



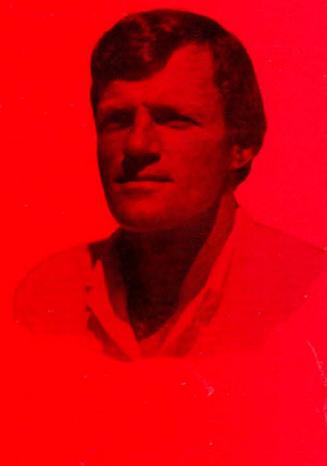
chemical engineering education

WINTER 1973

VOL. 7, NO. 1

*Steve Whitaker*

OF CALIFORNIA  
AT DAVIS



**CHE AT TEXAS**

- CATALYST:** effectiveness factor . . . . . Cassiere & Carberry
- CURRICULUM:** cpm network . . . . . Cunningham & Sommerfield
- CALTECH:** polymer program . . . . . Cohen & Tschoegl
- POLLUTANT:** dispersion . . . . . Miller & Cadman
- CATALYSIS:** short course . . . . . Luss & Richardson
- DESIGN:** control system . . . . . Paul
- VIEWPOINT:** frosh course . . . . . Hunter
- APL:** modern analysis . . . . . Pham & Cloutier

*Also 1972 Award Lecture:*

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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 32601. 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 © 1973. 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.

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**Experimentation and Modeling**

Sir: The article on kinetics of yeast growth (*Chem. Eng. Education*, 6, 134-7 (1972)) should not go unchallenged, for the lesson it teaches is not what designers of the experiments have intended. Oxygen or some constituent other than sugar must have limited growth of the yeast, despite apparent agreement of the data with a simple model.

One can overlook the unexplained failure of Beer's Law to describe turbidity of a yeast suspension or what one hopes is a typographical confusion between corn sugar and cane sugar. (If the latter were indeed used, consistent results for sugar analysis would have been difficult even with a detailed recipe!) Of more consequence is a failure to recognize that the experiment is not at all "patterned after the commercial process for growing yeast," (which employs a low concentration of sugar so as to avoid catabolite repression of respiratory enzymes—the kinetic behavior can be complex).

Results of the published experiment showing departure from exponential growth after only five hours, when the sugar content was still 15 gm/liter, should have alerted the designers to some other rate-limiting constituent like oxygen. Having called attention to such possibilities in presenting theoretical background, the author neglected to perform even the simple test of trying oxygen-enriched air once the rate of growth declined. More elegant of course would have been to use a dissolved oxygen probe. The data suggest that after about five hours growth became linear, a very nice example of mass transfer limitation of a kinetic process.

The sought-for relationship between growth rate and sugar concentration cannot be found with any accuracy by taking slopes off an integral curve as proposed. The correct concentration for half-maximal rate ( $1/b_s$ ) is so small that in any properly conducted experiment the rate curve remains exponential until just before complete exhaustion of sugar when it bends over sharply to zero. Initial rate data were used by Monod; others have used continuous backmix reactors to obtain the desired relationships.

Except for the nagging question of how fractions of a volume per cent of yeast can be measured in 12-ml centrifuge tubes, the experiment itself is a good one. It provides a first-class example of the hazard of overzealous fitting of kinetic data to an *a priori* mathematical model—a hazard fully emphasized in Levenspiel's text.

R. K. Finn  
Cornell University

**Anderson Replies**

Sir: Professor Finn has restated one of the conclusions reached by several of the students who have run the experiment: Another factor may partially limit the growth of the yeast. Those students received top marks, and with a lab report written without jumping to conclusions Professor Finn might also receive top marks. In fact, data of other groups have yielded lower values for ( $1/b_s$ ), but

in all cases the yeast stop growing when the sugar runs out. A simple check on the effect of the oxygen supply can be obtained by varying the air feed rate. Regarding corn vs. cane read corn but buy dextrose from a laboratory supply house. Of course, "patterned after" does not imply exact duplication of a commercial process but merely similarity. The use of 12-ml centrifuge tubes for measuring yeast cell volume is quite simple and gives surprisingly reproducible results as shown by sample replication.

The objectives and requirements of research investigations and undergraduate experiments differ in several important respects. In the former the limitations of time and complexity are not near as severe as in the latter. The time available in an undergraduate course laboratory precludes the use of both initial rate measurements and continuous backmix reactors as suggested by Finn. The data obtained in most batch experiments are adequately represented by the accepted model, which includes the effects of many constituents other than sugar. The model is certainly not an *a priori* model since it results from the "shrewd scientific detective work" (1) of a number of workers over a period of years.

J. B. Anderson  
Yale University

(1) O. Levenspiel, "Chemical Reaction Engineering," Wiley & Sons, Inc., New York, 1962, p. 31.

**Tenn Tech Is Accredited**

Sir: The chemistry survey reported by Dr. James Cobb in the summer 1972 issue of *Chemical Engineering Education* may leave the impression that the Department of Chemical Engineering at Tennessee Technological University is not presently accredited. Without worrying about the merits of achieving accredited status I would like to point out that this department, formed as a department in the fall of 1966, was inspected in the spring of 1970 and accredited by action of the AIChE and ECPD in the summer of 1970. I see other universities in the list that may have similar comments.

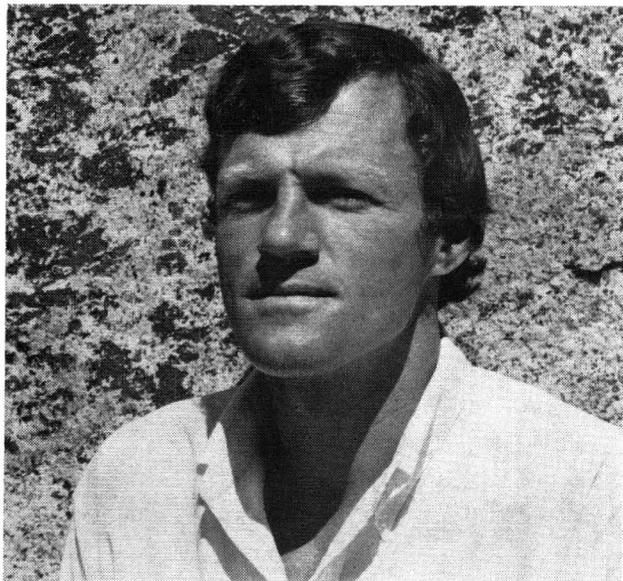
While I have this opportunity let me express my appreciation for the efforts you and your associates put into *Chemical Engineering Education*. I find it both interesting and useful.

John C. McGee, Chairman  
Tennessee Technological University

**Steam Table Correction**

Sir: For those chemical engineering teachers of thermodynamics who are accustomed to using the little steam table booklets prepared by Combustion Engineering, Inc., the most recent edition contains an erroneous enthalpy value that might cause a few anxious moments in class for the unwarned. Whereas most of us are familiar with the convention of assigning the value zero to the enthalpy and entropy of "saturated" liquid water at 32°F, the latest edition of "Steam Tables" shows the disquieting value of 0.0179 Btu/lb<sub>m</sub> for the enthalpy  $h_f$  at this point.

(Continued on page 52)



## *Steve Whitaker of* **CALIFORNIA AT DAVIS**

**I**N CARMEL-BY-THE-SEA there once lived a blacksmith who fashioned hot iron into wondrous objects while a son watched wide-eyed and took note of each step as drill stock was fashioned into candlestick and sheet iron into weather vane. But the Golden Bear from Berkeley beckoned and an artisan was lost from the diminishing ranks of "smithies" in order to swell the ranks of another Smith. So it was that Steve Whitaker began his undertaking as a chemistry major at Berkeley when that campus was known for its grassy glades, the pleasures of Strawberry Canyon, and a clear view of the now disappearing San Francisco skyline. A persuasive upper classman, "Skip" Scriven, effected the change to chemical engineering while also demanding participation in the Sunday afternoon volleyball game at Bowles Hall. Ever since, these two activities have been interfering with each other, one always diminishing the success of the other.

In 1954 Steve Whitaker started his graduate studies at the University of Delaware working with Professor R. L. Pigford on the problem of interfacial resistance to gas absorption. The re-

*This article was submitted to CEE by J. M. Smith of the Chemical Engineering Department of the University of California at Davis.*

**Underneath lay the perplexing question of how to incorporate a rigorous treatment of fluid mechanics into the chemical engineering program . . . and move logically to a problem solving technique with which the practical problems of engineering could be solved with confidence.**

sults of that study have remained anonymous, but the view of ubiquitous Bob Pigford was inspiring and Professor Whitaker's long-time interest in interfacial phenomena can be traced to that early encounter with the subject. When life in the laboratory became too gruesome, Scriven was always waiting with the Delaware Engineers volleyball team, ready to sally forth to do battle with the Four Corners Tuesday Night Recreational Volleyball Club. Lee Brown offered fantastic sailing on the Chesapeake Bay and was brave enough to let novice Whitaker handle the main in a howling October gale. After an hour of clinging to the side of Lee's capsized boat, Whitaker was relegated to crewing for Mary Wilkenson who was fast enough at the tiller to offset the many blunders made by her crew.

After completing graduate work in 1958 Steve Whitaker moved to the nearby Du Pont Experimental Station and began working in the area of fluid mechanics while attending Jim Carberry's weekly seminars on casualty and modern man — the study of an evolutionary society. Although his PhD thesis dealt with the use of frequency-response techniques to study interfacial mass transfer, Whitaker's graduate school experience left him with the impression that fluid mechanics was the weakest link in the chemical engineers training, and his research at the Engineering Research Laboratory provided an opportunity to study this subject. A confused attitude prevailed until visiting lecturer Bob Bird

**California provided Steve the opportunity to renew his acquaintance with the High Sierra.**



provided one of his inimitable multi-colored presentations, and the elements of transport phenomena were unfolded across a sixty foot blackboard. Bird's ideas were in marked contrast to the pragmatic attitude at Du Pont where engineers struggled to describe the vagaries of the real world in terms of a finite number of previously derived equations. A more attractive alternative was lurking in Bird's comments; namely the ability to analyze any and all real processes in terms of the finite set of *laws of continuum physics*.

A brief discussion with George Bankoff at an AIChE meeting in Mexico City eventually led to an appointment on the faculty at Northwestern University in 1961, and there Whitaker's understanding of fluid mechanics began to take on some recognizable form. This was due in no small measure to the necessity of explaining the subject to the undergraduates, and to endless discussions with John Slattery. Interest in surface phenomena, generated by the work with Pigford, led to a series of research efforts on the fluid mechanics of interfacial phenomena, while the persistent nagging by Slattery about the inadvisability of using Darcy's law for two-dimensional flows led to a permanent interest in the subject of transport processes in multi-phase systems.

**L**IFE AT NORTHWESTERN was not all academic, and dream of glory nurtured by earlier victories with the Bowles Hall Chargers and the Delaware Engineers, led Professor Whitaker to join the much-traveled (10,000 miles per year) Chicago volleyball team. While holding records for travel, the Chicago team reached in vain for a national championship. Always finishing among the top ten teams in the country yielded

but a mediocre thrill. Sailing on Lake Michigan provided some sport in the off season, and as co-owner with George Brown of an ageless and nameless racing sloop a more definitive competitive position was assumed, i.e. dead last.

Underneath these activities lay the perplexing question of how to incorporate a rigorous treatment of fluid mechanics into the chemical engineering program, and how to structure an approach to engineering analysis that would "begin at the beginning," i.e. the fundamental postulates of continuum physics, and move logically to a problem solving technique with which the practical problems of engineering could be solved with confidence. The crux of the matter seemed to be to break away from the luxury of using previously derived equations, and build directly on the fundamental postulates in their most elementary form.\* Calculus, linear algebra, and vector analysis, all standard lower division subjects, would provide the tools if they could only be put to use.

**. . . dream of glory nurtured by earlier victories with the Bowles Hall Chargers and the Delaware Engineers, led Steve to join the much-traveled Chicago volleyball team.**



Lunchtime activity on the UCD sandcourts.

In 1964 Professor Whitaker returned to California to join Joe Smith's new chemical engineering program at the University of California at Davis. The unstructured nature of the new College of Engineering provided the opportunity of teaching both fluid and solid mechanics in the

\* In this respect Bertrand Russell once noted, "The habit of simply assuming results, once one is persuaded they are true, rather than trying to prove them, has all the advantages of thievery over honest toil."

**Steve and Suzanne plus Suzy, Collin Walter, Larry, Lynn and Jimmy on a Sunday afternoon outing.**



common core courses. A few (very few) polite conversations regarding course content and level were always held, but angry debate would more accurately describe the discussions about the common core courses. A heavy dose of "slings and arrows" will usually clear ones head, and Professor Whitaker's thoughts on fluid mechanics were crystallized in the book, *Introduction to Fluid Mechanics*, which had its beginnings at Northwestern. Although the common core courses have essentially disappeared, Professor Whitaker's interest in the undergraduate program has not waned, and an introductory text on heat transfer is currently being prepared.

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**Other climbing activities led to an assault on 21,000 ft Mt. Ausangati in Peru and a 28 hour off-route climb of the East face of Mt. Whitney.**

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**T**HE RETURN TO CALIFORNIA also provided Steve Whitaker the opportunity to renew his acquaintance with the High Sierra where many a boyhood summer was spent hiking and fishing; however, the population explosion in California had flooded his favorite haunts and heavier loads had to be carried higher and further to avoid the crowds. Charlie Sleicher provided some relief with excursions to the Northwest and the spectacular Ptarmigan Traverse. Other climbing activities led to an assault on 21,000 ft Mt. Ausangati in Peru (failure occurred at 19,000 ft when the tent blew apart), and a 28 hour off-route climb of the east face of Mt. Whitney. Springtime will usually find Steve Whitaker sneaking out of his office early on Fridays, squeezing in three-day week ends with his wife Suzanne at Yosemite Valley where the "big walls" are contemplated, but avoided in favor of the

smaller and less strenuous climbs that abound in the valley. The Whitaker boys, Larry and Jimmy, have participated in some small climbs, while the girls, Lynn and Suzy, must wait a few summers before they can join their brothers on the rock. Suzanne views this activity benignly from below, but leads the way when it's time to take the high country trails.

In 1964 Davis was a town without a volleyball team, and like a true devotee Steve Whitaker organized and coached the UCD Volleyball Club during its early years. After 16 straight defeats at the hands of southern California teams, he recognized that coaching was not his game and he threw his talents in with a group of misfits from several northern California cities known as "Friends of Fred." Friends indeed they were not, and the team was known far and wide for its internal strife if not for its ability to win matches. Personal opinions were put aside for the 1970 National AAU Masters (over 35) Volleyball Championships and the team at last managed to bring home the first place medal. In 1972 everyone was two years older and fourth place was the best that "Friends" could do in the same tournament.

While national competition is a thing of the past, the local players are still easy pickings. Fran Woods and Steve Whitaker have never lost a coed doubles match on the UCD volleyball sand courts, and lunch time will usually find Jim Hurley (Physics) and Steve Whitaker tenaciously holding the number one court against an array of frustrated undergraduates. That too must pass, but there will always be a bright-eyed chemical engineering student intent on mastering the laws of physics for some good purpose, and there is much to be done in that domain. □

# Beneath this soft and warm exterior, there lies a heart of plastic.



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## ChE department

### TEXAS

*This paper was submitted by the Chemical Engineering faculty, University of Texas, Austin.*

#### **How did chemical engineering get started at Texas?**

The parallelism that exists between the Department of Chemical Engineering at The University of Texas at Austin and the hydrocarbons processing industry of the state is not accidental. Each has complemented the other since before World War I, when the late Dr. E. P. Schoch foresaw the need to apply his profound knowledge of chemistry to develop uses for the crude oil which production was increasing daily. As a result of Dr. Schoch's direct effort, a degree program leading to the Bachelor's Degree in Chemical Engineering was authorized by the Regents early in 1916 and the first two degrees were awarded in June 1919. Official recognition was given to the new Department through the changing of Dr. Schoch's title from "Professor of Physical Chemistry" to "Professor of Chemical Engineering and Physical Chemistry."

For almost 20 years Dr. Schoch was the only permanent faculty member, but as the student load became heavier he was given assistance by the appointment of full time instructors on a year to year basis. In 1938 Chemical Engineering was established as a full Department in the College of Engineering with Dr. E. P. Schoch as Chairman. Among the early faculty members were Drs.

J. S. Swearington, John Griswold, W. A. Cunningham, and K. A. Kobe. Physically, the Departmental activities were housed within the Chemistry Building until a new building for Chemical Engineering was authorized and constructed during the years immediately preceding the World War II. The building, containing 33,000 sq. ft. of floor space is devoted exclusively to office and laboratory usage.

The accrediting program of the AIChE was suspended nationally early in World War II, but this Department was given provisional accreditation in 1943, and after the war full accreditation was received and has been retained since that time.

#### **How big is your department?**

Prior to 1935 only 130 bachelors degrees had been granted with an average of 8 graduating seniors per year, but this number jumped to 24 in 1935 and reached a pre-war peak of 54 in 1939. With the onset of the war, the normal undergraduate activities slowed very substantially, but picked up again in 1947 when 80 degrees were awarded and reached a peak in 1948 with 105 Bachelor's Degrees. Since that time the average annual number of B.S. graduates has been approximately 60. Total undergraduate enrollment is currently about 350 full time students. Graduate enrollment increased steadily after 1948 until 1965, reaching a level of 50 to 60 full time students per year.

### How does your undergraduate curriculum compare to that of other ChE departments?

Chemical Engineering curricula among the various schools have many similar features. We require the usual freshman courses in the areas of mathematics, physics, chemistry, drawing, etc., but in addition recently introduced a PSI course (see below) in computer programming for entering freshmen. One feature of this course, in addition to the development of programming skills, is the motivation of the students toward chemical engineering by means of a series of talks by Professor Schechter, the departmental chairman.

After the freshman year the typical student takes a series of core courses in chemical engineering consisting of material and energy balances, transport phenomena, thermodynamics, unit operations, kinetics, plant design, and laboratory. In addition, he takes courses in mathematics, chemistry, some engineering, physics, English, government, and history. He also takes eight elective courses generally grouped into blocks of similar content, such as

- Computer applications, process analysis, control
- Materials engineering and chemistry
- Management and management decision making
- Environmental improvement
- Chemical processing
- Biomedical engineering

It takes the average student four years plus a semester to complete the undergraduate program. Cooperative students spend three semesters working in industry in addition to their academic work.

### What type of laboratory courses do you have?

A distinct upswing in the quality of our laboratory courses and facilities has taken place in the last three or four years. We believe that modern methods of data acquisition, real time analysis, and graphical display can be of value in making the undergraduate laboratory experience more meaningful for students. To implement this philosophy we have assembled an 8K mini-computer, A/D and D/A converters, magnetic tape drives, teletype, and CRT display, and interconnected them to the main university computer (see Table 1). The system is used in a variety of ways in the experiments from presenting tutorial material to the calculation of final results. The computer is incorporated into the procedure in a manner that improves student's understanding of the experiment while not isolating him from it.



R. S. Schechter, Department Chairman

The three main undergraduate laboratory courses in which the system is used are transport phenomena, process control, and the unit operations laboratory.

In general the work assigned in these laboratory courses has the principal objective of bringing students into actual contact with the physical world. Students are expected to see the correspondence between terms in an equation and the corresponding physical quantities; to make valid approximations while avoiding unwarranted assumptions; and establish that the theory they have learned does describe real world systems. To

Table 1. Characteristics of the Department of Chemical Engineering Computer System

- I. Nova Mini-computer
  - A. 16 bit word length
  - B. 8 K words of memory
  - C. Integer arithmetic
  - D. 1.2 microsecond memory cycle time
  - E. 4 accumulators
- II. Data Acquisition
  - A. 12 channel multiplexer
  - B. Binary-gain range amplifier
  - C. Analog-to-digital converter
- III. Analog Output on 4 Channels
- IV. Peripherals
  - A. Computek graphics terminal
  - B. Dual deck magnetic tape cassette unit
  - C. ASR 33 teletype
- V. Communications Interfaces (for communication with XDS-930, Sigma 5, and CDC-6600)
  - A. 110 bits/sec. to teletype
  - B. 110 bits/sec. to Bell type 103A data set
  - C. 1200 bits/sec. to Bell type 202 data set
  - D. Optional 2400 bit/sec. interface to the Computek terminal

realize these objectives, laboratory equipment has been designed and built for appropriate experiments some of which involve extensive computation. Efficient techniques have been implemented to acquire data, put it in the form having the greatest significance, and present the information to the student during the laboratory period.

