W_o^2 + 2R_v W_o \Delta W \quad (22)$$

$$P_{do} = R_v W_o^2 \text{ or } W_o = \sqrt{\frac{P_{do}}{R_v}}$$

$$\Delta P_d = 2R_v W_o \Delta W \text{ or } \Delta W = \frac{\Delta P_d}{2R_v W_o}$$

$$W_o = 1000 \text{ lb/hr; } P_{do} = 15 \text{ psi; then } R_v = 15 \times 10^{-6}$$

$$\Delta W = \Delta P_d / (2 \times 15 \times 10^{-6} \times 1 \times 10^3) = \Delta P_d / 3 \times 10^{-2}$$

Thus the same configuration on the analog can be employed except that now the flow W_o and ΔW must be expressed in terms of P_{do} and ΔP_d .

The plot on the following page gives the results from the analog computer runs. It gives the steady

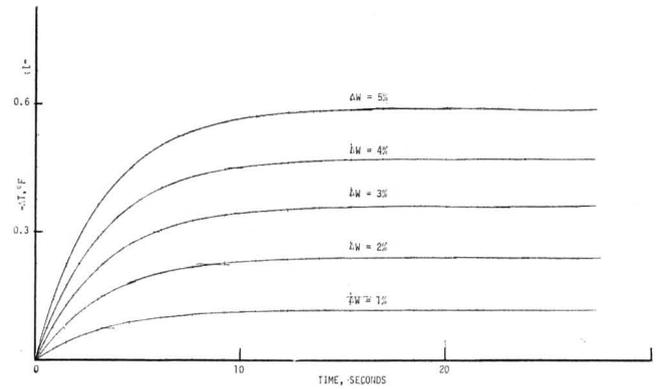


Figure 3
ANALOG SOLUTION OF PERTURBATION EQUATION

temperature T_o , plus the incremental change ΔT for five values of ΔW .

RESULTS

THE RESULTS OF THE ANALOG computer runs for ΔT for the five increments in ΔW agree with the digital computer runs. The data from the digital computer runs are tabulated in Table 4. The first column gives the percentage change in ΔW for each run. The second column gives the percent change in T resulting from the increment ΔW . The third column gives the predicted error in the perturbation equation found by evaluating the small term $\Delta W \Delta T/k_2$ which was dropped from the equation. The last column gives the measured error which was found by computing ΔT as the difference between the nominal value T_o and T which was calculated by perturbing the original equation and getting the result to eight significant figures, and comparing

TABLE 4

Comparison of Errors

ΔW	=	$\frac{\Delta T}{T \text{ max.}}$		
		ΔT max.	E pred.	E meas.
1%		.0528%	.125%	.429%
2%		.1056%	.25%	.818%
3%		.1585%	.375%	1.214%
4%		.2113%	.50%	1.616%
5%		.2641%	.625%	2.008%

this with the value of ΔT computed by the perturbation equation.

It can be seen that the measured error, although somewhat larger than predicted, is reasonably small for small perturbations. It can be con-