**Is it true that you have a tutoring service for undergraduates via the telephone?**

Yes we do. Professor Rase realized several years ago that an undergraduate student who has difficulty in solving a homework problem often can resolve the difficulty with the help of a key suggestion. The telephone tutoring service enables the student to call a phone number at any hour of the day or night and receive hints that assist in the solution of homework assignments. Individual tutorial assistance in person or by phone can be routinely obtained from tutors on duty Monday through Friday from 3 P.M. to 5 P.M. Based on the questions asked each day, the tutors record or tape hints and suggestions for these homework problems that seem to cause students difficulty. The recorded material is activated when a student dials the proper number. If the student does not understand the information presented on the first reading, he can hang up and dial again. Another call re-initiates the tape.

**What is the student evaluation of the program?**

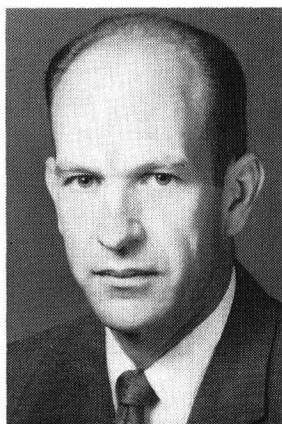
Almost every student who has used it believes it is very helpful, especially when credit on a homework problem is important.

**What improvements are planned for the system in the future?**

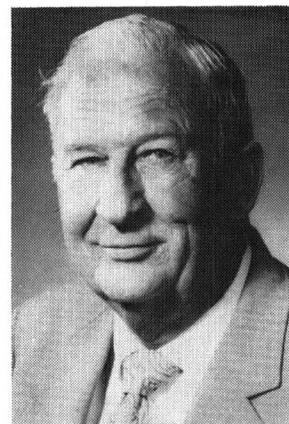
We are working on a way to computerize the system so that after the student dials the main number, he can dial an extension corresponding to the course number and receive a message for that course without having to listen to the whole tape.

**Do you use the Personalized System of Instruction to any extent?**

The College of Engineering at the University of Texas at Austin has been very active in developing applications of the Keller Plan, also known as the Personalized System of Instruction (PSI). PSI is distinguished by an initial careful analysis by the teacher of what the students are



Rase



Cunningham

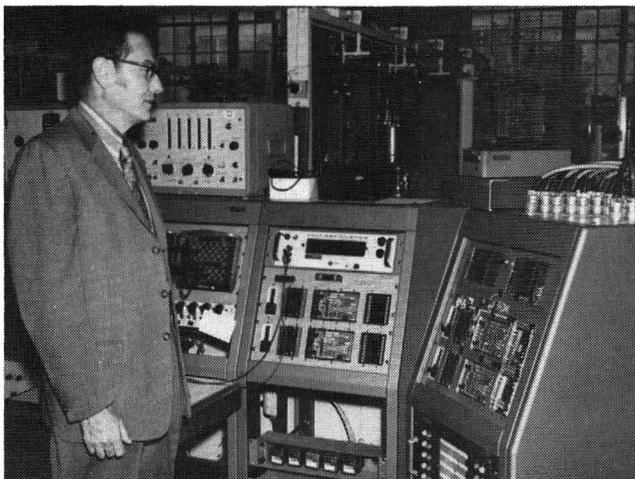
to learn in his course. Once the terminal and intermediate objectives are fixed, he then divides the course into units, each containing a reading assignment, study questions, collateral references, study problems and any necessary introductory or explanatory material. The student studies the units sequentially at the rate, time and place he prefers. When he feels that he has completely mastered the material for a given unit, a proctor gives him a "readiness test" to determine if he is ready to pass on to the next unit. The proctor is a student who has been carefully chosen for his mastery of the course material. The student must make a grade of 100 on the "readiness test," and if he does not, he is told to restudy the unit more thoroughly. He receives a different test form each time he appears to be tested. All students who demonstrate mastery of all course units receive a grade of A.

Lectures are given at stated intervals during the course to students who have completed a specified number of units and can therefore understand the material to be covered. The students who qualify for a lecture are not required to attend them, and the lecture material is not covered on any examination.

**Is PSI an improvement over the lecture-recitation system of instruction?**

The Keller Plan has worked well for us. Students like the flexibility that it gives them. Most (80 to 90 percent) prefer it to the more conventional methods of instruction; they report that it taught them how to study, and our results indicate that they learn more and learn it better.

Next year there are plans to develop eight new PSI courses in the College of Engineering, including Material and Energy Balances and Pro-



D. M. Himmelblau with Data Processing Equipment

cess Analysis and Simulation in the Chemical Engineering Department.

There are some problems, of course. Students who are poorly prepared are often forced to drop a course (they probably would have flunked in a conventional course), and those who haven't developed self-discipline are prone to procrastinate. And very little data are available on whether the PSI student's better grasp of course materials at the end of a course results in better long-term mastery. We hope that our continuing study of the method will throw some light on these matters.

#### **Do you have a big graduate program?**

We have a relatively large graduate study body, with 50 to 60 full time students being enrolled each year. About one-half are working toward the doctoral degree and the other half toward the M.S. In the last ten years 72 students completed their Ph.D. degrees in our department.

#### **What do you do in your M.S. program?**

In the future we actually will have two types of M.S. programs, one with a thesis and the other without; the latter program was just introduced. A student can complete the requirements for the M.S. in one year but the average student takes about a year plus a semester. A wide variety of courses are available both within and outside of the Ch.E. department. We do not encourage students to specialize in any one area of course work but instead try to provide them with as broad a background as possible so that their future job potential will not be too constrained. The research completed for the M.S. degree is not nearly as extensive as that for the Ph.D.

#### **How does your Ph.D. program operate?**

One of the main goals of our doctoral program, as in other universities, is to provide a student with the opportunity to carry out an independent study under the general supervision of an expert, his professor. Our faculty take pride in their close personal contact with their graduate students and we feel that this interaction is a big contributor to high student morale. As with the M.S. students, doctoral students are not expected to limit their course work solely to the area of their research, and are encouraged to broaden their interests. We require no specific count of courses or hours completed for a Ph.D. so that the doctoral program is completely flexible and can nicely fit in with the student's needs and interests. We do require successful completion of preliminary written qualifying examinations and a foreign language test of some type before a student can become a doctoral candidate. However, the bulk of the student's time, beyond the M.S. requirements, is spent in his research.

#### **What types of research programs are underway?**

We have a full time faculty of 14 and consequently have a broad spectrum of on-going research projects. Because of proximity of the University to the vast chemical and petroleum developments on the Gulf Coast of Texas, an active interest is maintained in the fundamental problems of a wide variety of process plants. The Department has earned a reputation for excellence in research in materials, separation processes, polymers, fluid properties, surface and aerosol physics, catalysis and kinetics, automatic control, process simulation and optimization, and biomedical engineering. A summary of the individual faculty and their research interests is as follows:

##### **James R. Brock**

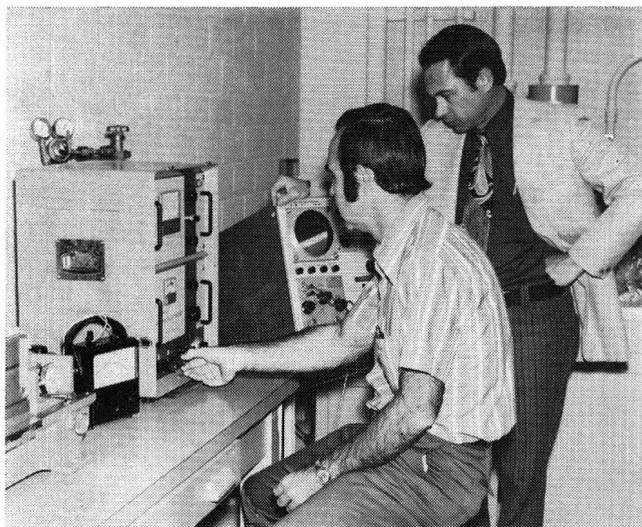
Aerosol physics and chemistry, nucleation processes, coagulation and condensation, deposition and filtration of particles, particle charging, the surface properties of particles, and quantitative human ecology as related to environmental problems of air and water pollution.

##### **William F. Bradley**

Crystal structure analysis and crystal chemistry, in particular studies of natural fine-grained mineral and the associations of organic matter with fine-grained minerals.

##### **Tom F. Edgar**

Process identification, optimization and control, energy systems engineering.



D. R. Paul (right) with Carl Locke in polymer lab

**Robert P. Popovich**

Physiological transport parameters in a patient's artificial kidney system; extracorporeal treatment of blood to alleviate major disease states; enzymatic detoxification of endogenous and exogenous toxins (artificial liver); pathogenesis and treatment of atherosclerosis.

**David M. Himmelblau**

Process analysis and simulation, and system analysis, optimization, stochastic modeling.

**Joel O. Hougen**

Process dynamics and control system design.

**John J. McKetta, Jr.**

Phase equilibria, thermodynamic properties and high pressure P-V-T.

**Donald R. Paul**

Polymer physics and chemistry. In particular the thermodynamics and transport properties of polymers in bulk and solution with applications to polymer processing.

**Howard F. Rase**

Reaction kinetics and catalysis with particular emphasis on catalyst geometry and specificity, new catalyst development and also enzyme model catalysts, process and chemical reactor design techniques.

**Robert S. Schechter**

Surface transport phenomena, surface viscosity, elasticity and diffusion, hydrodynamic stability, and the application of acids in oil reservoirs.

**Hugo Steinfink**

Crystal chemistry, magnetic, electrical, and optical properties of rare earth compounds, crystal chemistry of silicate-organic complexes.

**James E. Stice**

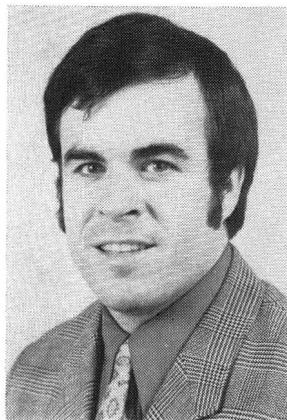
Computer assisted instruction, research in engineering teaching.

**Matthew Van Winkle**

Azeotropic and extractive distillation, solvent requirements and prediction of vapor liquid equilibria for multicomponent solvent-containing systems. Studies of efficiency in perforated tray columns including entrainment and frothing characteristics related to efficiency.

**Eugene H. Wissler**

Properties of aerosol particles, aerosol beams, simulation of the human thermal system, and non-Newtonian fluids.

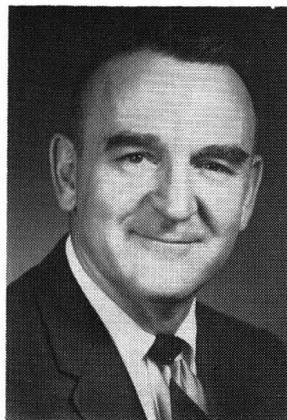


Edgar



Van Winkle

Members of the Chemical Engineering faculty are not only recognized leaders in their individual areas of expertise, but have been called on to take positions of leadership in University administrative functions, as well as in the AIChE and other professional organizations, in civic, and other activities of a broad nature. Dr. McKetta is a member of the National Academy of Engineering. □



McKetta



Steinfink

**Mathematical Methods in  
Chemical Engineering,  
Volume II, First-Order  
Partial Differential**

**Equations with Applications**

RUTHERFORD B. ARIS  
and NEAL R. AMUNDSON,  
both of the University of  
Minnesota

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January 1973, approx. 416 pp., (013-561092-3), \$16.50

# Chemical Engineering BOOKS

**Dynamic Behavior of  
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Provides a complete and systematic study of the analysis of unsteady state phenomena. Emphasizes physical interpretation of dynamic linear and nonlinear responses as well as methods of analysis. Covers both distributed parameter and lumped systems. Classes of system models prepare reader to generalize readily to other systems and to diverse fields of application. Over 100 detailed examples illustrate the fundamentals and varieties of applications. Over 200 figures present results graphically. Appendices include vector and matrix manipulation and Laplace transform pairs for easy reference.

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**Electrochemical Systems**

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January 1973, approx. 440 pp., (013-248922-8), \$18.95

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## FRESHMAN ENGINEERING - A Student Viewpoint

DAVID L. HUNTER,  
*University of Colorado*  
*Boulder, Colo. 80302*

Too often faculty members neglect students' "non-academic deficiencies" in designing their freshman engineering courses. Unfortunately, these problems can be bigger "roadblocks" than any academic deficiency. Adjustment to the University environment and learning the "rules of the game" is more important than any basic course. Thus, a department interested in success of its students would be well advised to devote some effort to helping students solve their adjustment problems. This effort, coupled with the difficult problem of what to present to freshman chemical engineers gave rise to a novel course at the University of Colorado.

The course was designed (with a little help from his friends) and is taught by Dr. R. Curtis Johnson, Department Chairman. It makes use of undergraduate teaching assistants and the entire department faculty. The purposes of the course are to answer students "quasi-academic" questions about the University and the Department, to provide fundamentals useful in other courses, and to identify other student problems, academic and non-academic, so that appropriate solutions may be sought.

The "medium" of the course is environmental awareness. The course tries to emphasize the relationship of the engineer to society. The text, *Population/Resources/Environment*, by Paul R. and Anne H. Ehrlich is supplemented by reprints from Chemical and Engineering News. The topics are loosely defined to encourage the students to discuss the topics with the senior assistants, the faculty members and among themselves. Interaction and discussion rather than presentation of specific material is stressed.

The course carries two credit hours and meets once per week for two hours. The first hour is devoted primarily to lectures and testing. During the second hour the class is split into groups of about ten. One senior assistant is responsible for each group. The time is spent dis-

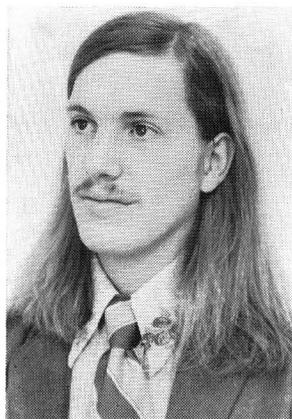
cussing the topic for the week with a member of the faculty. Each week the group discusses a different topic with a different member of the faculty. This affords each student an opportunity to meet every faculty member on a personal basis. Table 1 presents the activities of the classes taught in the fall of 1971.

It is important to all freshman chemical engineers to find out what a chemical engineer really does. This information is communicated in many ways. The AIChE film *The Chemical Engineer* is an excellent primer. Two field trips give the students a better idea. One trip to a research facility, such as the National Bureau of Standards, and one to an operating plant are usually scheduled. Of course, contact with the faculty, older students and the regular student AIChE chapter speakers aid in the communication process.

Insuring that students are familiar with the college, its facilities, and the services it offers aids the adjustment process. Brief tours are conducted so that students can become familiar with important facilities such as the Chemical Engineering Laboratory, the Computing Center, the Engineering Library and the Administrative Offices. The tours are designed to be instructional. University personnel are on hand to see that the students are familiar with the available facilities. In addition, student leaders are invited to speak to the class to inform the students of services provided by the student government and to encourage them to become more involved.

Setting up appropriate counseling sessions is facilitated by having all the freshmen in one class. Little counseling is done in class, but academic counseling sessions are scheduled with the department chairman. Senior students are given a class period to present a student viewpoint of the curriculum and the faculty. Additional counseling sessions are scheduled with faculty, student, or administrative counselors for freshmen who so desire.

In addition to a general environmental awareness, the course tries to impart some basic skills



David L. Hunter is presently "taking it easy" in Boulder, Colorado. He earned BS degrees in ChE and Business, University of Colorado, 1972 and hopes to attend law school and work in environmental law.

that will be valuable in both future courses and other endeavors. Basic sessions are conducted in laboratory safety and fire fighting. Extensive instruction is given in the use of the slide rule. Basic math relationships and flow diagrams are covered in homework assignments and exams.

Each student is required to prepare a paper on a topic of his choice in the environmental area. If the student wishes to continue his research on the project he can obtain one hour of independent study credit by expanding the project during the following semester.

The response of freshmen at the end of the semester was somewhat mixed. Most freshmen were probably not able to appreciate the uniqueness of the course. The course and the professor received high ratings in the formal student evaluation of teaching that is conducted each semester. The course seemed to reach its target students. Most of the students who were enthusiastic about the course were, in the opinion of the senior assistants, students that were having scholastic difficulty. Some students who are doing well in other courses felt that they wanted more technical material.

Students who had taken the same course previously had much higher opinions of the course. The "non-academic" aspects of the course were particularly appreciated.

The senior assistants who have participated in the program during its three years of existence are unqualifiedly enthusiastic about the course, from both the standpoint of their own experience and what they feel the freshmen have gained.

**Adjustments to the University environment and learning the "rules of the game" are more important than any basic course.**

TABLE 1 — Activity Charts for ChE 130, 1971.

Week	1st Hour All Groups	2nd Hour Small Groups
1	Introduction, R. C. Johnson	Photos and Introduction
2	Reading Test College Counselor	Tours of ChE Lab Eng. Library
3	Reading Results and talks by Student AIChE officers	Tours of Numerical Analysis Center & Computer facilities
4	Safety lecture and Demonstration	Safety lecture and Demonstration
5	Slide Rule Instruc- tion, J. F. Carley	Topic: Pesticides Paul Barrick
6	Slide Rule	Topic: Chemical Mutagens Igor Gamow
7	Slide Rule	Topic: Population W. B. Krantz
8	Slide Rule	Topic: Air-Water Pollution Frank Kreith
9	Slide Rule EXAM	Exam Followup Senior Assistants
10	Pre-advising Session, R. C. Johnson	Topic: Environmental Research, L. F. Brown
11	Academic Advising by Student Advisors	Topic: Colo. Environment, M. S. Peters
12	Slide Rule Make-up Exam	Topic: Mathematic Modeling, W. F. Ramirez
13	Cryogenics, K. D. Timmerhaus	Topic: Peter Principle, G. J. Maler
14	Field Trip: National Bureau of Standards	Field Trip
15	Review	Review
16	Final Exam	Final Exam

#### Supplemental Readings

- 1) *Report of the Secretary's Commission on Pesticides and their relationship to Environmental Health*, U.S. Department of Health, Education, and Welfare, Washington, D. C., December, 1969.
- 2) Sanders, Howard J., *Chemical and Engineering News*, "Chemical Mutagens, The Road to Genetic Disaster?", Vol. 47, May 19, 1969.

(Continued on page 17)

# APPLICATIONS OF HETEROGENEOUS CATALYSIS

DAN LUSS and JAMES T. RICHARDSON  
*University of Houston*  
*Houston, Texas 77004*

Chemical Engineering Departments provide a useful service to the industrial community by offering short courses on topics of current interest. Many universities have found this to be so profitable a utilization of faculty and facilities that available courses proliferate during the summer months. The most valuable courses are those which are tailor-made to suit the needs of potential attendees and not the predilections of the available faculty.

The Chemical Engineering Department of the University of Houston organized two short course on the applications of heterogeneous catalysis during the summers of 1971 and 1972. The program was so successful that essentially the same course is being repeated this year. Other short courses in catalysis have been presented before at Rice University, Lehigh, Berkeley and Delaware. However, our program is sufficiently different from these others so that it is worthwhile to outline the philosophy, organization and logistics of the course.

There are two types of practitioners in catalysis—the researchers and the users. A short course should be organized from the beginning with one or the other of these groups in mind. This course was aimed at the wide audience of users. These individuals have usually a considerable practical experience in a relatively narrow area but do not have a systematic and comprehensive coverage of the theory of catalysis and catalytic reactor design. Moreover they usually have little knowledge of the principles and techniques used by others.

We decided upon a “how to” theme—how to select, prepare, characterize, test and use a catalyst. The program was built around these five points with emphasis on practical implications and applications of current theory and know how and not on building an in-depth understanding of the latest research developments.

In order to present a comprehensive coverage of the subject and to expose the students to a

variety of viewpoints we selected as instructors two industrial and three academic experts. Each lecturer was instructed on the material to be included in his section in order to avoid gaps in the coverage and to prevent repetitious discussions of certain material. A comprehensive set of notes for classroom use was collected from each. These were reproduced, bound and distributed to each attendee before the start of the course. The class schedule for 1972 is shown in Table 1.

Table 1 - COURSE OUTLINE AND LECTURERS  
(Summer 1972)

1. **Catalyst Selection** (0.5 day) J. T. Richardson
  - A. Introduction to catalysis
  - B. Theories of catalysis
  - C. Prediction of catalytic properties
  - D. Catalytic process development
2. **Catalyst Preparation and applications** (1 day) C. L. Thomas - Sun Oil Company (retired)
  - A. General principles
  - B. Preparation and use of non-supported catalysts
  - C. Preparation of catalyst supports
  - D. Preparation of supported catalysts
  - E. Proven catalysts and catalytic processes
3. **Catalyst Characterization** (0.5 day) J. T. Richardson
  - A. Common mechanical properties
  - B. Measurements of surface area, pore size distribution, acidity, metal surface area, effective diffusivity and dispersion
  - C. Survey of instrumental techniques
4. **Kinetics, Mechanisms and Experimental Reactors** (0.5 day) J. W. Hightower - Rice University
  - A. Theory of adsorption
  - B. Langmuir Hinshelwood kinetics
  - C. Discussion of some examples
  - D. Comparisons of various experimental reactors
  - E. Practical suggestions
5. **Diffusional Effects** (0.5 day) D. Luss
  - A. Isothermal inter and intra-particle diffusional disguise of activity and kinetics
  - B. Effect of external and internal temperature gradients
  - C. Diffusional disguise of selectivity
  - D. Experimental methods of determining these effects
6. **Poisoning of Catalysts** (0.5 day) J. T. Richardson and D. Luss
  - A. Mechanisms of sintering, poisoning, and fouling
  - B. Determination of mechanisms by single pellet studies



James T. Richardson received his PhD ('56) degree in solid state physics from Rice University. Following a year of postdoctoral research in low temperature physics, he joined Humble Oil and Refining Company (later Esso Research and Engineering) at Baytown Texas. During the next thirteen years, his research activities included all phases of fundamental and applied heterogeneous catalysis, with emphasis on correlation between catalyst properties and kinetics. In 1969 he joined the ChE Department of the University of Houston. Dr. Richardson is one of the organizers and a past chairman of the Southwest Catalyst Society. (left photo)

Dan Luss received his BS and MS from the Technion-Israel and his PhD from the University of Minnesota. His areas of specialization are analysis and control of chemical reactors and heat and mass diffusional intrusion in catalytic reactor behavior. He received the Allan P. Colburn award of the AIChE in 1972.

- C. Effects of diffusion on poisoning and regeneration
- D. Shell progressive non-catalytic gas solid reactions
- 7. **Catalytic Emission Control Devices for Automobiles** (0.5 day) J. W. Hightower - Rice University
  - A. Federal standards and testing procedures
  - B. Engine parametric effects on emissions
  - C. Chemistry of control systems
  - D. Choice of possible catalysts
  - E. Cold start up, poisoning and melting problems
- 8. **Aspects of Catalytic Reactor Engineering** (0.5 day)
  - D. Luss
    - A. Effect of poisoning on operation of catalytic reactors
    - B. Regeneration of cokes packed reactors
    - C. Design aspects of exothermic reactors
    - D. Sensitivity and stability
- 9. **Industrial Applications** (0.5 day) V. W. Weekman, Jr. Mobil Research and Development Company
  - A. Modelling techniques of complex processes
  - B. Modelling of catalytic cracking kinetics
  - C. Modelling of a regenerator for catalytic cracking processes
  - D. Modelling of catalytic mufflers

An important part of organizing such a course is to attract a sufficient number of attendees. The publicity for our course consisted primarily of a brochure, outlining the aims and details of the

course, which was mailed to local members of the ACS and AIChE, and to members of the Catalysis Society of North America. This was followed by individual letters to various industrial research organizations, catalyst manufacturers, etc. This procedure was found to be very effective and in 1972 we had to reject 21 applicants due to restrictions on the maximal size of the class (40 students).

The students, representatives of a wide range of industries, responded most favorably to this format. Classes were informal with valuable contributions being made by many of the group. Using suggestions of the 1971 participants, we expanded in 1972 the discussions of proven catalysts and methods of catalyst preparation as well as of problems related to the design of catalytic mufflers for automobiles.

Short courses similar to this may, no doubt, be organized in many other fields of chemical engineering. The needs of industry for further education are continually changing. Courses of this nature help to fill the gap between formal university curricula and the demands of our profession. In addition, exposure to groups such as this is a rewarding and revitalizing experience for any faculty member. □

#### HUNTER: (Continued from page 15)

- 3) Kiefer, David M., *Chemical and Engineering News*, "Population," Vol. 46, October 14, 1968.
- 4) Levitt, Arnold, *Chemical and Engineering News*, "Pollution; Causes, Costs, Controls," Vol. 47, June 9, 1969.
- 5) *Cleaning Our Environment* (Supplement), "The Chemical Basis for Action," American Chemical Society, Washington, D. C., 1971.
- 6) "Second Interim Report," Colorado Environmental Commission, December, 1971.
- 7) Forrester, Jay W., *Technology Review*, "Counter-intuitive Behavior of Social Systems," Vol. 73, Number 3, January, 1971.
- 8) Peter, Laurence J., and Hull Raymond, *The Peter Principle*, Bantam Books, New York, N. Y. 4th Printing, 1970.

#### Acknowledgements

I would like to acknowledge the work and suggestions of the other twelve senior assistants during the past three years; Don Hedden, Craig Farmer, Bob Powell, John McMartin, Jim Roberts, Craig Miller, Ed Heubach, Bill Barker, Chris Harris, Craig Runyan, John Hayes and Steve Hammill. □

# NETWORK PLANNING & THE CHE CURRICULUM

R. C. CUNNINGHAM and J. T. SOMMERFIELD  
*Georgia Institute of Technology*  
*Atlanta, Georgia 30332*

**F**OR MANY YEARS now industry has found the Critical Path Method (CPM) to be a considerable aid in planning and scheduling activities. This method determines the shortest period of time required for the completion of a system of activities in the following manner. Each activity is listed with (1) its activity number, (2) its time required for completion (activity duration), (3) those activities which must be completed before starting the activity in question (preceding activities), (4) those activities which cannot be started before the completion of the activity in question (succeeding activities), and (5) any other constraints which are found necessary to be placed on the particular activity, e.g., activity start or finish times.

Once the activities have been listed with this information, the activities may be graphed by activity as in Figure 1 wherein the ordinate has some arbitrary units of time. Those activities having no preceding activities are listed by activity number at the extreme left and the succeeding activities are placed on the graph further to the right according to the time scale. Preceding and succeeding activities are connected with lines to show their relationships with other activities. The time element should never be forgotten with respect to activity duration and specified activity start or finish times.

Once all of the activities have been included on this graph, the activity finding itself to the extreme right is the last activity in a series of activities which define the critical path. The remaining critical path activities can be found by following the lines connecting activity to activity which exhibit no time lag (slack) from the finish of one activity to the start of the next. When this procedure has been completed, the critical path has been defined. If the system of activities is to be completed in the shortest possible time, these critical path activities must be completed in a continuous manner, one right after another with no interruption.

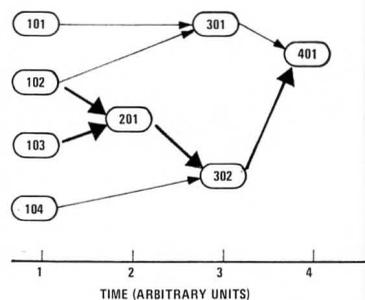
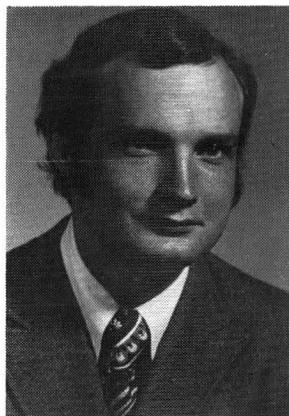
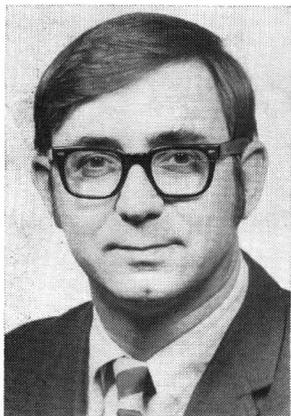


Fig. 1. Sketch of a CPM diagram. Critical path activities (101, 102, 201, 302, 401) are connected by heavy lines.

Now that the critical path has been delineated all the activities can be listed with their earliest start times, latest finish times and slacks such that there will be no increase in the critical path and therefore no increase in the time necessary to complete the entire system of activities. This list of earliest start times, latest finish times and slack offers a framework around which a schedule can be built.

With the advent of computers, programs have been written which can aid in scheduling a system of activities by using CPM. The necessary information is the same as that which is required to complete the CPM diagram as described above, but the time and effort required to obtain the necessary earliest start time and latest finish time for each activity is greatly reduced.

**N**OW THAT THE GROUND WORK has been laid, it is time to introduce the primary purpose of this article, namely, CPM as an aid in formulating curricula. The question might be asked why such a method is necessary; it can be seen today that universities are changing their curricula at an ever increasing rate, and at the same time complexities are being introduced when departments offer new options to better meet the personal needs and desires of individual students. Keeping this in mind, a tool such as CPM could greatly alleviate much of the toil involved with adapting curricula.



Robert C. Cunningham is a field service engineer with the Babcock & Wilcox Co. and is based in their Denver office. He received his BSChE from Georgia Tech in 1972. He had co-op experience with the Savannah River Plant of the AEC in Aiken, S.C. The work described in this paper was performed as an undergraduate special project.

Jude T. Sommerfeld received his BSChE from the University of Detroit and MS and PhD from the University of Michigan. His activities include teaching, research and consulting in the areas of reactor design and computer applications. He has had 10 years of engineering and management experience with BASF-Wyandotte Corp., Monsanto Co., Parke, Davis & Co. and Ethyl Corp., and is a member of AIChE, ACS, and ISA. He is also a registered professional engineer in Georgia. (left photo)

The method for reducing curriculum information as it appears in a university catalog so that it can be accepted by a CPM computer program is quite easy. The individual courses are assigned activity numbers by which the computer can recognize them. An activity duration whether on a semester, quarter or any other time basis is given to each course. The prerequisite courses fill the

preceding activities category and the courses for which this particular course is a prerequisite fall into the succeeding activities category. If a certain course is required to be taken in a specified year of study or before a specified time in a program of study, the constraints can be accepted by the CPM program by listing a start time or finish time for that course.

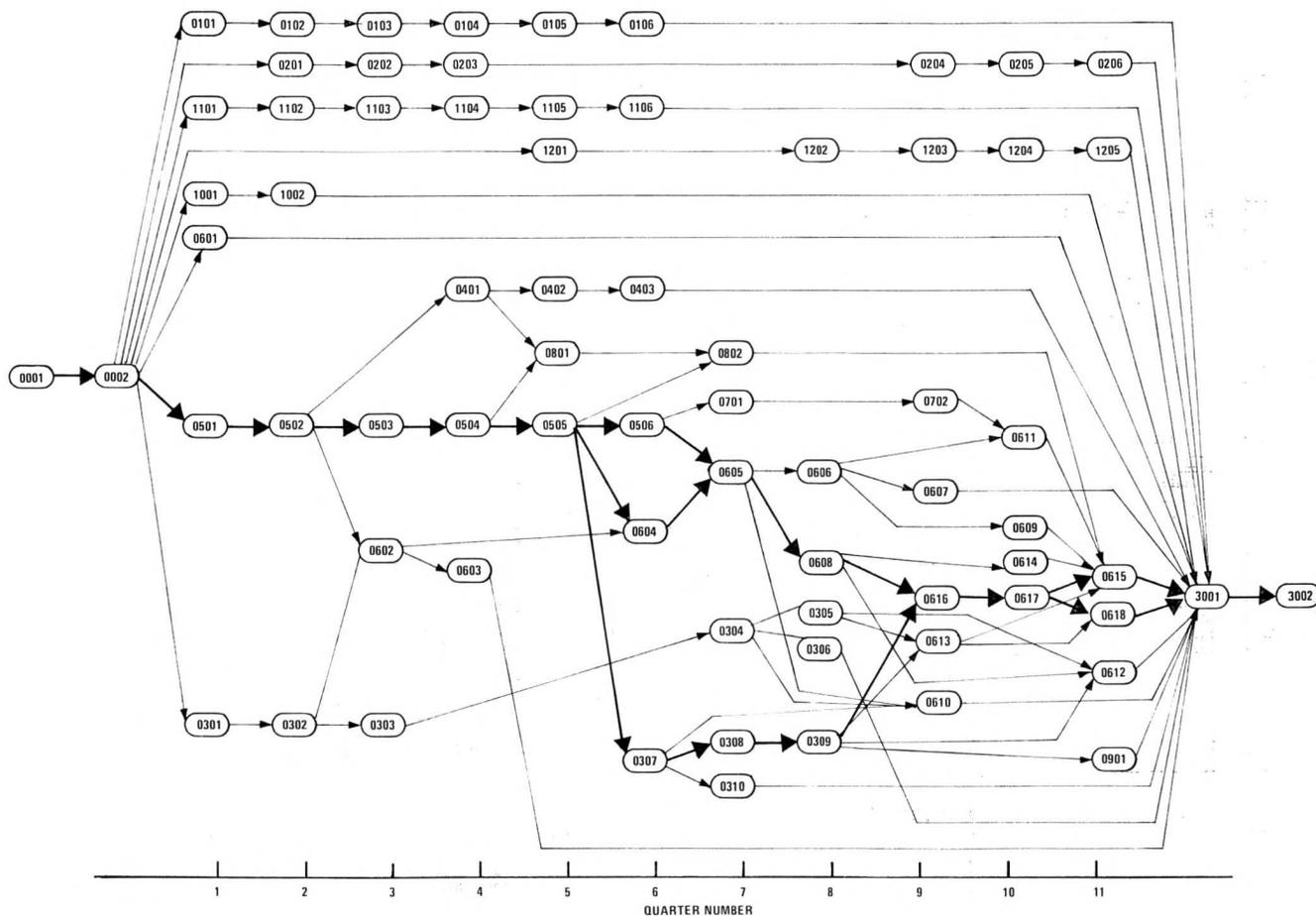


Fig. 2. CPM diagram of chemical engineering curriculum. Critical path activities are connected by heavy lines.

With this information the CPM program determines an earliest start time, latest finish time and slack for each course in the particular curriculum. All of the courses which comprise the critical path are fixed as to when they must be

The CPM diagram is helpful in testing time feasibility of proposed curricula and in offering a model which can answer some of the questions dealing with curricula practicality.

Table I. Accelerated Chemical Engineering Curriculum (Eleven Quarters).

Qtr. No.	Activity Number	Course Name	Cr. Hrs.	Prereq. Activities	Earliest Start	Latest Start	Slack
1	501	Calculus I	5	-	1	1	0
1	301	General Chemistry I	5	-	1	3	2
1	101	Humanities I	3	-	1	6	5
1	1101	Physical Training I	1	-	1	6	5
1	1001	Eng. Graphics I	3	-	1	10	9
1	601	Chem. Eng. Orientation	1	-	1	11	10
			18				
2	502	Calculus II	5	501	2	2	0
2	302	General Chemistry II	5	301	2	4	2
2	201	Social Science I	3	-	1	6	5
2	102	Humanities II	3	101	2	7	5
2	1102	Physical Training II	1	1101	2	7	5
2	1002	Eng. Graphics II	3	1001	2	11	9
			20				
3	503	Calculus III	5	502	3	3	0
3	303	General Chemistry III	4	302	3	5	2
3	602	Material Balances	3	302,502	3	5	2
3	202	Social Science II	3	201	2	7	5
3	103	Humanities III	3	102	3	8	5
3	1103	Physical Training III	1	1102	3	8	5
			19				
4	504	Calculus IV	5	503	4	4	0
4	401	Physics I	5	502	3	4	1
4	603	Energy Balances	3	602	4	11	7
4	203	Social Science III	3	202	3	8	5
4	104	Humanities IV	3	103	4	9	5
4	1104	Physical Training IV	1	1103	4	9	5
			20				
5	505	Calculus V	5	504	5	5	0
5	402	Physics II	5	401	4	5	1
5	801	Statics	3	401,504	5	9	4
5	1201	Elective I	3	-	1	7	6
5	105	Humanities V	3	104	5	10	5
5	1105	Physical Training V	1	1104	5	10	5
			20				
6	506	Differential Equations	5	505	6	6	0
6	307	Physical Chemistry I	3	303,402,505	6	6	0
6	604	Computers in Chem. Eng.	3	505,602	6	6	0
6	403	Physics III	5	402	5	11	6
6	106	Humanities VI	3	105	6	11	5
6	1106	Physical Training VI	1	1105	6	11	5
			20				
7	310	Physical Chemistry Lab.	2	307	7	11	4
7	308	Physical Chemistry II	3	307	7	7	0
7	605	Transport Phenomena I	4	506,604	7	7	0
7	304	Organic Chemistry I	3	303	4	8	4
7	701	Electric Fields-Circuits	3	402,506	7	8	1
7	802	Material Science	3	505,801	6	10	4
			18				
8	309	Physical Chemistry III	3	308	8	8	0
8	608	Stagewise Operations	4	605	8	8	0
8	606	Transport Phenomena II	4	605	8	9	1
8	305	Organic Chemistry II	3	304	5	9	4
8	306	Organic Chemistry Lab	2	304	5	11	6
8	1202	Elective II	3	1201	2	8	6
			19				
9	616	Thermodynamics I	3	309,608	9	9	0
9	607	Momentum-Heat Transfer	3	606	9	11	2
9	613	Chemical Kinetics	3	305,309,608	9	10	1
9	610	Chem. Eng. Literature	1	304,307,605	8	11	3
9	702	Elem. Electronics	3	701	8	9	1
9	1203	Elective III	3	1202	3	9	6
9	204	Social Science IV	3	203	4	9	5
			19				
10	617	Thermodynamics II	3	616	10	10	0
10	614	Chem. Eng. Economics	3	608	9	10	1
10	611	Process Instrumentation	3	606,702	9	10	1
10	609	Mass Transfer	4	606	9	10	1
10	1204	Elective IV	3	1203	4	10	6
10	205	Social Science V	3	204	5	10	5
			19				
11	618	Comprehensive Prob.	3	613,614,617	11	11	0
11	615	Chemical Plant Design	3	609,611,613	11	11	0
				614,617,802			
11	612	Polymer Science	3	305,309,608	9	11	2
11	901	General Metallurgy	3	309	9	11	2
11	1205	Elective V	3	1204	5	11	6
11	206	Social Science VI	3	205	6	11	5
			18				

Table II. Typical Chemical Engineering Curriculum (Twelve Quarters).