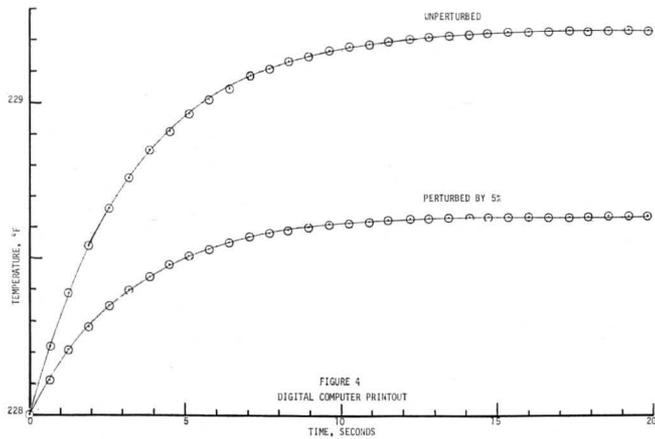


Figure 4
DIGITAL COMPUTER PRINTOUT

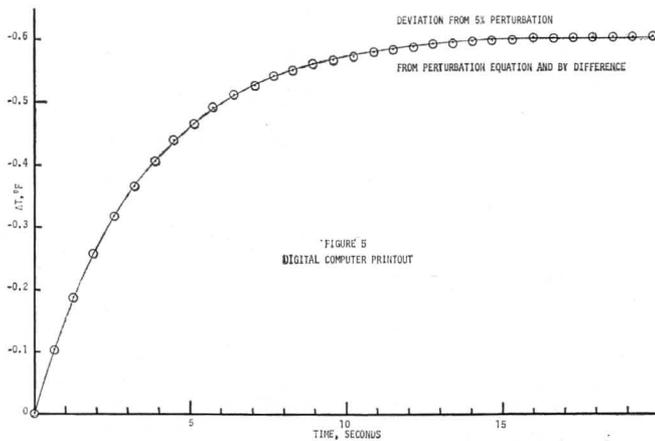


Figure 5
DIGITAL COMPUTER PRINTOUT

cluded then that using the perturbation equation on the analog computer will give much better results than perturbing the original equation and trying to take the difference of nearly equal numbers.

The problem with using conventional techniques, especially on the analog computer, is that the effect on the system response is slight and the isolating of the change by subtraction of nearly equal numbers can produce serious errors. By solving the perturbation equation directly, we can achieve a result which is scaled to the full range of the computer minimizing the error. □

REFERENCES

1. Levine, Leon: "Methods for Solving Engineering Problems", McGraw-Hill, New York 1964.
2. "8400 Hytran Simulation Language Programming

Manual", Electronic Associates, Inc. 1967.

3. Coughanowr, D. R., L.B. Koppel, "Process Systems Analysis and Control", McGraw-Hill Book Co., New York 1965.
4. Meissinger, Hans F., "The Use of Parameter Influence Coefficients in Computer Analysis of Dynamic Systems", presented at a Western Simulation Council meeting in 1960.
5. Bush and Orlando, "A Perturbation Technique for Analog Computers", Cornell Aeronautical Lab., Buffalo, N.Y., presented at the National Simulation Conference in Dallas on October 24, 1958.
6. McDonnel, J.A., IBM, "Simulation Using Perturbation Methods", Instruments and Control Systems, February 1964, pp. 127-8.
7. Luyben, William L., "Process Modeling, Simulation, and Control for Chemical Engineers", McGraw-Hill, New York 1973.
8. Dorf, Richard C.: "Modern Control Systems", 2nd Ed., Addison-Wesley, 1974.

TABLE 2

Pot#	Parameter	Value	Time Scaled
1	1/2.5	.4	.4
2	$T_i/250$.8	.8
3	1/2.5	.4	.4
4	$K_i/2.5$.0704	.704
5	$2W_o/5.K_2$.05	.50
6	W_o/K_2	.125	1.25
7	K_i	.176	1.76
8	$100 W/K_2$.125	1.25
9	$T_s/250$.9999	.9999

TABLE 3

CASE 2

1	1/2.5	SAME AS ABOVE
2	$T_i/250$	
3	1/2.5	
4	$K_i/2.5$	
5	$(2/5) \frac{\sqrt{P_{do/R_v}}}{K_2}$	
6	$\frac{\sqrt{P_{do/R_v}}}{K_2}$	
7	K_i	
8	$10 \frac{\Delta P_d}{R_v W_o K_2} = 10 \left(\frac{\Delta P_d}{K_2 \sqrt{P_{do/R_v}}} \right)$	
9	$T_s/250$	

AN INEXPENSIVE TIME BOMB

NOEL DE NEVERS

University of Utah

Salt Lake City, Utah 84112

PURPOSE

This experiment demonstrates:

1. Bernoulli's Equation
2. Unsteady-state flow
3. Flame velocity and flame stabilization
4. Mathematical model building.

APPARATUS

The apparatus consists of a can with a snug-fitting lid. One-gallon paint cans or 2-lb. coffee cans are ideal. The lid is loosely attached to the body of the can by a 6" length of 1/8" chain or strong flexible wire, which is soldered to both lid and body. The can has two holes in it. One hole about 1/4" O.D. is in the center of the lid, the other about 1/2" O.D. is on the side near the bottom. In addition the demonstrator needs a stopwatch, a book of matches, and a roll of masking tape.