Qtr. No.	Activity Number	Course Name	Cr. Hrs.	Prereq. Activities	Earliest Start	Latest Start	Slack
1	501	Calculus I	5	-	1	2	1
1	301	General Chemistry I	5	-	1	4	3
1	101	Humanities I	3	-	1	7	6
1	1101	Physical Training I	1	-	1	7	6
1	601	Chem. Eng. Orientation	1	-	1	12	11
1	1201	Elective I	3	-	1	8	7
			18				
2	502	Calculus II	5	501	2	3	1
2	302	General Chemistry II	5	301	2	5	3
2	102	Humanities II	3	101	2	8	6
2	1001	Eng. Graphics I	3	-	1	11	10
2	1102	Physical Training II	1	1101	2	8	6
			17				
3	503	Calculus III	5	502	3	4	1
3	303	General Chemistry III	4	302	3	6	3
3	103	Humanities III	3	102	3	9	6
3	1002	Eng. Graphics II	3	1001	2	12	10
3	1103	Physical Training III	1	1102	3	9	6
3	1202	Elective II	3	1201	2	9	7
			19				
4	504	Calculus IV	5	503	4	5	1
4	401	Physics I	5	502	3	5	2
4	602	Material Balances	3	302,502	3	6	3
4	104	Humanities IV	3	103	4	10	6
4	1104	Physical Training IV	1	1103	4	10	6
			17				
5	505	Calculus V	5	504	5	6	1
5	402	Physics II	5	401	4	6	2
5	603	Energy Balances	3	602	4	12	8
5	105	Humanities V	3	104	5	11	6
5	1105	Physical Training V	1	1104	5	11	6
			17				
6	506	Differential Equations	5	505	6	7	1
6	403	Physics III	5	502	5	12	7
6	604	Computers in Chem. Eng.	3	505,602	6	7	1
6	106	Humanities VI	3	105	6	12	6
6	1106	Physical Training VI	1	1105	6	12	6
			17				
7	605	Transport Phenomena I	4	506,604	7	8	1
7	304	Organic Chemistry I	3	303	4	9	5
7	307	Physical Chemistry I	3	303,402,505	6	7	1
7	801	Statics	3	401,504	5	10	5
7	201	Social Science I	3	-	1	7	6
7	1203	Electives III	3	1202	3	10	7
			19				
8	606	Transport Phenomena II	4	605	8	10	2
8	305	Organic Chemistry II	3	304	5	10	5
8	308	Physical Chemistry II	3	307	7	8	1
8	310	Physical Chemistry Lab	2	307	7	12	5
8	802	Material Science	3	505,801	6	11	5
8	202	Social Science II	3	201	2	8	6
			18				
9	607	Momentum-Heat Transfer	3	606	9	12	3
9	608	Stagewise Operations	4	605	8	9	1
9	306	Organic Chemistry Lab	2	304	5	12	7
9	309	Physical Chemistry III	3	308	8	9	1
9	203	Social Science III	3	202	3	9	6
9	701	Elec. Fields Circuits	3	402,506	7	9	2
			18				
10	616	Thermodynamics I	3	309,608	9	10	1
10	612	Polymer Science	3	305,309,608	9	12	3
10	609	Mass Transfer	3	606	9	11	2
10	610	Chem. Eng. Literature	1	304,307,605	8	12	4
10	702	Elem. Electronics	3	701	8	10	2
10	204	Social Science IV	3	203	4	10	6
			17				
11	617	Thermodynamics II	3	616	10	11	1
11	613	Chemical Kinetics	3	305,309,608	9	11	2
11	611	Process Instrumentation	3	606,702	9	11	2
11	614	Chem. Eng. Economics	3	608	9	11	2
11	1204	Elective IV	3	1203	4	11	7
11	205	Social Science V	3	204	5	11	6
			18				
12	618	Comprehensive Prob.	3	613,614,617	11	12	1
				609,611,613			
12	615	Chemical Plant Design	3	614,616,802	11	12	1
12	901	General Metallurgy	3	309	9	12	3
12	206	Social Science VI	3	205	6	12	6
12	1205	Elective V	3	1204	5	12	7
			15				

started or completed; however, the remainder of the courses can be taken at any time within the constraints of the earliest start and latest finish times. In order to assist in selecting definite start dates for these courses which are not part of the critical path, various programs, e.g., RAMPS (Resource Allocation and Multiple Project Scheduling)\*, can be used to devise the final schedule. These programs distribute the various courses within the limits of their earliest start and latest finish times such that there will be a nearly constant number of credit hours per school term throughout the entire program of study.

A typical undergraduate chemical engineering curriculum is used as an example to illustrate the concept of CPM as a scheduling aid. Figure 2 is a CPM diagram of this curriculum wherein the activity numbers represent various courses (the two activities at the extreme left and the two activities at the extreme right, 0001, 0002, and 3002, are dummy activities and are included only to facilitate the operation of the particular CPM program which was used). This figure illustrates the role prerequisites play in scheduling courses.

Table I shows the final schedule which was derived from the CPM program. The earliest start times, latest finish times and slacks were provided by the CPM program enabling the critical path to be defined and also giving the shortest time for completion of the entire program of study. The courses which do not lie on the critical path and are accompanied by slacks were distributed manually, and the final product is a schedule which breaks the individual courses down into school quarters.

The actual schedule for this curriculum as it might have appeared in a university catalog is listed in Table II and consists of twelve quarters. The information obtained from the CPM program showed that the curriculum could be completed in an accelerated program of eleven quarters in which no more than 20 credit hours are required per quarter.

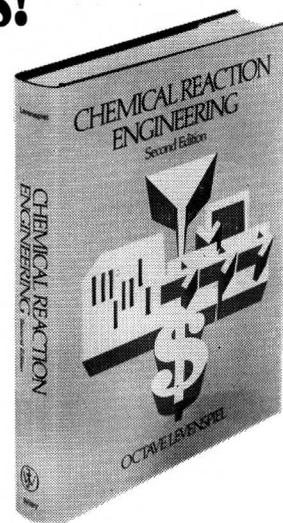
Referring once again to Figure 2 it is seen that the courses have been distributed among the eleven quarters of the accelerated program as they appear in Table I. This type of CPM diagram can be helpful not only in testing feasibility of the time considerations of proposed curricula but also in offering a model which can answer some of the questions dealing with curricula practicality. □

\*Kurzeja, J. T., *Hydrocarbon Processing*, April, 1965, p. 171.

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# THE INTERPHASE CATALYTIC EFFECTIVENESS FACTOR: Activity, Yield and Non-isothermality

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An essential component of any course in Chemical Reaction Engineering is the Diffusion-Catalytic Reaction topic. In an introductory course, it is deemed imperative that the student gain an insight into the key features which characterize the behavior of a reaction network in which diffusion of heat and/or mass affects the observed, global rate of catalytic reaction. In sum, how does heat and mass transport intrusions affect:

- activity for various reaction orders?
- Yield/selectivity for multipathed reaction networks?
- Observed reaction order and activation energy? and finally
- how can diffusional intrusions be detected in terms of laboratory observables?

We acknowledge two regions of diffusional transport in the typical porous solid catalyzed reaction:

- 1) Intraphase; diffusion of heat and mass within the porous catalyst with simultaneous reaction.
- 2) Interphase: Diffusion of heat and mass through boundary layers surrounding the catalyst pellet or extrusion. Reaction occurs in series with interphase (external) diffusion.

The global (observed) rate is that phrased in terms of observables. In general, external surface and internal concentrations and temperatures are beyond direct measurement. So a global rate,  $R_o$  is

$$R_o = k_x g(C_o)^\alpha$$

where  $k_x$  is a rate coefficient based upon observed rate, concentration  $C_o$  and order  $\alpha$ . The intrinsic, surface catalytic rate is, of course, a complex function of surface concentrations and temperature. Thus the concept of catalytic effectiveness (Thiele) was invoked and elaborated to relate the

intrinsic rate function to the observed functionality.<sup>1,2,3</sup>

Insofar as one or more steps of a complex, multipathed, reaction network can be altered by diffusion of heat and/or mass, yield/selectivity can be affected. By yield we mean the rate of desired product formation relative to that of key reactive consumption. Selectivity is merely the ratio of two-point yields.

## Isothermal Inter-intraphase Effectiveness and Yield

The modern undergraduate readily handles the problems of isothermal first order reaction with both external and internal diffusional events. For a flat plate

$$D \frac{d^2 C}{dx^2} = k_o C \quad (1)$$

with b.c.

$$x = L \quad k_g (C_o - C) = -D \frac{dC}{dx}$$

$$x = 0 \quad dC/dx = 0$$

the solution to which is in terms of overall catalytic effectiveness

$$\eta = \frac{\frac{1}{L} \int_0^L k_o C dx}{k_o C_o} \quad (2)$$

is

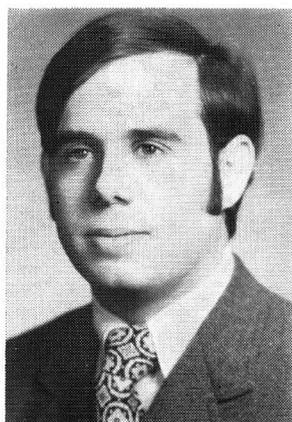
$$\eta = \frac{\tanh \phi}{\phi \left[ 1 + \frac{\phi \tanh \phi}{(Bi)_m} \right]} \quad (3)$$

where

$$\phi = L \sqrt{\frac{k_o}{D}} = \text{Thiele Modulus}; (Bi)_m = \frac{k_g L}{D} = \text{Mass Biot Number}$$

The diffusion affected yield for consecutive reaction is also readily analyzed by the undergraduate for isothermal conditions.<sup>2,4</sup>

However, for nonlinear kinetics and non-isothermal environments, analytical solutions are not to be found, and the more sophisticated approximate mathematical treatments are usually beyond the undergraduate, or if within his grasp, the very journey through that mathematical jungle may cause the student to lose sight of the physics of the problem and the engineering consequences. A simple alternative exists requiring no more than the use of a slide rule, whereby key features of the more complex internal diffusion-



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Germain Cassiere is from Shreveport, La. and attended the University of Notre Dame, graduating magna cum laude with a BSChE in May 1972. He is a member of Tau Beta Pi and was employed during previous summers with the chemical process division of Universal Oil Products in Shreveport. Presently, he is attending Louisiana State University Medical School in New Orleans.

reaction problem become manifest. We simply deal with the external (interphase) problem.

### Isothermal External Diffusion-Reaction

In steady state reaction of  $n$ th order over a flat nonporous catalytic plate, equating mass transport to surface reaction, we have

$$k_g a (C_o - C) = k_s C^n \quad (4)$$

Dividing by  $k_g a C_o$ , where  $f = C/C_o$

$$1 - f = \left[ \frac{k_o C_o^{n-1}}{k_g a} \right] f^n = Da_o f^n \quad (5)$$

where

$$Da_o = \frac{k_o C_o^{n-1}}{k_g a} = \text{Damköhler Number}$$

External isothermal effectiveness is

$$\eta = \frac{\text{Actual Surface rate at } C}{\text{Rate if } C = C_o} \quad (6)$$

or

$$\eta = \frac{k_o C^n}{k_o C_o^n} = \left( \frac{C}{C_o} \right)^n = f^n$$

Equation (5) is easily solved for  $n = 1, 1/2, 2$  and  $-1$ . The negative first order reflects abnormal kinetics (i.e. rate increases with conversion). Such a case is found in transition metal

catalyzed oxidation of CO at CO concentrations above 1%.<sup>5</sup> The solutions are:

$$n = 1 \quad \eta = \frac{1}{1 + Da_o} \quad (7)$$

$$n = 1/2 \quad \eta = \sqrt{\frac{(2 + Da_o^2)}{2} \left[ 1 - \sqrt{1 - \frac{4}{(2 + Da_o^2)^2}} \right]} \quad (8)$$

$$n = 2 \quad \eta = \left[ \frac{\sqrt{1 + 4 Da_o} - 1}{2 Da_o} \right]^2 \quad (9)$$

$$n = -1 \quad \eta = \frac{2}{1 + \sqrt{1 - 4 Da_o}}, \text{ no solution exists for } Da_o > 1/4 \quad (10)$$

These external isothermal effectiveness factors are displayed in Figure 1 on log-log co-ordinates. The similarity to internal effectiveness behavior for linear and nonlinear kinetics is evident. We learn by this simple arithmetic manipulation that

- The greater the reaction order, the greater the diffusional taxation for a given value of  $Da_o$ .
- An effectiveness greater than unity is possible if an adsorbable species inhibits the rate.
- At large values of the modulus, all  $\eta$  values approach the reciprocal of the modulus.

Now the global rate is, of course,

$$R_o = \eta k_o C_o^n \quad (11)$$

At large values of  $Da_o$ ,  $\eta \rightarrow 1/Da_o$

$$R_o = \frac{k_o}{\frac{k_o C_o^{n-1}}{k_g a}} \cdot C_o^n = k_g a C_o$$

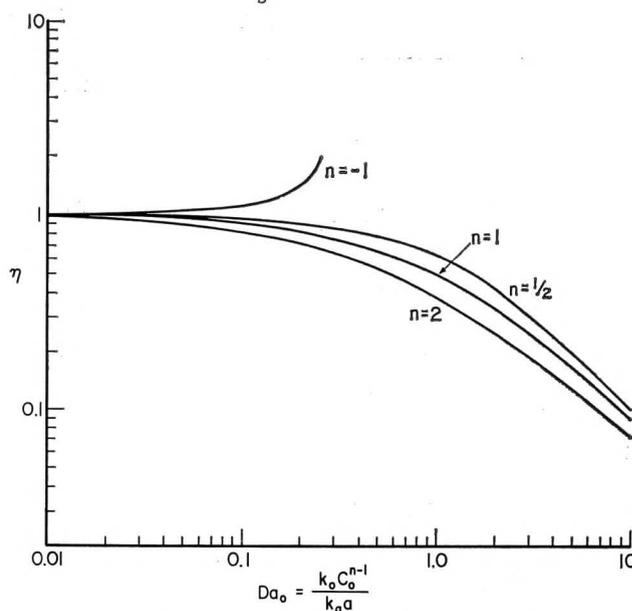


Fig. 1. Isothermal External Catalytic Effectiveness for Reaction Order  $n$

so the experimental rate coefficient  $k_x$  is  $k_g a$  and the reaction order changes from  $n$  to unity. Activation energy changes from its true value when  $\eta = 1$  to a small value characteristic of a mass transfer coefficient  $k_g a$ .

The students readily realize however that Fig. 1, while instructive, is of little use unless  $k_o$  is known *a priori* to permit computation of  $Da_o$ . They soon learn that Fig. 1 is easily re-expressed in terms of observables. Dividing both sides of equation (11) by  $k_g a C_o$

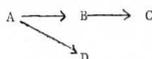
$$\frac{R_o}{k_g a C_o} = \eta \frac{k_o}{k_g a} C_o^{n-1} = \eta Da_o \quad (12)$$

Hence by replotting Fig. 1 in terms of  $\eta$  vs  $\eta Da_o$ , we secure Fig. 2 which permits determination of  $\eta$  from the observed rate  $R_o$ , bulk concentration  $C_o$  and a calculatable transport coefficient  $k_g a$ . Fig. 2 also teaches that the ultimate observed rate is that of bulk mass transport, i.e., at  $\eta Da_o = 1$ . Aris\* points out that by eq's (7-10) and (5) Figure 2 obeys the equation:

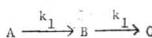
$$\eta = (1 + \eta Da_o)^n$$

### Isothermal Yield/Selectivity

A multipathed network, such as



is obviously a combination of consecutive and simultaneous reaction. Consider consecutive reaction



In the absence of mass diffusional limitations, surface concentrations equal those in the bulk stream, so for linear kinetics

$$-R_A = k_1 A_o \quad (13)$$

$$R_B = k_1 A_o - k_2 B_o$$

Dividing, we secure the point yield

$$-\frac{dB}{dA} = Y_B = 1 - \frac{k_2}{k_1} \frac{B_o}{A_o} \quad (14)$$

Anticipating diffusion, then

$$k_g a (A_o - A) = k_1 A \quad (15)$$

$$k_g a (B - B_o) = k_1 A - k_2 B \quad (16)$$

and solving for B, then the ratio of rates (yield)

Solving for A in (15), substituting in (16)

is

$$-\frac{dB}{dA} = Y_B = \frac{1}{1 + Da_2} - \frac{k_2}{k_1} \frac{(1 + Da_1)}{(1 + Da_2)} \frac{B_o}{A_o} \quad (17)$$

or

$$Y_B = \eta_2 - \frac{\eta_2 k_2}{\eta_1 k_1} \frac{B_o}{A_o} \quad (18)$$

\*Aris, R. Personal Communication Sept. 1972.

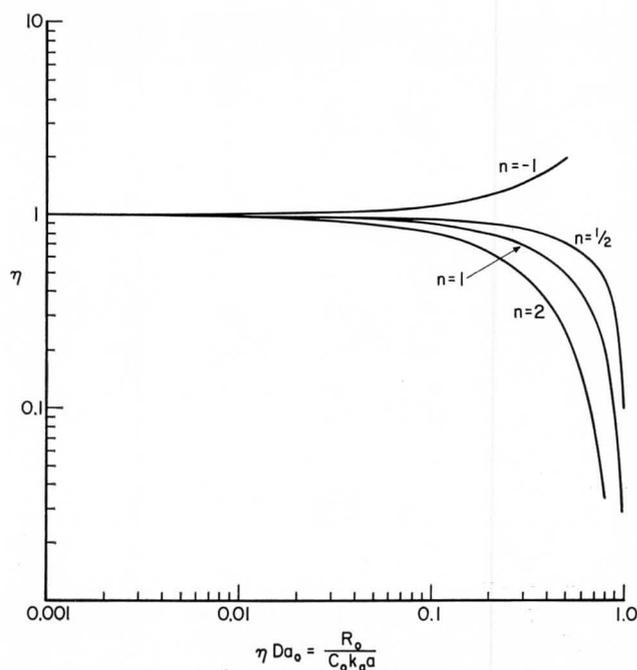


Fig. 2. Isothermal External Catalytic Effectiveness in terms of Observables for orders  $n$

When  $B_o = 0$ , initial point yield is

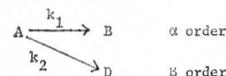
$$-\frac{dB}{dA} = \frac{1}{1 + Da_2} \quad (19)$$

or selectivity is, when  $B_o = 0$

$$\frac{dB}{dC} = \frac{1}{Da_2} = \frac{k_g a}{k_2} \quad (20)$$

Thus with mass diffusion, the survival of B depends upon the ratio of the escape rate from the surface to its rate of destruction on the surface.

For simultaneous reaction



Selectivity, 
$$s = \frac{dB}{dD} = \frac{k_1}{k_2} A_o^{\alpha-\beta} \quad (21)$$

With no diffusional gradient

$$S_o = \frac{k_1}{k_2} A_o^{\alpha-\beta} \quad (22)$$

OR

$$\frac{S}{S_o} = \frac{k_1/k_2}{(k_1/k_2)_o} \left( \frac{A}{A_o} \right)^{\alpha-\beta} \quad (23)$$

Isothermal selectivity alteration is then

$$s/s_o = \left( \frac{A}{A_o} \right)^{\alpha-\beta} \quad (24)$$

As  $A < A_o$ , we readily see that when  $A < A_o$  (diffusion intrusion)

$\alpha = \beta$  no affect upon selectivity

$\alpha > \beta$  selectivity for B declines

$\alpha < \beta$  selectivity for B improves

This finding follows from Fig. 1: The reaction of highest order is most taxed by mass diffusion.

## Non-isothermal Effectiveness and Yield

Here the analysis in terms of external effectiveness is truly fruitful since the corresponding internal problem is only solved rigorously by numerical means even for linear kinetics.<sup>6,7,8,9</sup>

The non-isothermal external effectiveness is

$$\bar{\eta} = \frac{k}{k_0} \left( \frac{C}{C_0} \right)^n \quad (25)$$

The linear case is quite easily handled in terms of observables as follows:\*

\*In view of equations (5) and (25), the non-isothermal external effectiveness for any order is

$$\bar{\eta} = \frac{k}{k_0} (1 - \bar{\eta} Da_0)^n$$

k the rate coefficient as the surface temperature is, relative to  $k_0$

$$k = k_0 \exp \left[ -\epsilon \left( \frac{1}{t} - 1 \right) \right] \quad (26)$$

where  $\epsilon = E/RT_0$  and  $t = T/T_0$

$$\text{also } \frac{C}{C_0} = \frac{1}{1 + Da} \text{ and } Da = Da_0 \exp \left[ -\epsilon \left( \frac{1}{t} - 1 \right) \right] \quad (27)$$

$$\text{so } \bar{\eta} = \frac{\exp \left[ -\epsilon \left( \frac{1}{t} - 1 \right) \right]}{1 + Da_0 \exp \left[ -\epsilon \left( \frac{1}{t} - 1 \right) \right]} \quad (28)$$

$$\text{rearranging } \bar{\eta} = (1 - \bar{\eta} Da_0) \exp \left[ -\epsilon \left( \frac{1}{t} - 1 \right) \right] \quad (29)$$

Note that  $\bar{\eta} Da_0 = \frac{R_0}{C_0 k_0 a}$ , is the observable.

We now evaluate  $t$  by heat balance

$$ha(T - T_0) = (-\Delta H) R_0$$

we divide both sides by  $k_g a C_0 T_0$

$$\frac{h}{k_g C_0} (t-1) = \left( \frac{-\Delta H}{T_0} \right) \frac{R_0}{k_g a C_0} = \left( \frac{-\Delta H}{T_0} \right) \bar{\eta} Da_0$$

Invoking the  $j$  factor analogy

$$\frac{k_g}{u} (Sc)^{2/3} = \frac{h}{\rho u C_p} (Pr)^{2/3}$$

then

$$\frac{h}{k_g} = \rho C_p \left( \frac{Sc}{Pr} \right)^{2/3}$$

thus

$$t = 1 + \left[ \frac{(-\Delta H) C_0}{\rho C_p T_0} \right] \bar{\eta} Da_0 (Le)^{2/3} \quad (30)$$

or

$$t = 1 + \beta \bar{\eta} Da_0 \text{ where } \beta = \left[ \frac{(-\Delta H) C_0}{\rho C_p T_0} \right] (Le)^{2/3}$$

and  $Le$  is the Lewis number  $D/\alpha$ .

The student now chooses a value of  $\epsilon$ , and  $\beta$  as fixed. Then for a series of  $\bar{\eta} Da_0$  values (say 0.001 to the limiting value of unity), he or she\* computes  $t$  and by equation (29) the  $\bar{\eta}$  -  $\bar{\eta} Da_0$  values are obtained. This simple procedure is re-

\*Ycs, Virginia, there is a co-ed Notre Dame

peated at other positive (exothermic) and negative (endothermic) value of  $\beta$  for the fixed  $\epsilon$ . Results are shown in Figs. 3 and 4 for  $\epsilon$  of 20 and 10, and a range of  $\beta$  values.

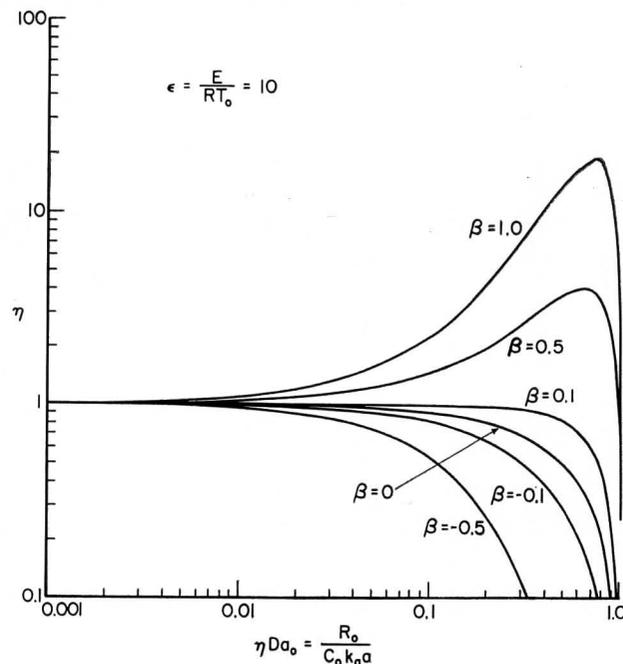


Fig. 3. Non-Isothermal External Catalytic Effectiveness in terms of Observables—First Order,  $\epsilon = 10$

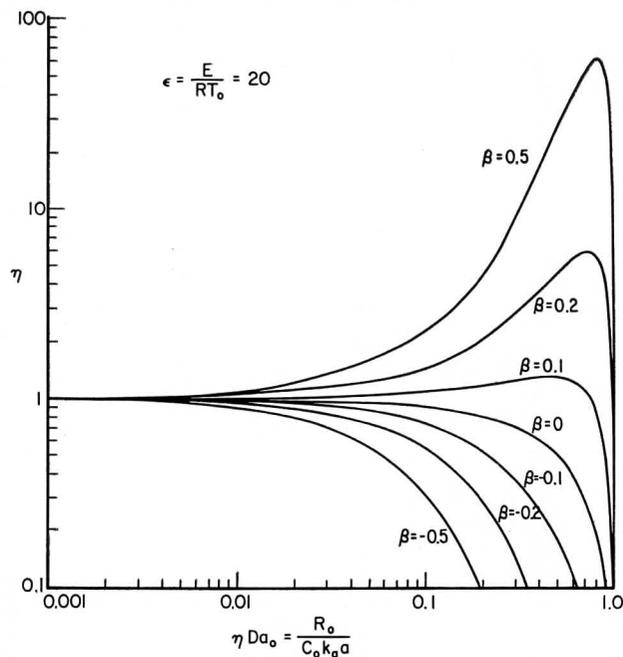


Fig. 4. Non-Isothermal External Catalytic Effectiveness in terms of Observables—First Order,  $\epsilon = 20$

We see that the chief characteristics of the non-isothermal intraphase (internal) effectiveness factor are displayed by the very easily calculated external effectiveness behaviour:

- (a)  $\bar{\eta}$  values much greater than unity are found for exothermic reactions.
- (b) the Arrhenius number,  $\epsilon$  is more important than  $\beta$  in determining  $\bar{\eta}$  and
- (c) at high values of the modulus  $\bar{\eta}$  falls well below unity.

Yield/selectivity in a non-isothermal atmosphere is readily treated. In equations (17) and (23), the ratio  $k_1/k_2$  at surface temperature appears. This ratio relative to its value at bulk temperature  $T_0$ , is

$$\frac{(k_1/k_2)_T}{(k_1/k_2)_0} = \exp \left[ -\Delta\epsilon \left( \frac{1}{T} - 1 \right) \right]$$

where

$$\Delta\epsilon = \epsilon_1 - \epsilon_2 = \frac{(E_1 - E_2)}{RT_0}$$

A valuable qualitative insight into non-isothermal yield/selectivity trends is secured by the student by consideration of Fig. 5.

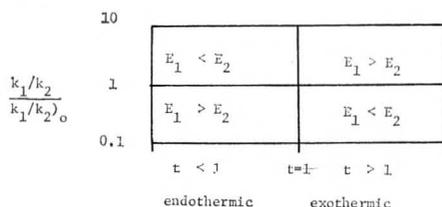


Fig. 5. Yield/Selectivity Trends in Non-Isothermal Atmosphere.

In the light of Fig. 5, consider non-isothermal selectivity in simultaneous reaction, equation (23)

$$\frac{S}{S_0} = \frac{k_1/k_2}{(k_1/k_2)_0} \left( \frac{A}{A_0} \right)^{\alpha-\beta} \quad (23)$$

From a knowledge of the sign of  $\Delta\epsilon$  and the thermochemistry of the reactions, the student can predict whether mass and heat transfer limitation will enhance or tax selectivity, or over a range of conditions the heat transport limitation may just compensate the taxation of mass transport.

### Transient Isothermal Effectiveness

The analysis of transient external effectiveness is also simple yet instructive. Consider a case where reactant is exposed to the catalytic surface at  $\tau = 0$ . A first order reaction is assumed under isothermal conditions. What is the  $\eta\tau$  relationship?

$$k_g a(C_0 - C) = kC + \frac{dC}{d\tau}$$

or

$$1 - \eta = Da_0 \eta + \frac{d\eta}{d\theta}$$

where

$$\eta = C/C_0 \text{ and } \theta = k_g a \tau$$

the desired solution is

$$\eta = \frac{Da_0 + \exp \theta}{(1 + Da_0) \exp \theta}$$

Which is more conveniently expressed in terms of  $\eta$  at any time relative to  $\eta_{ss}$  at final steady-state.

$$\frac{1 - \eta}{1 - \eta_{ss}} = \frac{\exp \theta - 1}{\exp \theta}$$

This equation teaches that the dimensionless group  $k_g a \tau$  determines the rate of approach to steady-state. In the case of the internal effectiveness in transient, approach to steady-state is governed by an analogous dimensionless group

$$\theta^* = \frac{D\tau}{L^2}$$

where  $D$  is internal diffusivity and  $L$  the pellet dimension<sup>10</sup>

### Practical Applications

While the primary purpose of the development of external effectiveness is its instructive value in shedding light on the internal problem, it should not be forgotten that there exists some quite important catalytic systems involving gaseous reaction over nonporous catalysts. For example,  $NH_3$  is oxidized to  $NO$  and  $HCN$  is synthesized from  $NH_3$ ,  $O_2$  and methane over platinum alloy wire matrices. Methanol may be oxidized to formaldehyde over nonporous silver. Such systems are susceptible to analyses in terms of the external effectiveness.

### Conclusions

The diffusion-reaction problem is profitably viewed in terms of external mass and heat transport affected activity and selectivity in a simple analytical fashion with readily calculated results which bear very fruitful analogy to features revealed by the often much more difficult-to-solve internal diffusion-reaction problems.  $\square$

### REFERENCES

1. Thiele, E., *Ind. Eng. Chem.* **31**, 916 (1939).
2. Wheeler, A. in *Catalysis* (P. H. Emmet, Ed.). Vol. 2 Reinhold, N. Y. 1955.
3. Weisz, P. B., *Z. Physik. Chem. N.F.* **11**, 1 (1957).
4. Carberry, J. J., *Chem. Eng. Science* **17**, 675 (1962).
5. Tajbl, D. G., Simons, J. and Carberry, J. J., *Ind. Eng. Chem. (Fund.)* **5**, 171 (1966).
6. Carberry, J. J., *A.I.Ch.E. J.* **7**, 350 (1961).
7. Tinkler, J. D., and Metzner, A. B., *Ind. Eng. Chem.* **53**, 663 (1961).
8. Weisz, P. B., and Hicks, J. S., *Chem. Eng. Science* **17**, 265 (1962).
9. Hutchings, John and Carberry, J. J., *A.I.Ch.E. J.* **12**, 30 (1966).
10. Hutchings, John, Ph.D. Thesis, Chem. Eng., Univ. of Notre Dame (1968).

# He's locked into childhood by a disease that's already licked.

What happened was measles. Common measles. And what's tragic is that it should never have happened at all.

To most people, measles is simply a childhood nuisance. But statistics don't bear them out.

During the height of the measles season, 10,000 children are stricken every three days. 60 are hospitalized, 10 develop inflammation of the brain, 3 become mentally retarded. And one dies.

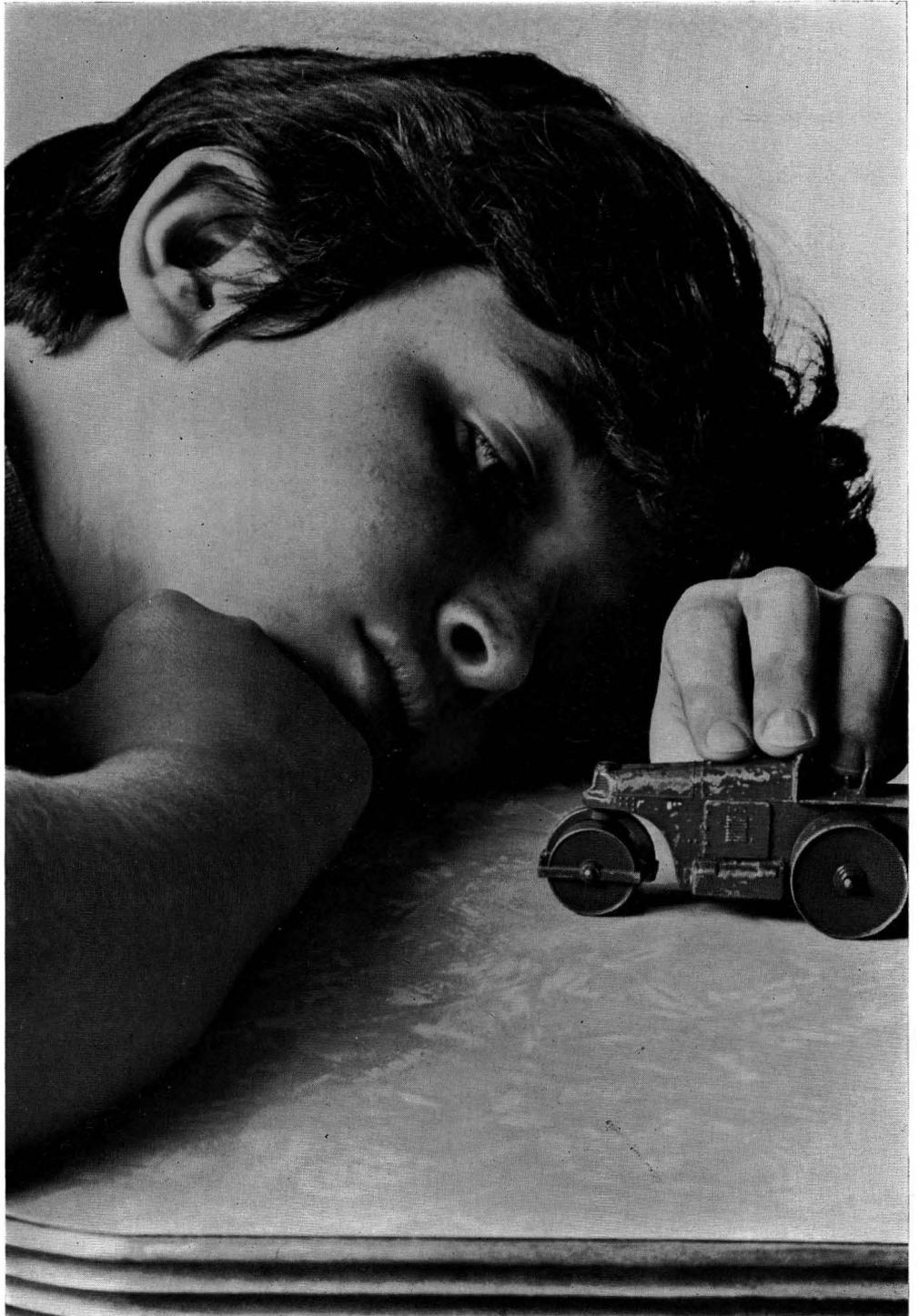
There's just no excuse for this disastrous waste. Since 1965, the measles vaccine developed by Dow has more than proved its worth. And the cost of immunization is low compared to the consequences of the disease, the staggering expenditure in medical care and the enormous number of school days missed.

But after several years of dramatic decline, measles is now galloping back. Because even the best preventive is powerless if people refuse to use it.

The answer is not more of our vaccine. There's already plenty of that. It's community awareness of the threat measles poses to our children. And community action to stop the disease in its tracks.

At Dow, we're concerned with more than chemistry. We're concerned with life. And despite our imperfections, we're determined to share its promise. Wisely.

For a booklet on measles vaccination and your children, write to: The Dow Chemical Company, Midland, Michigan 48640.



## ChE book reviews

*Chemical Plant Simulation*, Crowe, Hamielec, Hoffman, Johnson, Shannon, Woods, xiv+368 pp., Prentice-Hall, Englewood Cliffs, N. J., 1971.

Process engineers have long used computers to provide refined, detailed studies of individual process equipment. But the real virtue of large, high-speed computers is the ability to classify, file, and analyze masses of data. With a sufficiently powerful computer system, we are able to analyze complete processes. This attractive prospect has led to many attempts to build up special systems for chemical analysis. In a recent survey, I was able to identify 31 distinct systems; many more undoubtedly exist in proprietary situations. Most of these are directed towards "simulation," but this differs greatly from the stochastic simulation of the systems engineers. For chemical plants, simulation means the generation and calculation of the many material, heat, and pressure balances needed to relate the flows, temperatures, pressures, and compositions in a complex process. Simulation can be applied to the material balance studies of a process under design; it can be used to provide cases for scheduling an operating process; or it can be used for control studies of an existing plant.

Of course, a simulation really evaluates only one operating condition or one design. The job of the process engineer is to make decisions; for him, simulation is just a first step, — he must explore many possible solutions, changing the simulation variables through changes in input data. This is really optimization, but optimization systems seem to be either too specialized or unable to accommodate efficiently the general building-block units of the process simulators. In any event, the recent widespread use of simulation systems in industry indicates that these systems do perform useful tasks. At the very least they provide an improved, up-to-date way of assembling and retaining the data needed for complex processes. To be efficient and competitive, all process engineering groups today must be facile in their use. Thus, the young engineer's first process assignment often involves computer simulation.

How do we take account of this in the chemical engineering curriculum? One solution,—fully demonstrated in a number of universities in the U.S. and Canada, — is to have students work realistic process simulations using a well-

maintained computer system. The group at McMaster University, headed for many years by Prof. Ab Johnson, built up an expertise in this area through joint cooperative effort of students and faculty in several full-scale simulation studies. This effort was based on the PACER system first developed at Purdue by Prof. Paul Shannon and his student, Mosler, in 1964. The important results of this collaboration are now available in a well-constructed and carefully edited book. The preliminary paper-bound version has been in use at McMaster and elsewhere since 1969. With so many tables, figures, and charts, the new edition is much easier to use.

Of course, the use of simulation studies in the undergraduate curriculum does require time. The student should not be asked to make such studies if it detracts from his ability to think about the process. If his major concern becomes one of getting the cards punched in the right places, rather than thinking about the effect of the numerical input values on the properties and flows, then the simulation study is not really worthwhile. Adequate time must be provided to evaluate carefully the significance of the process behavior underlying the simulation. However, if the system is properly used, simulations supply a good idea of the nature of real processes. Simple examples may give the student a clear understanding of process structure, but may also mislead him, through oversimplification of complex relationships.

The book is oriented to, and illustrated with, a specific system, PACER (and in particular the McMaster version, MACSIM), but it is a suitable introduction to many of the general ideas and principles of simulation. In spite of differences in programming and data handling, all of these simulation systems rely on the same basic ideas:

1. The existence of general-purpose equipment modules interrelated by streams.
2. The use of equipment vectors to store the particular characteristics of the equipment involved in a particular process.
3. The use of stream vectors to describe the properties of the streams, and more generally, of the information flow.
4. The characterization of the information flowsheet in terms of a process matrix.
5. The use of numerical iteration to calculate systems with recycle.
6. The ability to develop and use in the

simulation system general-purpose prediction routines or data libraries for physical and chemical properties.

Many of these concepts are fundamentally simple and are illustrated in elementary courses in stoichiometry and thermodynamics through simple, clearly described examples. However, computer application to large, practical problems results in system complexity and in multiplicity of detail. It is difficult to impress the undergraduate with the nature of this complexity and at the same time keep him from complete confusion. The straightforward how-to-do-it approach in this text is a good solution. Careful study of the text, with a simultaneous application to a realistic example project should give the student a good appreciation of the value of computers in process analysis.

The first two chapters provide an elementary introduction of the basic ideas, using simple process flows and simple equipment modules for mixing, separation, etc. In these chapters, there is a description of the recycle problem and its solution by iteration, and a brief review of techniques for analyzing process structure. Chapter 3 introduces PACER and describes the many control elements needed for this specific system. Even though the reader may be using some other simulation system, the specific description supplied may be the best way to understand clearly the nature and extent of control information required by large systems.

The central portion of the book is a detailed description, section by section, of the classic McMaster example, the contact sulphuric acid plant simulation. After a general description of the plant (Chapter 4), the two major decisions about modelling are described (Chapter 5). This is one of the most important chapters in the book since it emphasizes the way in which the engineer can control the sophistication, adaptability, and accuracy of the simulation at the expense of greater development time, more knowledge of basic data, and greater demands on the computer. Then, (Chapters 6-10), the various types of equipment modules are developed in some detail, using those for the sulphuric acid plant as basic examples. Here, the need for various levels of sophistication is described and illustrated. In spite of the specific nature of the examples, the discussion covers all the major types of equipment. Moreover, the problems at the end of each chapter are often oriented to other systems which have been studied by the McMaster group. In Chapter 11,

the authors describe the use of the simulation, and the results obtained in some particular studies of the sulphuric acid plant. With a thorough study of these chapters, the reader should be able to apply PACER to other chemical processes with which he is familiar. And he would probably find it helpful even with another simulation system. Often, the users' manual is written for skilled or experienced engineers. Here, the descriptions and illustrations are definitely oriented to use as a text, or basic reference. In addition to the bare details, the book also includes a full description of some of the tricks which are essential for efficient simulation of real processes. For example, the sulphuric acid plant simulation uses a special pressure module to handle the pressure balances in the system without excessive information recycle.

In the closing chapters, several more general ideas are covered. Chapter 12 briefly describes optimization, using small-dimension direct-search techniques. Of course, optimization is the only efficient way to make decisions in large, multi-variable problems, yet the need for optimization is not always recognized. In the survey mentioned earlier, only CHEOPS (which does not take advantage of the new developments in computers) and RPMS (which is limited to linear models) are truly oriented to optimization. The other systems, like PACER, require excessive duplication in the computation of each case. Optimization calls for several thousand cases in a typical direct search of ten to fifteen variables. Early versions of PACER are much too clumsy and slow to make such computations efficiently, since each case is treated as a complete simulation. There has recently been some recognition of this handicap, and it is possible that some of the proprietary systems now short-cut duplicated computation. But the description in Chapter 12 is little more than an introduction to basic ideas which can only be applied in a limited way to PACER models.

Chapter 13 is much more successful and important. This is a critique and summary of the strategy of tackling a simulation. It includes a detailed and complicated flowchart of simulation procedures which is well worth careful study. The authors are among the most experienced users of simulation. Their comments about their past experience are intelligent and significant. Finally, Chapter 14 provides a look ahead to possible future developments in the use of simu-

(Continued on page 32)

# THE POLYMER PROGRAM AT CALTECH

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The California Institute of Technology (Caltech) is a small private school with a total enrollment of about 1500 students, about half of whom are graduates. The faculty consists of about 250 professors of all ranks, about 130 visiting professors and associates, and some 240 research (postdoctoral) fellows. With this unusual student-faculty ratio classes at Caltech are generally small, interpersonal relations are fostered, and course programs and research activities tend to be closely interwoven.