DESCRIPTION OF DEMONSTRATION

Beforehand the demonstrator fills the can (lid in place) with natural gas. This is done by blowing gas from a gas jet in the bottom hole, while the can is in a hood. Two to three minutes will do. Then, before shutting off the gas, the demonstrator tapes over the lid hole with masking tape, then removes the can from the gas jet, and tapes over the bottom hole.

To begin the demonstration the demonstrator sets the can on a table, removes the bottom masking tape, then removes the tape over the lid hole and starts the stopwatch immediately. He then strikes a match and lights the gas issuing from the lid hole.

The flame burns brightly for a while, then dies down to the point where it is invisible in a well-lighted room. Finally the gas-air mixture in the



can explodes with a loud bang blowing off the lid and emitting a flash of blue flame. By watching his stopwatch the demonstrator (who knows in advance when this explosion will occur) can time his lecture to reach a dramatic point just when the explosion occurs.

THEORY

The theory is easier to discuss on the assumption that the hole in the bottom is very large. If it were large the pressure drop through it would be negligible. However, if the hole actually is large the resulting explosion is not as dramatic as if it is small.

We may apply the classical Bernoulli's equation across the hole in the top, with the well-known orifice velocity formula resulting

$$v = c \sqrt{2\Delta p / \rho_{\text{gas}}} \quad (1)$$

(See the table of nomenclature).

We will now consider the start of the experiment, when the can is full of natural gas. If the hole in the bottom is large, the gas pressure at the

bottom of the can is P_{atm} . The value of Δp is found by noting the pressure drop as one moves up in a column of gas and a column of air,

$$P_{air} = P_{atm} - \rho_{air} g \Delta Z \quad (2)$$

$$P_{gas} = P_{atm} - \rho_{gas} g \Delta Z \quad (3)$$

$$\Delta p = P_{gas} - P_{air} = g \Delta Z (\rho_{air} - \rho_{gas}). \quad (4)$$

Substituting this in equation 1 we obtain

$$v = c \sqrt{\frac{2g \Delta Z (\rho_{air} - \rho_{gas})}{\rho_{gas}}} \quad (5)$$

This is a steady-state solution, because the classical Bernoulli's equation is a steady-state equation. As shown in most fluid mechanics textbooks, this result is an excellent approximation of the instantaneous velocity for unsteady-state processes like the one here, in which the velocities are small compared with the speed of sound.

At this point we will introduce two models of the behavior of the gas, and determine the velocity-time curve for each. The experimental explosion time is bracketed by these calculated curves, as we would naturally expect.

Model 1—The diaphragm or plugflow model

Let us assume there is no mixing between inflowing air and the gas in the container. Since the gas is lighter than the air, it will always be above the air. We may imagine it separated from the air by a moving flexible diaphragm. If we now construct the ratio v/v_0 from equation (5), we get

$$\frac{v}{v_0} = \sqrt{\frac{\frac{\rho_{air}}{\rho_{gas}} - 1}{\frac{\rho_{air}}{\rho_{gas_0}} - 1} \frac{\Delta Z}{\Delta Z_0}} \quad (6)$$

However the values of gas density on the right cancel so,

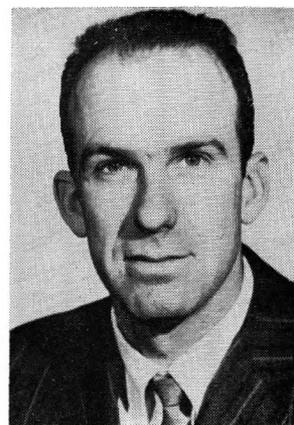
$$\frac{v}{v_0} = \sqrt{\frac{\Delta Z}{\Delta Z_0}} \quad (7)$$

Here ΔZ is the instantaneous value of the distance from diaphragm to lid hole and ΔZ_0 is the initial value.