These typical Caltech tendencies are reflected in the Polymer Program in Chemical Engineering. Two lecture courses and a laboratory course are offered as part of the ChE program. The research group in the Polymer Laboratory currently comprises six graduate students, a visiting scientist, and three research fellows, representing five different countries. The polymer activities of the Polymer Research Section of Caltech's Jet Propulsion Laboratory are brought to the campus by its head, Dr. R. F. Landel, and Member of the Technical Staff, Dr. A. Rembaum. Both serve as part-time Lecturers in Chemical Engineering. A series of weekly seminars keeps the group in touch with advances being made in the study of polymers outside of the Caltech community.

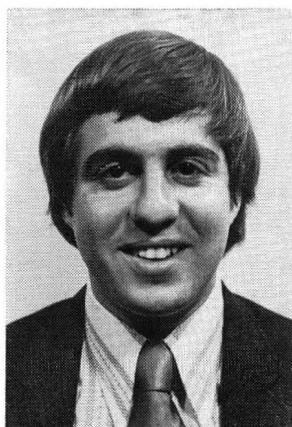
## COURSES

A basic course, Polymer Science, is offered for graduate students and for those undergraduates who have had a sufficient background in physical and organic chemistry. The first term's lectures, presented by A. Rembaum, cover polymer chemistry. Topics discussed include: the nature and classification of polymers, methods of synthesis, polymerization kinetics and molecular weight distribution, copolymerization and cross-linking. The second and third terms' lectures are given by N. W. Tschoegl. During the second term, attention is focused on the physical char-

acterization of polymers by solution methods and physical methods in bulk. A detailed treatment of polymer properties is the subject of the third term which includes a discussion of the principles of polymer technology. Throughout the course the emphasis is on an understanding of polymer properties in terms of polymer structure.

During the third term, students can elect to take the Polymer Science Laboratory course. This course has been developed by R. E. Cohen on a trial basis over the past two years and was offered for credit for the first time in 1971-72. The laboratory course acquaints students with a selection of techniques employed in the synthesis and characterization of polymeric materials. The techniques have been chosen for their practical importance and instructional value. The student first synthesizes a polymer, following the kinetics of the free radical polymerization reaction. He then characterizes his reaction product by determining number average and viscosity average molecular weights and the glass transition temperature. Finally, he studies the mechanical properties of his polymer by carrying out stress relaxation measurements. A laboratory manual with a discussion of the procedures and background material has been prepared for the course.

Polymer Science is essentially an introductory course, although the presentation is fairly advanced, being on the level of P. J. Flory's *Principles of Polymer Chemistry*. The course alternates every second year with a more specialized course on the Mechanical Behavior and Ultimate Properties of Polymers, open to graduate students. Students enrolling in the latter course are expected to have completed studies equivalent to the Polymer Science course. The course begins with an introduction to the theory of viscoelastic behavior. The discussion centers on material functions and their interconversion, model representation, time-temperature equiva-



Robert E. Cohen obtained his BSChE degree with distinction from Cornell University and his ('72) PhD from Caltech. He is currently a Research Fellow at Caltech, and will take up a similar position in the Department of Engineering Science at Oxford University in England in the Fall of 1972. In the Fall of 1973 he will be an Assistant Professor at MIT. (right photo)

Nicholas W. Tschoegl obtained the degree of BSc (Hons.) in Physical Chemistry for the New South Wales University of Technology in Sydney, Australia, and the ('58) PhD degree from the same institution which is now the University of New South Wales. He spent two years each at the University of Wisconsin and Stanford Research Institute before coming to Caltech in 1965.

lence, and the molecular theories of polymer behavior. During the second term consideration is given to the mechanical behavior of various polymer systems including amorphous, crystalline, and cross-linked polymers, copolymers, elastomers, filled and plasticized systems, blends and melts, and to the elements of large deformation theory. The first two terms' lectures are given by N. W. Tschoegl. The third term, presented by R. F. Landel, is devoted to a discussion of the phenomenology and the molecular and statistical theories of rupture in polymeric materials. Throughout the course special attention is given to controlling molecular parameters.

In accordance with Caltech's small enrollment, a typical class in the polymer courses consists of about ten students. Thus an informal atmosphere and close interpersonal contacts are insured. Each student prepares an individual term paper on a topic related to the course once during this academic year. These papers are presented in form of a lecture to the class and the research group in a common seminar. Graduate teaching assistants (drawn from the research group) are given opportunities for preparing and presenting lectures within the framework of each course.

## RESEARCH

Research activities in the Polymer Laboratory are directed toward obtaining an understanding of the molecular basis of the engineering properties of rubbery materials (elastomers). The majority of the research projects is of an experimental nature, dealing with the study of elastomeric materials through the measurement of various mechanical properties. Theory is developed as needed as an integral part of the research activity.

Mechanical tests with both transient and dynamic loading patterns are used to evaluate the properties of a variety of elastomers at atmospheric pressure, in isothermal and isochronal modes of testing. A new rheometer with a wide modulus, frequency, and temperature range has been developed. Two Instron testers are available for large deformation studies.

The Polymer Laboratory is uniquely equipped for the study of pressure effects on polymer properties. Pressurized testing equipment is being used to study the pressure dependence of mechanical properties, failure criteria for filled and unfilled elastomers in uniaxial and biaxial deformation under superposed hydrostatic pressure, and the internal energy contribution to rubber elasticity.

With the help of A. Rembaum, some synthesis is carried out in conjunction with the research effort. The capability of synthesizing particular polymers as part of the mechanical properties research distinguishes the Caltech program from most polymer programs in other ChE Departments. The laboratory has a high-vacuum apparatus which is used for the anionic polymerizations of block copolymers. The synthesis of special elastomers containing a known amount of chains tagged at both ends by a heavy atom is expected to lead to X-ray scattering studies of the end-to-end separation of chains as a function of temperature and strain. Ample characterization equipment is available so that the molecular structure of newly synthesized materials can be determined.

A good deal of the effort is concerned with the properties of novel elastomers. Thus, triblock copolymer elastomers (thermoplastic rubbers) are used as model substances for the elucidation of properties which are difficult to study in conventional elastomers. These studies have led to the development of a theory for the superposition of time and temperature effects in thermorheo-

**With this unusual student-faculty ratio, classes at Caltech are generally small, interpersonal relations are fostered, and course programs and research activities tend to be closely interwoven.**

logically complex two-phase polymer systems. A study was also made of terminal chains and their entanglements in triblock-diblock blends in which the proportion, length, and distribution of the terminal chains could be controlled. A study of rubbers consisting of two interpenetrating networks is expected to begin in the Fall of 1972.

Research activities are not restricted to the Polymer Laboratory. Thus, within Chemical Engineering, Professors W. H. Corcoran and N. W. Tschoegl collaborate in an effort to assess the effect of mechanical deformations on diffusion through membranes. A joint effort on segmental motion by NMR techniques is being planned with Professor R. W. Vaughan. Outside of Chemical Engineering, the Polymer Laboratory has maintained close contact with Professor W. G. Knauss's group in Aeronautics whose interests lie in the field of crack propagation and fracture in elastomers. Close liaison is also maintained with the Materials Science group at the Institute. Because of its small size, such interdepartmental contacts are easy to maintain at Caltech.

In the past, both Materials and Chemistry students have received Ph.D. or M.S. degrees for thesis work done in the Polymer Laboratory. Chemistry and Chemical Engineering form a single division at Caltech, and the polymer courses attract an increasing number of chemistry students. Chemistry undergraduates receive credit for undergraduate research performed in the Laboratory.

### **SEMINARS**

During the academic year, the polymer group meets weekly for an informal luncheon seminar held in Professor N. W. Tschoegl's office. These seminars have the character of a special topics course for which, however, no credit is given. Approximately half of the seminar speakers come from outside Caltech. An effort is made to invite speakers who do research which is different from that of the group or who can supplement the expertise of the lecturers presenting the regular courses. Since it is recognized that many of the group's graduates will go into industry, a special effort is made to invite speak-

ers from industrial R&D laboratories to acquaint group members with the directions and values of high-level industrial research and development work. Through the seminars the members of the group meet the many well-known polymer scientists who regularly pass through Caltech. The seminars contribute to the broadening of the group's concept of polymer research beyond the study of mechanical properties and rubbers.

The seminars also serve as a forum for periodic reporting by members of the group on the progress of their research. A graduate student is expected to present an average of three to four talks per year and in this manner gains valuable experience in the art of oral expression and communication. Every group member is expected to be sufficiently familiar with everybody else's research to be able to interact and such interaction is encouraged. This has led to intensive mutual reinforcement of interest and to cohesion within the group, and has sensitized group members to the demands and advantages of the team work so often essential to successful work in industry.

The seminar program has been very successful and has attracted interest from other groups at Caltech and also from outside the Campus. A major advantage of the seminars is, however, that they are normally restricted to a small group of about 15 people to encourage free-wheeling and uninhibited discussion. □

### **BOOK REVIEW: (Continued from page 29)**

lation: the extension to design; the relationship of process simulation to the stochastic simulation of the systems engineer; and the strong dependence of simulation systems on new hardware developments.

In summary, this book is recommended as a basic source reference on simulation systems. The reader should find it valuable either as an undergraduate text or for self-study. With its use he should be able to understand the fundamental elements of a simulation, and have less confusion as to the application of simulation systems to large complex processes.

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# Analog Simulation of the Dispersion of Atmospheric Pollutants

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## PROBLEM

The problem is to devise an analog program for simulation of the dispersion of atmospheric pollutants. Beginning with a commonly accepted dispersion model, which is analytical in nature, show the steps involved in the analog simulation of the vertical concentration profile at successive points downwind of a line source. This problem can be used as a very effective demonstration or as an introductory problem at various stages of a course on analog simulation.

## SOLUTION

The most commonly used models of atmospheric dispersion from continuous sources are the Gaussian Plume Models (D. B. Turner, Workbook of Atmospheric Dispersion Estimates, U. S. Department of HEW, 1967). For an infinite line source such as might be used to simulate automotive emissions on a freeway, the model has the following analytical form

$$\chi = \frac{q}{\sqrt{2\pi} \sin\phi \sigma_z u} \left\{ \exp\left[-\frac{(z-H)^2}{2\sigma_z^2}\right] + \exp\left[-\frac{(z+H)^2}{2\sigma_z^2}\right] \right\} \quad (1)$$

where

H is the effective height at which the emissions occur (meters).

z is the vertical distance above the ground (meters).

u is the wind speed (meters/sec).

$\phi$  is the angle between the source line and the wind direction (limited to  $\phi \geq 45^\circ$ )

q is the rate of emission per unit length (grams/(meter sec)).

$\chi$  is the concentration of the pollutant (grams/cubic meter).

$\sigma_z$  is called the vertical dispersion coefficient (meters).

$\sigma_z$  has been empirically related to the distance, x meters, from the line source to the point of interest and to the stability condition of the atmosphere. Suggested correlations are given by Turner. As approximations to these correlations:

$$\sigma_z \approx 0.023 x \quad (2)$$

when the turbulent nature of the atmosphere is minimal to

$$\sigma_z \approx 0.14 x \quad (3)$$

when the atmosphere is very turbulent.

Models very similar in nature are also presented by Turner for point and instantaneous source emissions.

## Analog Simulations

Using the model described above, two situations will now be considered for analog simulation. The first is the simulation of the vertical concentration profile at a fixed distance downwind assuming, q,  $\phi$ ,  $\sigma_z$ , u, and H are fixed. The second is the simulation of the vertical profile in an automated manner as the distance downwind increases linearly.

### • Vertical Profile at Fixed Downwind Distance

To develop a model suitable for analog simulation, the basic dispersion model is first written as

$$X = \frac{q}{\sqrt{2\pi} \sin\phi \sigma_z u} (\alpha + \beta) \quad (4)$$

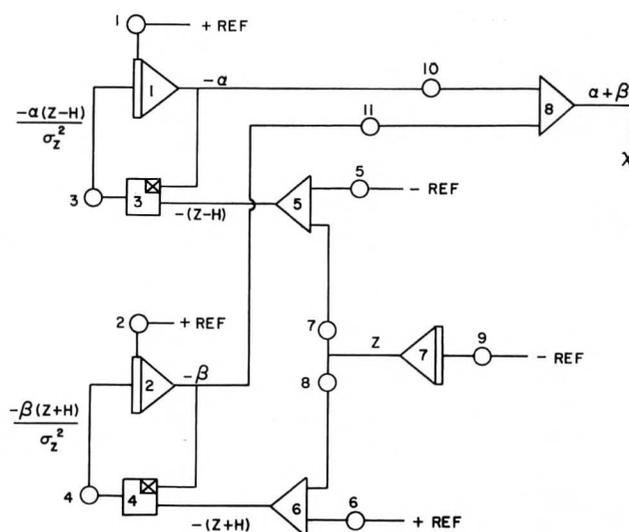
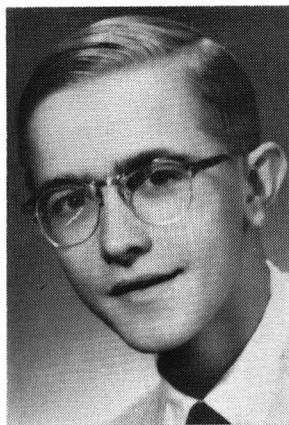
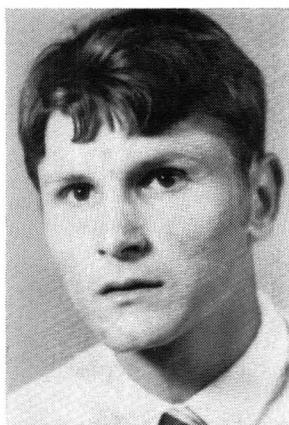


Fig. 1. Vertical Profile Generation



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Theodore W. Cadman received his BS, MS, and PhD from Carnegie Mellon University. Since 1965 he has been engaged in teaching and research in the Department of Chemical Engineering at the University of Maryland. His primary interests are in process simulation. He is the faculty advisor for the student AIChE and a member of Analog Hybrid Educational Users Group, AIChE, ACS and IST. (right photo).

where

$$\alpha = \exp \left[ -\frac{(z-H)^2}{2\sigma_z^2} \right]; \quad \beta = \exp \left[ -\frac{(z+H)^2}{2\sigma_z^2} \right] \quad (5,6)$$

The variables  $\alpha$  and  $\beta$  are then differentiated with respect to  $z$  to yield the following differential equations for the purposes of analog solution.

$$\frac{d\alpha}{dz} = -\frac{(z-H)}{\sigma_z^2} \alpha \quad (7)$$

$$\frac{d\beta}{dz} = -\frac{(z+H)}{\sigma_z^2} \beta \quad (8)$$

By reference to Equations (5) and (6), the appropriate initial conditions are found to be

$$\alpha(z=0) = \exp \left[ -\frac{H^2}{2\sigma_z^2} \right] = \beta(z=0) \quad (9)$$

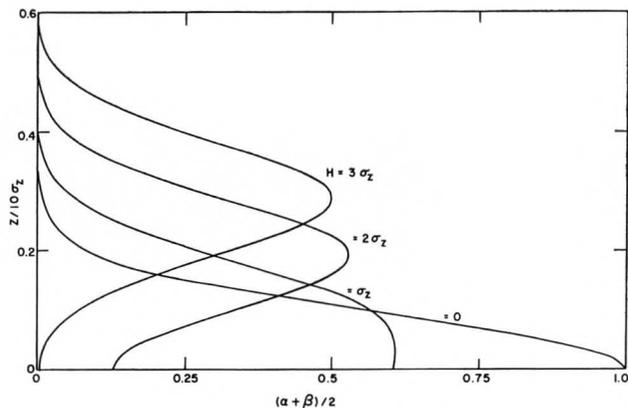


Fig. 2. Vertical Profiles for Various H.

Using Equations (7) and (8), the analog diagram presented in Figure 1 can be used to compute  $\chi$  as a function of  $z$  for fixed  $q$ ,  $\Phi$ ,  $u$ ,  $\sigma_z$ , and  $H$ . Table 1 below details the variables and

TABLE 1. ANALOG VARIABLES AND PARAMETERS

	Before Scaling	After Scaling
Amp 1	$-\alpha$	$-\alpha/\alpha^*$
Amp 2	$-\beta$	$-\beta/\beta^*$
Amp 3	$-\alpha(z-H)$	$-\alpha(z-H)/(\alpha^*(z-H)^*)$
Amp 4	$-\beta(z+H)$	$-\beta(z+H)/(\beta^*(z+H)^*)$
Amp 5	$-(z-H)$	$-(z-H)/(z-H)^*$
Amp 6	$-(z+H)$	$-(z+H)/(z+H)^*$
Amp 7	$z$	$z/z^*$
Amp 8	$\alpha+\beta$	$(\alpha+\beta)/(\alpha+\beta)^*$
Pot 1	$\alpha(0)$	$\alpha(0)/\alpha^*$
Pot 2	$\beta(0)$	$\beta(0)/\beta^*$
Pot 3	$1/\sigma_z^2$	$(z-H)^*/(\sigma_z^2 B)$
Pot 4	$1/\sigma_z^2$	$(z+H)^*/(\sigma_z^2 B)$
Pot 5	$H$	$H/(z-H)^*$
Pot 6	$H$	$H/(z+H)^*$
Pot 7	$1$	$z^*/(z-H)^*$
Pot 8	$1$	$z^*/(z+H)^*$
Pot 9	$1$	$1/(z^* B)$
Pot 10	$1$	$\alpha^*/(\alpha+\beta)^*$
Pot 11	$1$	$\beta^*/(\alpha+\beta)^*$

parameters of the circuit before and after scaling. For convenience in this table a superscript  $*$  is used to indicate the maximum magnitude and  $B$  is used to represent the time scaling factor.

Using the values given in Table 2, the sample results given in Figure 2 were obtained by varying  $H$  from 0 to  $3\sigma_z$ .

TABLE 2. EXAMPLE NUMERICAL PARAMETERS

Parameter	Value
$\alpha^*$	1
$\beta^*$	1
$z^*$	$10\sigma_z$
$(z-H)^*$	$10\sigma_z$
$(z+H)^*$	$20\sigma_z$
$(\alpha+\beta)^*$	2
$\sigma_z$	10

As indicated in Figure 2, at low values of  $H$  the maximum concentration occurs at ground level. In this context, it is worth noting that the model assumes complete reflection of the pollutant at the ground. At higher values of  $H$ , the profile becomes more symmetric, and the maximum value of  $(\alpha+\beta)$  approaches  $1/\sigma_z$  as  $\alpha$  be-

comes increasing dominant in the sum. It may be further observed by reference to Equations 7, 8, and 9 that  $z$  and  $H$  may be related to  $\sigma_z$  as suggested in Figure 2 in order to obtain a general solution valid for  $\sigma_z$ .

### • Spread of Profile in Downwind Direction

To simulate the dispersion as a function of the downwind distance, it is necessary to change  $\sigma_z$  as suggested by the approximations in Equations 2 and 3. If an analog capable of two speed integration, possessing a moderate amount of logic, is available, the simulation of this downwind dispersion can be automated to yield an effective demonstration. In essence, the automation procedure is to use a slowly continually operating analog circuit to generate  $\sigma_z$ ,  $\sigma(0)$ , and  $\beta(0)$  for use in the more rapidly repetitive operating circuit given in Figure 1. Pots 1 and 2 are, of course, eliminated and Pots 3 and 4 must be replaced by dividers to handle a varying  $\sigma_z$ . In addition, a final divider must be used to compute the  $(\alpha + \beta)/\sigma_z$  terms in  $x$  as indicated by

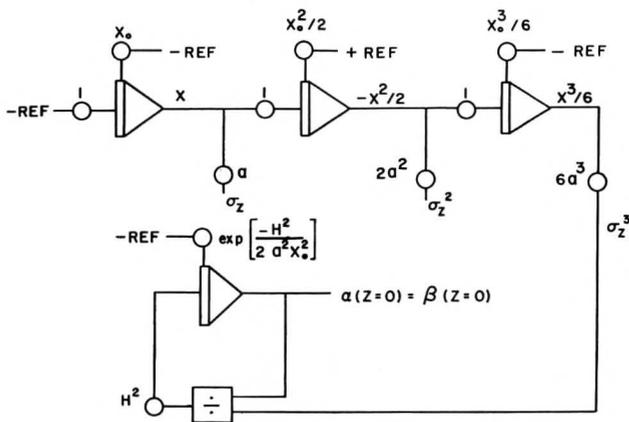


Fig. 3. Generation of Parameters

Equation 4.