If we square both sides and differentiate with respect to time we obtain

$$\frac{2v}{v_0^2} \frac{dv}{dt} = \frac{1}{\Delta Z_0} \frac{d(\Delta Z)}{dt} \quad (8)$$

Now we make a volume balance, ignoring the



Noel de Nevers earned his BSChE at Stanford and his PhD at the University of Michigan, with a year out in between to be a Fulbright exchange student at the Technical Institute in Karlsruhe, Germany. He spent five years with what is now Chervon Research and Chevron Oil-field Research, before joining the faculty of the University of Utah. He spent Academic 1971-72 on leave, working for the Office of Air Programs of the Environmental Protection Agency. He is the author of a textbook on Fluid Mechanics, and editor of a book of readings and discussions on Technology and Society.

minute compressibility effects of the gas, and obtain

$$d \left(\frac{\Delta Z}{dt} \right) = -v \frac{a_h}{a_c} \quad (9)$$

Substituting (9) in (8) and cancelling we obtain

$$\frac{dv}{dt} = - \frac{v_0^2 a_h}{\Delta Z_0 a_c} = \text{constant} \quad (10)$$

This may be readily integrated, and rearranged to obtain

$$\frac{v}{v_0} = - \frac{v_0 a_h t}{\Delta Z_0 a_c} \quad (11)$$

i.e., the velocity falls off linearly from its initial value to zero when one can-volume of gas has flowed out. This is plotted in Figure 1 for a 1-gallon paint can.

Model 2—The perfectly mixed model

Now let us assume that at any time the contents of the can are perfectly mixed. Returning to equation (6) we see that the only time-dependent quantity on the right-hand side of equation (6) is ρ_{gas} which increases steadily as gas flows out and air flows in. We may solve for it, as follows

$$\rho_{gas} = \frac{\text{mass of gas in container}}{\text{volume of container}} \quad (12)$$

$$\frac{d\rho_{gas}}{dt} = \frac{1}{V} (\text{mass flow rate in} - \text{mass flow rate out}) \quad (13)$$

$$= \frac{a_h v}{V} (\rho_{air} - \rho_{gas}) \quad (14)$$

OR

$$\frac{d\rho_{gas}}{(\rho_{air} - \rho_{gas})} = \frac{a_h v}{V} dt \quad (15)$$

integrating from time zero to time t

$$-\ln \left\{ \frac{(\rho_{air} - \rho_{gas})}{(\rho_{air} - \rho_{gas_0})} \right\} = \frac{a_h}{V} \int_{t=0}^t v dt = \frac{Q}{V} \quad (16)$$

here Q is the total volume of air which has flowed into the can. This is readily rearranged to

$$\rho_{gas} = \rho_{air} - (\rho_{air} - \rho_{gas_0}) \exp(-Q/V) \quad (17)$$

If we now substitute this in equation (6), cancel out the ΔZ 's, and rearrange, we obtain

$$\frac{v}{v_0} = \frac{\frac{\rho_{g_0}}{\rho_a} \exp(-Q/V)}{1 - (1 - \frac{\rho_{g_0}}{\rho_a}) \exp(-Q/V)} \quad (18)$$

This does not have an obvious analytical solution

for v as a function of t , but for a given value of $\frac{\rho_{g_0}}{\rho_a}$

one may easily prepare a plot of v/v_0 vs. Q/V , and solve for the v vs. t behavior numerically. Figure 1 shows such a plot for a 1-gallon paint can, together with the plot for Model 1. Note that the curves cross in the low-time region. This appears strange, but is consistent with the models chosen. In the early stages the mixed model should predict the more rapid decrease in velocity because, in equation (1) the density of the gas (which appears in the denominator) increases for the mixed model, but not for the diaphragm model. In the early stages, both models show a comparable decrease in Δp .

FLAME SPEED AND STABILIZATION

The previously discussed models allow us to predict how fast the gas is moving through the lid-hole for any instant of time. As discussed in texts on combustion (Ref. 1), in laminar flow of combustible gas and air, a flame propagates itself with a reproducible velocity. For methane-air, this is a function of composition, with a maximum value, for room-temperature gases of about 1.1 ft/sec.

As long as the velocity through the lid-hole is greater than the flame velocity, the flame burns above the can. When the two velocities are identi-

cal, the flame is exactly in the plane of the lid. When the velocity of the gas is slightly less than the flame velocity, the flame burns into the can, where the velocity of the gas is much less than in the lid hole, and an explosion (deflagration) results. In this way the lid-hole acts exactly as does the flame-stabilizer on a Fischer burner, or on a jet-engine combustor, or the small burner orifices on an ordinary gas stove.

If we assume that the flame velocity at the time of explosion is 1.1 ft/sec, then we can see the predicted time of explosion for each of the two above models. This is shown on Figure 1. The experimental results shown on Figure 1 indicate that the true behavior of the can is intermediate between those predicted by the two models, as common sense indicates it would be for these models.