Assuming  $\sigma_z = ax$  where  $a$  is a constant and noting that

$$\alpha(z=0) = \beta(z=0) = \exp\left[-\frac{H^2}{2\sigma_z^2}\right],$$

either  $x$  or  $\sigma_z$  can be used as the independent variable on the slowly operating circuit. As indicated in Figure 3,  $\sigma_z$  and  $\sigma_z^2$  are obtained by integration and  $\alpha(z=0) = \beta(z=0)$  are determined using

$$\frac{d}{d\sigma_z} \alpha(z=0) = \frac{H^2}{\sigma_z^3} \alpha(z=0) \quad (10)$$

Initial conditions on Equation (10) are chosen

at the lowest non-zero value of  $x$  to be simulated. Note that  $x = 0$  can not be assumed because it is a singular point in the model. Again referring to Figure 3, the generated values of  $\sigma_z$ ,  $\sigma_z^2$ ,  $\alpha(z=0)$ , and  $\beta(z=0)$  are fed to the repetitive operating circuit which computes  $\chi$ . If the secondary circuit operates very slowly,  $\sigma_z$  and  $\sigma_z^2$  will change negligible during any one repetitive run and thus can be used directly in the primary circuit. If the secondary circuit is fairly rapid, a pair of track and store units can be used to interface the two circuits and maintain  $\sigma_z$  and  $\sigma_z^2$  constant during each repetitive run. By plotting  $\chi + x$  versus  $z$  the dispersion of the pollutant as a function of the downwind direction can be automatically obtained. Figure 4 presents several example profiles obtained in this manner.  $\chi$  is chosen to have a maximum value of 0.1 at a distance of 100 meters downwind. The result-

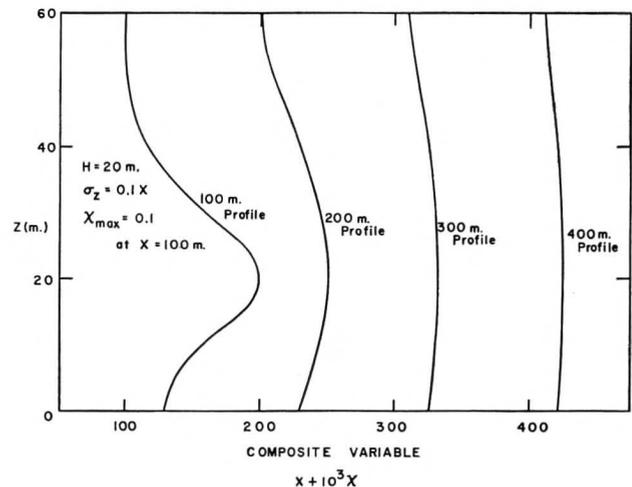


Fig. 4. Dispersion Downwind of Source.

ing dispersion downwind at 200, 300, and 400 meters is given.

### CONCLUSIONS

The analog simulation of the dispersion of atmospheric pollutants has been briefly examined in this paper. It has been shown that the problem can be used as an effective demonstration in order to examine the essential features of atmospheric dispersion. In addition, the problem presents several more difficult scaling problems for the student. The analytical nature of the solution provides, however, a ready check of the simulation and thus the simulation can prove to be an effective student problem at several stages of an analog course. □

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# MODERN ANALYSIS TECHNIQUES WITH THE APL SYSTEM

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*Laval University*

*Quebec, 10, Que., Canada*

## INTRODUCTION

Since the last decades, the discipline of Chemical Engineering has been subjected to a radical change with the now popular entry of Computer Science and its related techniques. In every field of Chemical Engineering, such as Transport Phenomena, Process Control, Chemical Reactor Design . . . a knowledge of Computer Science and its applications is evidently necessary. Applications of computer even permit the establishment of various special techniques of analysis to Chemical Engineering: Optimization,<sup>1</sup> Simulation,<sup>2</sup> Mathematical Modelings<sup>3,4</sup> and Computer Aided Design.<sup>5, 6</sup>

Although everybody recognizes the advantages of these modern techniques in Chemical Engineering, the incorporation of courses in these subjects often raises some problems for both the graduate students and the instructor.

Indeed, graduate students in Chemical Engineering seem reluctant to select, say, a course on Optimization of Chemical Processes, for the simple reason that they are aware that, to succeed in such a graduate-level course, they should have already passed or must follow various other courses: Computer Programming, Applied Mathematics, Numerical Analysis, Operational Research . . . . On the other hand, for the instructor, a common problem he must face is how to present such a wide-range but necessary background and the main content of the course under a rather heavy constraint: the limited time of a semester course with 2 or 3 hours weekly. Numerous instructors will share with the authors the regretful sentiment of lacking the time to attain their selfish desire: seeing their students being able to apply the shown techniques to a chemical engineering problem, rather than obtaining generally a vague notion of theoretical principles. In view of diminishing the difficulties mentioned, we, at Laval University, have tried to introduce a gradu-

ate course on the Modern Analysis Techniques for Chemical Engineering using extensively the advantages of the APL System, which we report here in this article.

## PURPOSES

The purposes of the course are two-fold: to give chemical engineering graduates an opportunity to be familiar with APL, one of the most scientific and advanced programming languages, and at the same time to get them acquainted with modern analysis techniques.

The organization of the course depends heavily on the APL system,<sup>7, 9</sup> hence a brief description of it is recommended. An APL system comprises a central computer and an indefinite number of typewriter-like terminals. A certain number of these remote terminals may be simultaneously linked to the computer, therefore easing the wide use of this computing tool. The user's instructions and programs can be stored in the center and copied for other use at any moment by some special instructions. As for the language itself, first defined by K.E. Iverson,<sup>7</sup> it is found to be the most convenient for mathematical and engineering computing purposes due to its logic and compactness. Moreover, the system's possibility of an interactive approach in problem solving makes it very attractive to the beginners. From the educational point of view, the characteristic advantages of the system have been exploited to give formal theorems demonstration<sup>10</sup> and engineering applications.<sup>11</sup>

## COURSE CONTENT AND ORGANIZATION

The course has been tested for the past 3 years at Laval University, Canada; after each session, the results were analyzed with hopes of making changes that would better suit the comprehension level and motivations of the "new-genera-

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tion" Chemical Engineering Graduates. The tests showed that good results were obtained by a well-balanced content of scientific programming and applied analysis techniques.

As a first part of the course, background on Computer Programming, especially on Time-Sharing Computing system, was given. After that, the APL language itself was showed to the students with particular reference to the scientific and engineering aspects of the system. In addition to formal lectures, students can learn the language by programmed lessons and do exercises which have been pre-registered in the system. This proves to be very helpful since it permits students to learn at their own rate while, by practicing directly with the system, they get acquainted quite easily with the rigid logic of a computer. As a consequence, the time of formal lectures was devoted more to the special topics students usually await from an instructor, such as the characteristics of the system, fundamentals of the techniques and particular hints for engineering students rather than some "dull" specific rules to write a program with an existing computing system.

After the first part, one can be assured that trainees can, from now on, master this useful tool of computing and are ready to see the analysis techniques in themselves with not much difficulties from the programming point of view. As for the second part of the course, some special-chosen modern techniques of analysis varying from Statistical Experimental Planning, Numerical Mathematics, Linear Programming to Simulation and Optimization were presented and it was particularly shown how they can be applied to solve chemical engineering problems in practice.

## DISCUSSION

As a result of our experience, it was found

that the organization of this course greatly improved the student's comprehension, which is usually difficult to attain in such a short period due to the rather wide-range nature of the covered subjects. Indeed, by using the pre-written programs of the system, students and instructor are free of the tedious work of having to re-write the computer program for the studied analysis technique. For example, when discussing optimal strategy for allocation of materials in chemical plants, we can apply directly pre-written programs related to transport and distribution problems<sup>12</sup> and concentrate much more on the mathematical philosophy of the technique and the chemical engineers' considerations. Trainees are better motivated when they can solve in applying the shown techniques, some real problems met in practice. As a short-term result, it was found that the course was also an immediate help to our graduate students confronting current research problems. Numerical computing, statistical tests, decision making . . . in nearly all our graduate dissertation thesis since the last years had been performed by the APL language rather than previously used cumbersome ones.

One of the reasons for this overwhelming victory of the APL language might be its scientific and unified approach, which is very welcomed in the engineering field.

As a counter-balance of all these advantages, some drawbacks were observed in our adopted way of course approach: firstly, the course required in fact a rather good background on mathematical analysis, and secondly its future utilities, especially for the industry-minded graduates, were handicapped by the rare presence of APL systems outside of the campus.

## CONCLUSION

The course served a definite need in introducing the modern analysis techniques to chemical engineering graduates. The course's approach enabled the student to gain a broad mastery of computer programming and some modern techniques to solve engineering problems.

From an instructor's point of view, the fact that his students can solve, store their solutions in the system and discuss and exchange afterward with his classmates, constitutes a real motivation for the continuing efforts to improve the course. Moreover, with the more and more widely spread use of the APL system in engineering

(Continued on page 43)

# DESIGN OF PROCESS CONTROL SYSTEMS

## Using Frequency Response And Analog Simulation Techniques

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**T**HE TIME REQUIRED to design control systems by analog simulation can be significantly reduced if initial approximations are made using frequency response methods. The tendency for most engineers is to use only one of the above techniques, the one with which they are the most familiar.

The object of this study is to present a method which will reduce the time involved in designing a control scheme for a process control system. The method itself combines the use of frequency response methods (Bode diagrams) and time domain methods (analog computer simulation) to give the most efficient design technique.

### DEVELOPMENT

**T**O ILLUSTRATE THE METHOD, let us consider a chemical process system described by the linear model shown in Fig. 1. The system to be studied is a spray dryer used to process an emulsion to obtain a powder. Control may be effected by regulating the feed to the diffuser vanes. The air heater consists of two non-interacting transfer lags of time constant 100 seconds each. The drum behaves as three transfer lags of time constant 12.5 seconds each, and one distance velocity lag of 2 seconds. A distance-velocity lag of 3 seconds exists between changes in air temperature at the heater and its appearance at the

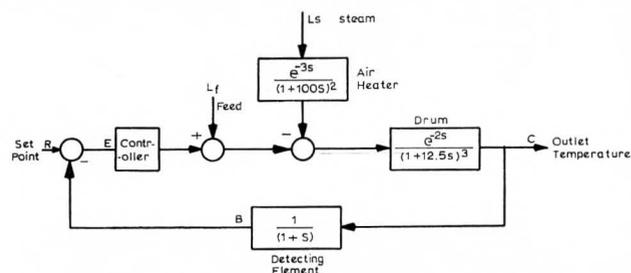


Fig. 1. Linear Model of Chemical Process System.

diffuser vanes. The detecting element has a transfer lag of time constant 1 second. We will neglect the time constant of the control valve. The block diagram of the system is given in Fig. 1.

Note that any controller designed should reduce the steady-state error to a step input at  $R$  to an arbitrarily small value, and at the same time minimize the effect of the load of less than 10% and have reasonable stability.

For a type zero system excited by a step input the steady-state error is defined as follows

$$e_{ss} = \frac{A}{1 + K_p} \quad (1)$$

where  $A$  = magnitude of step,  $K_p$  = position error constant defined as  $\lim_{s \rightarrow 0} G(s)$ . This steady-state error is equal to  $R-B$ . What we are actually interested in is  $R-C$ . However, since there is unity gain in the feed-back path  $B = C$  in the steady-state. For our system  $K_p = K_c$  which is the controller gain. Thus the steady-state specification will be met by values of  $K_c$  greater than 9. Let us now choose  $K_c = 10$ .

The Bode diagram of the system including controller gain, using straight line approximations, is given in Fig. 2. Using proportional control only we would have a slope of  $-3$  at cross-

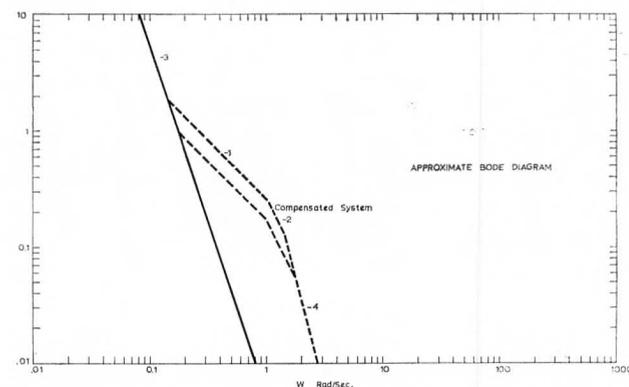
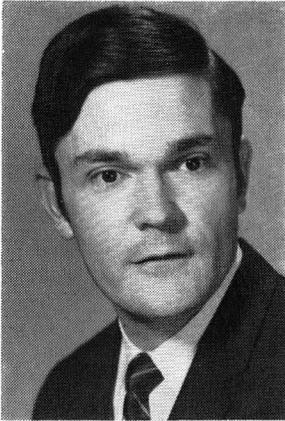


Fig. 2. Bode Diagram of System by straight line approximation.



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over which indicates the system would be unstable. However, the presence of dead-time terms requires that the phase angles be computed independently rather than from the magnitude curves using a tangent scale.

The crossover frequency occurs at 0.175 rad/sec. This is only an approximation however since we are using straight line approximations for the Bode diagram. The simulation on the analog computer will give us the true results for the model but the information from the Bode diagram is valuable in that it gives us approximate values and enables us to go to the computer where the optimal solution can be obtained by minor adjustment of the parameters.

We will now check the stability of the system using proportional control only, again by tabulating the phase angle contributions at the crossover frequency of all time constants and dead time terms.

$$\begin{array}{rcl}
 3 \tan^{-1}(.175) (12.5) & = & 3 \tan^{-1}(2.185) = -196.2^\circ \\
 \tan^{-1}(.175) (1) & = & \tan^{-1}(.175) = -9.9^\circ \\
 2(.175)180/3.14 & = & -20.0^\circ \\
 & & \underline{-226.1^\circ}
 \end{array}$$

The phase margin is  $-46.1^\circ$  and the system is clearly unstable.

In order to stabilize the system we must bring the slope of the curve at crossover up to a value of  $-1$ . This cannot be accomplished by a single lag-lead network (three mode controller) since the slope must be decreased by two. We will try a double lead network (two-proportional plus derivative controllers in series). The general form of the transfer function for this control

system is given as

$$\frac{K_c (1 + \tau_d s)^2}{(1 + \frac{\tau_d s}{\gamma})^2} \quad (2)$$

where  $\gamma = 10$ ,  $\tau_d =$  controller constant, and  $K_c =$  gain.

To check for stability we must select a value of  $\tau_d$  and compute the phase margin. Once again we stress that this will only be an approximation. For a first try, let  $\tau_d = 7.1$ . This is shown in Fig. 2. This gives a crossover frequency of 0.27 rad/sec from which we can compute the phase margin.

Tabulating the phase angle contributions we obtain

$$\begin{array}{rcl}
 3 \tan^{-1}(.27) (12.5) & = & 3 \tan^{-1}(3.38) = -220.5^\circ \\
 \tan^{-1}(.27) (1) & = & \tan^{-1}(.27) = -15.1^\circ \\
 2 \tan^{-1}(.27) (.71) & = & 2 \tan^{-1}(.193) = -21.8^\circ \\
 2 \tan^{-1}(.27) (7.1) & = & 2 \tan^{-1}(1.93) = +125.2^\circ \\
 & & 2(.27)180/3.14 = -30.9^\circ \\
 & & \underline{-163.1^\circ}
 \end{array}$$

This gives a phase margin of  $16.9^\circ$ . We will make a second try in an attempt to increase the phase margin. We will let  $\tau_d = 5.7$  which is also shown in Fig. 2. These values of  $\tau_d$  are selected by choosing a breakpoint on the curve.

Once again tabulating the phase angle contributions we obtain

$$\begin{array}{rcl}
 3 \tan^{-1}(.175) (12.5) & = & 3 \tan^{-1}(2.185) = -196.2^\circ \\
 \tan^{-1}(.175) (1) & = & \tan^{-1}(.175) = -9.9^\circ \\
 2 \tan^{-1}(.175) (.57) & = & 2 \tan^{-1}(.10) = -11.4^\circ \\
 2 \tan^{-1}(.175) (5.7) & = & 2 \tan^{-1}(1.0) = +90.0^\circ \\
 & & (2)(.175) 180/3.14 = -20.0^\circ \\
 & & \underline{-147.5^\circ}
 \end{array}$$

This gives a phase margin of  $32.5^\circ$  which is a safer margin of stability. A look at the calcu-

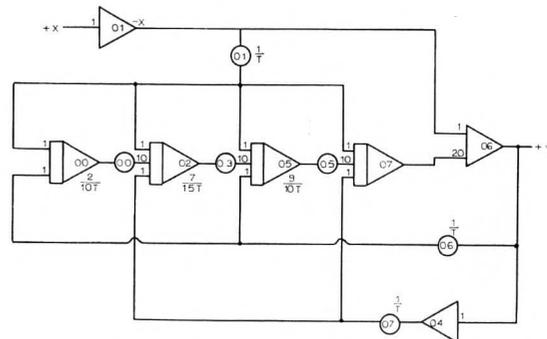


Fig. 3. Dead Time for Drum.

$$\begin{array}{lll}
 P_{00} = .1000, & P_{01} = .5000, & P_{03} = .2322, \\
 P_{05} = .4500, & P_{07} = .5000, & P_{07} = .5000.
 \end{array}$$

These integrators are run at times ten normal speed.

lations shows that moving the breakpoint in either direction will decrease the phase margin. If we make the breakpoint smaller we have a higher crossover frequency which yields a smaller phase margin, and if we make it larger we are back to the situation of a crossover slope of  $-3$ . Thus we are at the point of maximum relative stability. Therefore the transfer function for the compensated system is given as

$$\frac{10(1 + 5.7s)^2 e^{-2s}}{(1 + .57s)^2 (1 + 12.5s)^3 (1 + s)} \quad (3)$$

**T**HE NEXT STEP WILL BE to simulate the system on the analog computer. For this purpose the EAI-680 analog computer was utilized. The first phase of the study was to check the frequency

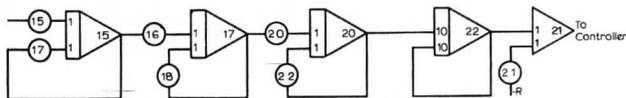


Fig. 4. Drum.

$$\begin{aligned} P_{15} &= 0.8000, & P_{16} &= 0.8000, & P_{17} &= 0.8000, \\ P_{18} &= 0.8000, & P_{20} &= 0.8000, & P_{21} &= 0.1000, \\ P_{22} &= 0.8000 \end{aligned}$$

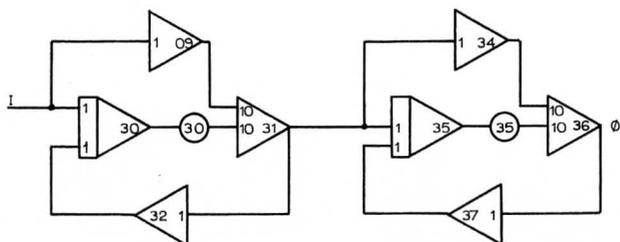


Fig. 5. Double Lead Controller.

$$P_{30} = P_{35} = 0.1750.$$

These integrators are run at ten times normal speed.

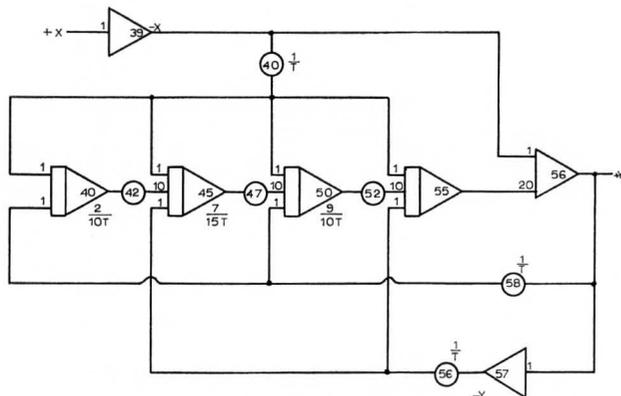


Fig. 6. Dead Time for Air Heater.

$$\begin{aligned} P_{40} &= 0.3333, & P_{42} &= 0.0667, & P_{47} &= 0.1558, \\ P_{52} &= 0.3000, & P_{56} &= 0.3333, & P_{58} &= 0.3333. \end{aligned}$$

These integrators are run at ten times normal speed.