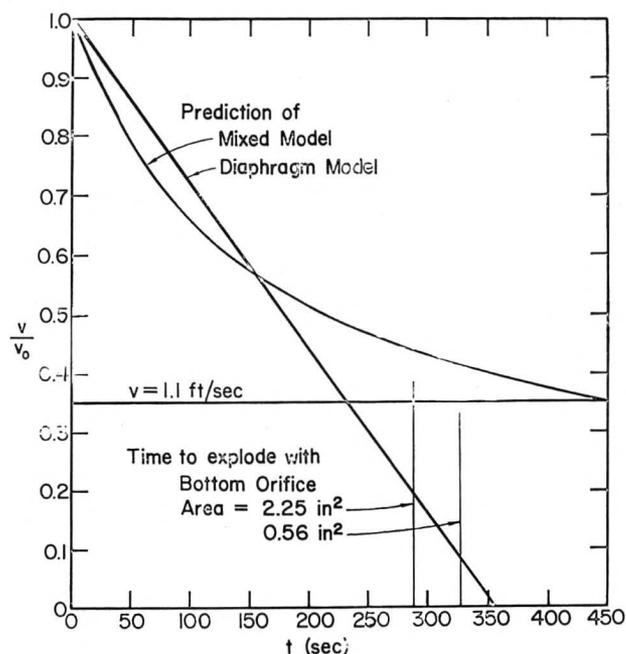


FIGURE 1

Calculated and Experimental Behavior of 1-Gallon Paint Can Bomb.
CAN DIMENSIONS

Diameter 6.75 in., Height 7.5 in., Lid hole 0.25 in.,
Assumed orifice coefficient $C = 0.6$, Assumed gas
MW = 17,
Calculated initial velocity $V_0 = 2.9$ ft/sec.

COMMENTS ON THE EXPERIMENT

1. The application of Bernoulli's equation is obvious. The teacher might note to the class that the flow here is quite analogous to the steady-state flow in chimneys, or for that matter to the steady-state flow in a room with a "radiator" at one side.

2. The mathematics shown should convince the students that unsteady-state flow is much more

ACKNOWLEDGMENT

The author learned this experiment from Fr. Pierre Jacobs, S. J. who used it purely for dramatic effect, at which he was very good.

difficult to analyze mathematically than steady-state flow. It might be offered as a general rule that an experiment which is easy to set up is generally hard to calculate, and vice-versa.

3. The two mathematical models chosen are the only two for which simple solutions are possible. This is typical of real engineering problems: by choosing limiting cases as mathematical models, one can bracket the observed behavior; but seldom is a real process simple enough to be accurately represented by such a model.

4. This demonstration can also be used for safety lectures. If we assume that the mixture which finally exploded was 10 mol % methane, then a gallon can contained about 0.3 gm of methane. Its destructive potential is made clear by the experiment. Annually in the United States several people kill themselves by taking cutting torches to "empty" oil drums. At the same mixture ratio, a 55-gallon drum would contain about 16 gm of methane (about 1/2 ounce). Normally these drums contain higher molecular weight vapors, but the quantity is such that they also pass for "empty", fatally.

A FEW PRACTICAL CONSIDERATIONS

1. This demonstration will not work outdoors, or in a very drafty room; the flame blows out.

2. Make the chain strong and keep your hands away when the can is about to explode. The can will jump up to one foot off the table, due to the kinetic energy of the lid.

3. Do not ever assume the flame is out because you cannot see it in a well-lighted room. In a darkened room you can always see it; the experiment is worth watching once in a darkened room.

4. The time to explode is a function of the size of the bottom hole. One can readily determine this function by making a large bottom hole and covering it with cardboard orifices held on my masking tape. If these cardboard orifices have various-size holes in them, one can make a plot of time to explode vs. hole area, and see that it asymptotically

approaches a value intermediate between that predicted by the two models as the area becomes large.

5. Top holes smaller than 1/8" do not work. They quench the flame, so that it cannot get through. This might be a good problem to go into in a graduate class. (See Ref. 1)

6. If the demonstrator wishes to use the timed explosion dramatically, he should time his can several times first. Reproducibility should be plus or minus 3 to 5 seconds in 3 to 10 minutes burning time. Reproducibility seems to be better for small bottom holes than large ones.

7. The author once tried to give this demonstration to a group of co-workers at the National Reactor Testing Station, Idaho Falls, Idaho. There he filled the can as described, removed the masking tapes, and applied a match. There was no flame. Another match failed to light a flame. After several minutes of head-scratching by the author and mild snickering by the audience, it occurred to the author to ask if the gas jets in the laboratory supplied natural gas. The answer was that they supplied propane. Thereupon the author applied a match to the bottom hole, producing a large flame. The can burned for 1/2 hour, and then went out without an explosion. The demonstration is not recommended for use with gases heavier than air. □

REFERENCE

1. B. Lewis and G. von Elbe, *Combustion, Flames and Explosions of Gases*, Academic Press (1951).

NOMENCLATURE

a	cross sectional area perpendicular to flow	ft ²
C	orifice coefficient	dimensionless
g	acceleration of gravity	ft/sec ²
p	pressure	lb _f /in ²
Δp	pressure difference across the top of the can	lb _f /in ²
Q	volume which has flowed into the can	ft ³
t	time	sec
V	volume of can	ft ³
v	velocity through lid hole	ft/sec
Z	elevation	ft
ΔZ	difference in elevation of two holes in can	ft
ρ	density	lb _m /ft ³

SUBSCRIPTS

atm	atmospheric
gas	pertains to gas in can
air	pertains to air
o	original condition, i.e. at start of demonstration
h	hole (in lid)
c	container

ChE book reviews

Chemical Kinetics and Reactor Design, A. R. Cooper and G. V. Jeffreys, Prentice Hall (1972). Reviewed by Dan Luss, University of Houston.

This is an undergraduate text on the analysis and design of chemical reactors. The approach is elementary with emphasis on the underlying concepts and techniques as is most proper for the first exposure to this subject. The coverage of several chapters is very good and the chapters on gas liquid and liquid-liquid reactors contain more material than most other texts. On the other hand, several other chapters, such as that on gas solid reactors, are rather superficial and leave much to be desired. In several cases, the authors make errors which indicate lack of knowledge of the literature. For example, they state on page 167 that for a system of first order reactions, "the reaction paths will not be straight lines," or that "the slope condition is sufficient for stability" even though both statements are not true in general. Similarly, the example on p. 133 applies a numerical solution for a problem for which an analytical solution was published already in 1962. Several definitions are rather unclear and that on catalysis fails to point out its important effect on selectivity. It is not clear why a modern text should apply the old height of reactor unit concept for design of packed bed reactors.

The book contains an appropriate number of suitable examples. It is, however, surprising to note that several of them have been taken, with only slight changes in the numerical values, from other texts without giving any proper credit to this fact. The example on butane decomposition is based on a 1939 kinetic investigation. In view of the many improved and more accurate recent studies, application of a more modern rate expression would have been desired. The text contains a rather large number of disturbing printing errors. For example, there is a consistent error in the sign for the rate expression developed on page 112. The captions for some figures are missing and in others there is no marking on the ordinate leaving the reader guessing.

The first chapter treats chemical reactor thermodynamics and applies them to some important processes such as methanol, SO_3 and NH_3 synthesis. Most of this material is covered in the U. S. in the thermodynamic course. The second

chapter discusses the kinetics of chemical reactions and the influence of concentration, temperature and changes in volume. This is followed by a discussion of rate expression for complex reactions, chain reactions, and heterogeneous catalysis. Several examples demonstrate techniques for the determination of rate constants from experimental data.

The third chapter contains a discussion of the batch and semi batch reactor for both isothermal and non-isothermal single reactions. A rather comprehensive chapter on the continuous stirred tank reactor follows. It includes a discussion of several optimization problems as well as of the stability and control. A description of plug flow and laminar flow tubular reactors is contained in the next chapter and it covers isothermal and non-isothermal operation, optimal operating temperature profile and the effect of laminar velocity on conversion.

The chapter on flow characteristics and their effects on the performance of continuous reactors presents an analysis of residence time distribution and dispersion models and their application to design for reactions with linear kinetics. A rather brief chapter is devoted to heterogeneous reactors. It describes briefly solid gas kinetics, the effect of diffusion on a first order isothermal reaction and non-isothermal operation. The last two chapters discuss gas liquid and liquid-liquid reactors, and several design examples demonstrate the effect of the chemical reaction on the mass transfer rate.

CACHE Computer Problem

(Continued from page 93.)

and TDEL, the assumed temperature change across the increment.

The subroutine checks if the calculated TB is greater than the specified maximum temperature, TMAXO ($^{\circ}\text{R}$). If so, TB is set equal to TMAXO and the enthalpy at TMAXO is calculated.

Subroutine PDROP

The pressure drop equation for a gas phase system at high velocities may be simplified to:*

*Hougen, O. A. and K. M. Watson, *Chem Process Principles III*, p. 869, John Wiley & Sons Inc., New York (1947).

$$\Delta P / \Delta L = \frac{0.0235}{D_1} \left(\frac{W}{1000} \right)^{1.8} \left(\frac{\mu^{0.2}}{\rho} \right) \quad [1]$$

where $\Delta P / \Delta L$ = pressure drop, psi/foot of pipe

D_1 = i.d. of tube, inches
 W = flow rate of gases, lbs./hr.
 μ = viscosity, micropoises
 ρ = density, lb./cu. ft.

This equation may be solved for ΔP by an iterative method; however, this can be avoided by defining ρ as:

$$\rho = \frac{W}{\bar{V}} = \frac{W}{\bar{N}_t R \bar{T} * FEED / \bar{\Pi}} \quad [2]$$

where $\bar{\Pi}$ = average pressure = $(PA + PB) / 2$
 \bar{N}_t = average number of moles/mole of feed
 \bar{T} = average temperature, $(TA + TB) / 2$
 \bar{V} = average specific volume
 $FEED$ = flow rate, lb. moles/hr.

Substituting [1] into [2] and grouping constant values

$$\Delta P = \frac{CONST * \bar{N}_t R \bar{T}}{\bar{\Pi}} * \Delta L = \frac{CONST 1}{\bar{\Pi}}$$

$$PA - PB = \frac{CONST 1}{(0.5 * (PA + PB))}$$

$$PA^2 - PB^2 = 2 * CONST 1$$

or

$$PB = \sqrt{PA^2 - 2 * CONST 1}$$

This is the final working equation for this subroutine. A flag, KPOP, is set to 2 if the group $(PA^2 - 2 * CONST 1) \leq 0.0$. In this case, calculations are stopped, and results to this point are printed out. The program then stops or if the data so provide, the tube size is incremented and the calculations are started anew.

Subroutine SCAN

This subroutine reads in the data, checks that the physical property cards are in the right order and that there are sufficient cards to agree with the specified number of components. The data is then printed out according to the input format.

The documentation accompanying the program

listing contains detailed descriptions of the input variables, and the data card specifications.

Subroutine VISCON (T)

Calculates viscosity according to equation proposed by Chapman-Cowling, *Mathematical Theory of Non-Uniform Gases*, Cambridge Univ. Press, Cambridge (1952) as given in *API Technical Data Book*, p. 11-47.

$$\mu_i = 0.001989 \frac{\sqrt{M_i T}}{\sigma^2 \Omega_v}$$

where μ_i = viscosity, cp.

M_i = molecular weight

T = temperature, °R

σ = Lennard Jones collision diameter, Å

Ω_v = collision integral = function $T / \epsilon / K$

ϵ / K = Lennard Jones potential parameter, °R

Ω_v is given by an empirical equation as a function of $(T / \epsilon / K)$ between TK / ϵ of 0.3 and 400 with an accuracy of $\pm 0.15\%$.

(See the program listing for the actual equation.)

The mixture viscosity is calculated according to

$$\mu_{mix} = (\sum y_i \mu_i \sqrt{M_i}) \div (\sum y_i \sqrt{M_i})$$

where y_i = mole fraction of component i.

This equation was suggested by Hering and Zipperer, *Gas Wasser-foch*, 79, 49 (1936) as reported in the *API Technical Data Book*, p. 11-51.

Values of ϵ / K (in °K) and T are listed in Reid and Sherwood, and many other sources. The group $T / (\epsilon / K)$ must be dimensionless.

REFERENCES

- Hougen, O. A., and K. M. Watson, *Chemical Process Principles, Vol. III*, John Wiley and Sons, New York (1947).
 Smith, J. M., *Chemical Engineering Kinetics, 2nd ed.*, pp. 214-223. McGraw-Hill Book Co., New York (1970).
 Amer. Petroleum Inst., *Technical Data Book-Petroleum Refining*, New York (1966).
 Reid, R. C. and T. K. Sherwood, *Properties of Gases and Liquids*, 2nd ed., McGraw-Hill Book Co., New York (1966).

DATA

The API Technical Data Book is a particularly convenient source of consistent data and tested methods of correlation. However, the required physical and thermal properties of compounds are readily available elsewhere.

What goes up must come down.



The tires of most jetliners lose traction on a half inch of snow.

That means runways must be kept free of snow and ice. Or airports must close and the planes land somewhere else.

Which causes a lot of inconvenience for passengers. Strange hotels. Long lines. Missed relatives. And dreary hours waiting for better weather.

But this winter the story may be different. Because of Union Carbide's Runway De-Icer.

We discovered a new combination of liquid chemicals that penetrates a covering of snow and ice and unglues it from the runway surface.

So it can easily be pushed away.

It can also be laid down before a storm to act as an anti-icer.

Last winter it was successfully used at over 20 busy metropolitan airports. This year we expect that more airports will be using UCAR Runway De-Icer.

So now instead of just talking about the weather, people can do something about it.



THE DISCOVERY COMPANY

Masters' Introduction to Environmental Science and Technology lets you cover today's most critical environmental problems with a single text

Masters covers the interrelated problems of population, pollution, and resource depletion so you can give your students a unified introduction to the major environmental problems facing mankind today . . . and that includes the energy crisis!

You'll find discussions of the world's growing demand for energy and its diminishing supply of natural resources . . . of the environmental disruption caused by the acquisition and use of these resources . . . and of the implications of America's growing dependence on foreign energy sources.

And you'll find detailed coverage of such new and future sources of energy as nuclear fission, fast-breeder reactors, and geothermal, solar, and fusion power.

Masters also includes full sections on—

- **"Ecology and Population,"** including the basic principles of ecology, and an analysis of population growth and the problems of providing food for our growing population

- **"Water Pollution,"** showing how man's activities can overload the natural ability of a body of water to purify itself, the importance of proper water and sewage treatment to public health, and the principles of operating a modern treatment plant

- **"Air Pollution,"** including the five principal types of emissions, the causes of inversion layers, the possible effects of air pollution on climate, and the technology of air pollution control—particularly in the automobile

And Masters makes it easy for students to understand by including graphs, tables, and illustrations, rather than complicated equation manipulations. And he provides both qualitative and quantitative questions at the end of each chapter.

Introduction to Environmental Science and Technology, by Gilbert M. Masters, University of Santa Clara
due March 1974 approx. 352 pages \$11.95 (tent.)

For a complimentary copy, contact your local Wiley representative
or write to Art Beck, Dept. 820, N.Y. office.
Please include course title, enrollment, and present text.



John Wiley & Sons, Inc.
605 Third Avenue, New York, N.Y. 10016
In Canada: 22 Worcester Road, Rexdale, Ontario
price subject to change without notice

In the energy field, there aren't any easy answers

which is one very good reason for considering Atlantic Richfield for your career.

It's energy that has created and maintains the fabric of today's civilization. That's basic.

But getting and using energy has also created some very large and basic problems: air pollution, ecological disruption, resources depletion—to name a few of the obvious ones.

Now, new answers must be found to developing and utilizing energy—and its by-products—if we are to maintain our energy-based standards of living.

We want the best brains we can find to help us arrive at these answers. We want people sensitive to the human and natural environment—and realistic enough to know that preserving both must come from tough, intelligent, dedicated work . . . backed by outstanding resources in capital, research and experience, such as those of Atlantic Richfield.

If tackling such large-scale, significant problems is one of your criteria in selecting a job, join us. We can offer you a career rich in challenge, rich in meaningful work, rich in personal reward.

We typically offer opportunities to engineers, accountants, financial analysts, auditors, geologists, geophysicists, sales representatives and programmers.

See our representative on campus or your Placement Director.

AtlanticRichfieldCompany 

An equal opportunity employer, M/F.