... although simulation is the only method which yields exact solutions for models . . . , the use of . . . the straight line Bode diagram gives ball park estimates . . .

response by developing a Bode diagram. The next phase was to study the dynamic operating response to changes in set point and load variables, and attempt to optimize the design by varying  $K_c$  and  $\gamma$ . The dead time was simulated by a modified fourth order Pade delay circuit. The complete set of analog diagrams is given in the Figs. 3, 4, 5, 6, 7, and 8.

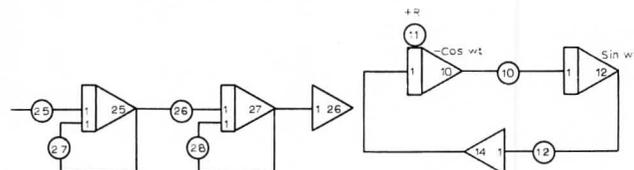


Fig. 7. Air Heater.

$$\begin{aligned} P_{25} &= 0.1000, \\ P_{26} &= 0.1000, \\ P_{27} &= 0.1000, \\ P_{28} &= 0.1000. \end{aligned}$$

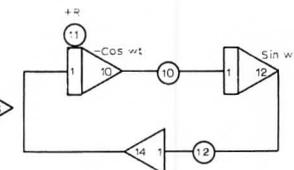


Fig. 8. Sine Wave Generator

$$\begin{aligned} P_{10} &= 0.1750, \\ P_{11} &= 0.1000, \\ P_{12} &= 0.1750. \end{aligned}$$

These integrators are run at ten times normal speed.

## RESULTS

**F**ROM APPROPRIATE CURVES, the open-loop frequency response of the system was determined and compared to the Bode diagram in Fig. 2.

The true frequency response of the model of the system was obtained by generating a sine wave over a range of frequencies and imposing it as an input to the set point of the system. Both the input and output of the system were recorded on a strip chart recorder. From the input and output curves the magnitude ratio and phase angle can be measured as functions of frequency. The results are plotted in Fig. 9. A comparison with Fig. 2 shows the error from the straight

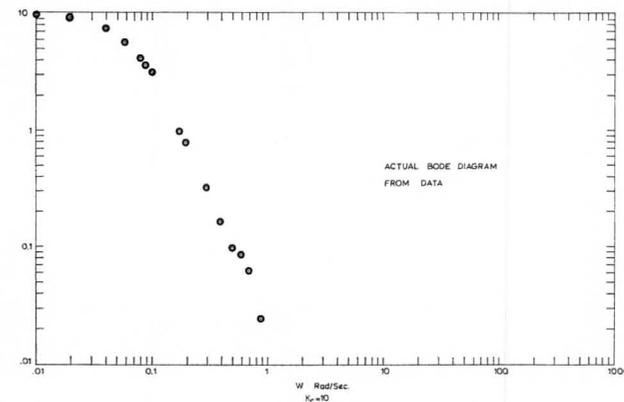


Fig. 9. Actual Bode Diagram of system.

line approximations. However, from Fig 9 we see that the crossover is about the same frequency as in Fig. 2. The phase shift at this frequency can be computed from the strip chart. In this case the phase shift was  $-170^\circ$  giving a phase margin of  $+10^\circ$ . This indicates that the response of the system will be stable but highly oscillatory.

The next step was to test the steady state error due to a step disturbance at the set point. A step of one volt was applied and the steady state error was calculated as 0.098 volt which is within the specification of 10%. The strip chart recording of the test is shown in Fig. 10.

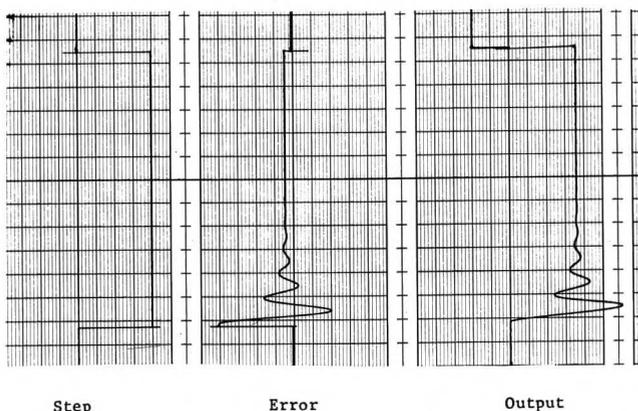


Fig. 10. Transient response of system to a step change in set point. 0.05 volts/div, 2mm/sec,  $K_c = 10$ .

A step disturbance was also applied at the load variable. This produced the same steady state error. This was expected since the steady state value  $B(t)$  is the same as  $C(t)$ .

The overshoot can be measured from Fig. 10 and is about 60% which is somewhat high. A run was made with  $K_c = 9$  which reduced the overshoot to 55% but gave a steady state error of 10% which is just on the limit of the specification. A third run was made with  $K_c = 8$  which gave an overshoot of 50% and a steady state error of 12.5%. It was felt then that the original value of  $K_c = 10$  was the best compromise.

Several more runs were made using this value of  $K_c$  and varying  $\tau_d$  in both directions. In all cases the overshoot was worse as predicted from the original Bode diagram.

A last set of runs was made in an attempt to optimize  $\gamma$ . For the first run  $K_c$  and  $\tau_d$  were kept the same and  $\gamma = 15$  was used. This gave an overshoot of 60% which was the same as  $\gamma = 10$ . A value of  $\gamma = 5$  was used and this gave an

overshoot of 80%. Therefore the original value of  $\gamma$  was retained.

## CONCLUSIONS

IT HAS BEEN PROVEN by this experiment that although simulation is the only method which yields exact solutions for models used for control system design, the use of approximations such as the straight line Bode diagram gives ball park estimates for the controller constants which are valuable starting points for the simulation study. Otherwise, one must hunt at random on the computer until the optimum values are found, which can be time consuming and wasteful. In this particular problem the values found by the approximate technique turned out to be the optimum values from the computer study.  $\square$

## APL: (Continued from page 39)

education circles, it is also possible to share the resulting programs with other educators having similar interests.  $\square$

## REFERENCES

- Himmelblau, D.M., "A Course on the Optimization of Large Scale Systems." Chem. Eng. Education, 5, No. 4, pp 196 (1971).
- Beamer, J.H., "Statistical Analysis and Simulation," Chem. Eng. Education, 5, No. 4, pp 192 (1971).
- Franks, R.G.E., "Mathematical Modeling in Chemical Engineering," John Wiley & Sons, Inc., N.Y. (1967).
- Kabel, R.L., "Mathematical Modeling," Chem. Eng. Education, 5, No. 4, pp 184 (1971).
- Carnahan, B., Seider, W.D. and Katz, D.L., "Computers in Engineering Design Education, Vol. II, Chemical Engineering," The University of Michigan, College of Engineering (1966).
- Westerberg, A.W., "Computer Aided Process Design," Chem. Eng. Education, 5, No. 4, pp 180 (1971).
- Iverson, K.E., "A Programming Language," John Wiley, New York (1962).
- Katzan, Harry Jr., "APL Programming and Computer Techniques," Van Nostrand (1970).
- Falkoff, A.D. and Iverson, K.E., "APL/360: User's Manual," I.B.M. (1968).
- Hatcher, W.S., and Rethier, P.E., "Une application du langage APL au problème de démonstration de théorèmes par ordinateur," in "Colloque APL," Institut de Recherche d'Informatique et d'Automatique, Paris, France (1971).
- de Vahl, Davis G., and Holmes, W.N., "The use of APL in Engineering Education," in "Colloque APL," Institut de Recherche d'Informatique et d'Automatique, Paris, France (1971).
- Smillie, K.W., "Statpack 2: An APL Statistical Package," Department of Computing Science, The University of Alberta, Edmonton, Alberta, Canada.

# PROCESS SYNTHESIS

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## INTRODUCTION

In the words of Webster, *synthesis* is "the combining of often diverse conceptions into a coherent whole" and *analysis* is "an examination of a complex, its elements and their relations." Synthesis refers to the more inventive aspects of engineering and analysis to the more scientific. Both are required in the development of industrial processes.

Since World War II engineering education has moved strongly towards analysis, with the introduction of courses which analyse individual process operations and phenomena. Transport phenomena, unit operations, process control, thermodynamics and other engineering science courses greatly strengthened engineering education by showing how things are and how they work.

Unfortunately, there was not a parallel development in the teaching of synthesis. The teaching of how things ought to be rather than how they are. This deficiency has been recognized for years, but the remedy awaited the development of sufficiently general principles about which to organize educational material.

The dominance of engineering science reveals a natural tilt in the educational landscape towards course material which possesses a natural organization. At the University, well organized and easily taught material rises to the surface.

A course in transport phenomena has the natural organization of the equations of change, thermodynamics has the first, second and third laws, unit operations can be organized about the various processing operations and so it is with the courses which dominate. This kept synthesis in the background in spite of the important role synthesis plays in the practice of engineering. Methods of synthesis were not well organized and easily taught, and for this reason synthesis could not rise to the surface.

In the late 1960's and early 1970's, research in process synthesis established the broad outlines of this field and it became apparent that a careful interlacing of synthesis and analysis is a

proper way to approach process development. In these theories of process development, each synthesis step defines an analysis problem the solution of which provides data required for further synthesis steps. Further, it became apparent that this organization of alternating synthesis and analysis steps begs the development of educational material for the early stages of engineering education.

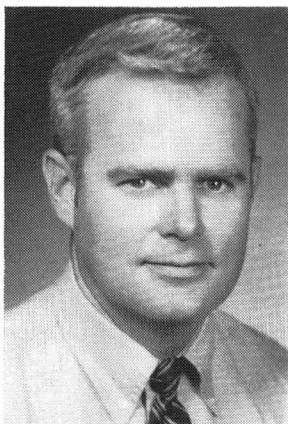
In this report we examine the development of a first course in engineering in which synthesis and analysis are taught simultaneously. Elementary new principles of process synthesis are combined with the classic analysis techniques of material and energy balancing. Emphasis is on the development of process technology rather than on the analysis of existing processes.

## RESEARCH IN PROCESS SYNTHESIS

Research in process synthesis has been adequately reviewed elsewhere and it would be a distraction here to go into any great detail.\* However, a brief discussion of the broad ways of thinking found in the research literature is necessary to set the stage for the educational developments. This, then, is a most superficial review of the emerging research leading to principles for the development of the process flow sheet. Three approaches to process synthesis are apparent; problem decomposition, evolution and optimization.

In process synthesis by *optimization* a combined design is proposed which is known to be redundant, containing process equipment and material flows in a greater number and diversity than is reasonable. However, somewhere hidden within the combined process design is an economically reasonable process. The desired process flow sheet is exposed by the methods of mathe-

\*J. E. Hendry, D. F. Rudd, J. D. Seader, *AIChE J.* (to appear)



Dale F. Rudd was born, raised and educated in Minnesota, receiving a Ph.D. degree in Chemical Engineering from the University of Minnesota in 1959. Most of his professional life has been spent at the University of Wisconsin where he is now Professor of Chemical Engineering. His research and teaching efforts have had a substantial influence on the chemical engineering profession in the United States and abroad. He has been recognized as an innovative and creative teacher, author, and lecturer.

Specializing in research on methods of process design, Professor Rudd has been a frequent consultant and lecturer in industry. In addition to contributions to the research literature, he is co-author of *Strategy of Process Engineering* and the forthcoming *Process Discovery*. In his books he has integrated modern mathematical concepts, a knowledge of industrial processes, and recent advances in econometrics to produce a novel treatment of process design and analysis.

Professor Rudd is the recipient of awards from the Canadian Institute of Chemistry, the AIChE, and the Mexican Institute of Chemical Engineers. He serves on the editorial boards of AIChE Journal, International Chemical Engineering, and Chemical Engineering Communications.

mathematical programming which trim away all but the flow sheet sought. This approach to design synthesis has been quite successful in specific problems such as heat exchanger network synthesis.

In process synthesis by *evolution* one begins with a reasonable design, a base design, which may not be the economically optimal one. Methods are then developed to detect the weak parts of the design, pointing to reactors which ought to be replaced, separation operations which ought to be reordered and so forth. From the base design there evolves better process designs.

Process synthesis by problem *decomposition* takes a completely different look at the problem, leading to the natural organization sought in the teaching of process synthesis. In decomposition a synthesis problem is decomposed into a sequence

**Science aims to analyze natural phenomena, and engineering aims to synthesize preferred situations from natural phenomena.**

of smaller and simpler problems which when solved generate the flow sheet for the original process development problem. The success of this approach depends on the accuracy with which the simpler problems can be identified. J. J. Sirola and G. J. Powers are largely responsible for the development of this approach.

In brief outline, flow sheet synthesis by problem decomposition occurs by the solution to these basic problems. First the chemical reaction path is established. This is the sequence of reactions which best transforms the raw materials into the products on the industrial scale. The second problem is one of species allocation in which a mapping of material flow is proposed from raw material and reaction site sources to product, waste and reaction site destinations. During species allocation the easiest set of separation problems are sought. The third problem is the selection of the physical and chemical phenomena which best accomplish the separation problems which arose from the species allocations. The final problem is task integration in which the several separate reaction and separation phenomena are integrated by the reuse of energy and material.

In the following section we give a glimpse of the detailed approach to process synthesis by problem decomposition, and emphasize the teaching of these methods as the first course in engineering.

#### TEACHING PROCESS SYNTHESIS

We now focus attention on undergraduate education in engineering, which in recent history, has a strong emphasis on the analysis of specific processing phenomena and operations. Our concern is to complement these courses with an introductory course which shows how these specific fields fit into the larger plan of process development. Along with this orientation, certain basic methods of engineering synthesis and analysis are taught.

We have had several years of classroom experience with this approach at the freshman and sophomore level. In mid 1973 Prentice-Hall Inc. will publish *Process Synthesis* by D. F. Rudd, G. J. Powers and J. J. Sirola.\* The chapters in this book are now reviewed.

\*D. F. Rudd, G. J. Powers, and J. J. Sirola, *Process Synthesis*, Prentice-Hall, Englewood Cliffs N.J. (1973).

## Engineering of Process Systems

First the students become acquainted with a bit of the history of processing to see how chemistry is used, how materials are separated and how economy is reached by the reuse of material and energy. In class we discuss the recovery of nitrogen from the atmosphere for use as a fertilizer, the conversion of vegetable protein into meat analog foods for human consumption and the treatment of sewage at the South Lake Tahoe plant, the most advanced sewage treatment facility in the world.

On their own, as home problems, the students prepare a short history of important process innovations. One project is to report on the events which led from Sir Alexander Fleming's discovery of penicillin to the massive process development campaign to provide enough penicillin to accompany the troops during Eisenhower's landing in Europe. A second project begins with this beer recipe from "Hints to Brewers," 1702.

"Thames water, taken up about Greenwich at low tide, when it is free of all the brackishness of the sea and has in it all the fat and sillage from this great city of London, makes a very strong drink. It will of itself ferment wonderfully, and after its due purgation and three times stinking, it will be so strong that several sea commanders have told me that it has often fuddled their murriners"

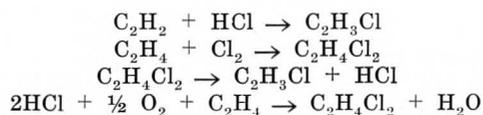
and traces the development of the activated sludge process for sewage treatment.

The students get a feel for processing, and discover the role that the engineer plays in supplying society's needs for food, water and other material items.

### Reaction Path Synthesis

The first major subproblem in process synthesis involves the selection and analysis of the chemistry of processing. The chemistry links the products of processing with cheap and readily available materials, and generates wastes and by-products with which we must contend. In this course we do not teach chemistry; we teach the assessment of chemical change.

For example, given these reactions which lead to vinyl chloride,



... research in process synthesis established the broad outlines of this field and it became apparent that a careful interlacing of synthesis and analysis is a proper way to approach process development.

the students learn to select the reaction sequences which require for each two molecules of vinyl chloride,

- two molecules of ethylene, one of chlorine and oxygen. This reaction path is to generate no by-products other than water.
- one molecule of ethylene, one of acetylene and one of chlorine. No by-products are allowed for this path.

The students also learn the basic principles of economic screening of the reaction paths they synthesize. The idea is that the products must be more valuable than the reactants if a reaction path is to be of any commercial interest.

Home problems include an analysis of the chemistry involved in these areas: the recycle of pickling liquor waste, acrylonitrile from propylene, titanium by chlorination, waste recycle in the solvay process, sodium bicarbonate by the solvay chemistry, superphosphate fertilizer, leaching copper ores, caustic manufacture the leBlanc process, soap manufacture, nitrogen fixation, fire retardant production, urea synthesis, and so forth.

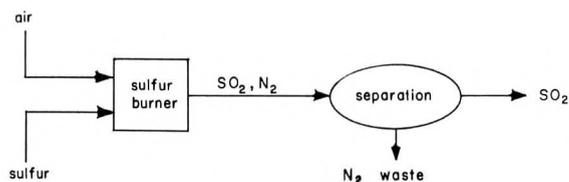
In summary, the students are acquainted with the chemistry of processing, synthesize alternate reaction paths from given chemistry and perform early economic screening of the chemistry.

### Materials Balancing and Species Allocation

Once the chemistry of processing is at hand, the problem arises of supplying the reactor feeds and disposing of the reactor effluents. This leads to the next major subproblem in process synthesis, species allocation. The purpose of species allocation is to identify the routes that the several species involved ought to take to support the chemistry and at the same time lead to the simplest separation problems. Given the needs of the chemistry, we allocate species for easy separation.

As a trivial example, suppose we are to manufacture sulfur dioxide by the direct oxidation of sulfur. Air and sulfur are the reactant sources and pure sulfur dioxide is needed as the product. A cold inert gas is needed to lower the reaction temperature. Figure 1 shows two allocations, one recycling sulfur dioxide as the inert and the other using nitrogen as the inert. The one allocation leads to the need to separate nitrogen from oxygen, a difficult problem and the other leads to the separation of sulfur dioxide from nitrogen, an easy problem. This illustrates how the engineer assesses the nature of separation problems and uses this information to impose the proper material flow on the emerging process flow sheet.

### Allocation 1



### Allocation 2

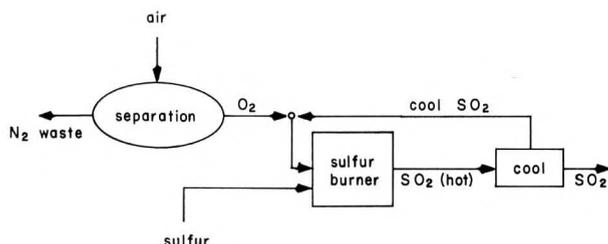


Fig. 1. Alternate Species Allocations During Sulfur Oxidation.

Before anything can be taught about species allocation as a technique in process synthesis, the students must have skill in material balancing. We spend the bulk of this chapter on material balancing, and it is only towards the end of the chapter that the idea is introduced that the real purpose of material balancing is to identify those allocations which involve easy separations.

Typical problems on material balancing and species allocation involve sugar refining, oil and meal from seed, soluble coffee powder production, phosphate rock beneficiation, city refuse composting, fish liver extraction, glycerine desalting, and the manufacture of styrene.

### Separation Technology

Species allocation is directed towards the identification of the easiest separation problems which have to be solved to support the process. This leads to the need for an understanding of the means by which materials are separated from each other. One seeks to identify the ways in which the materials differ, and develop equipment to exploit the proper differences. In this chapter we examine some of the separation processes, mainly to get an understanding of how the equipment works.

Equipment separating solids from solids are examined, along with equipment which accomplish separations based on volatility differences, and solubility differences. For example we examine the Nowak-Othmer scheme for separating the redmud waste from the Bayer Process, which

is a mixture of  $\text{Al}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$ ,  $\text{SiO}_2$ ,  $\text{TiO}_2$ ,  $\text{Na}_2\text{O}$  and  $\text{CaO}$ , by taking advantage of the differences in chloride forming affinity of the oxides, differences in volatility of the metal chlorides, and differences in water solubility. All of this orientation in separating technology is supported by material balance calculations and provides the background required to select the basis of separation, discussed in the next chapter.

Typical problems include municipal solid waste recycle, nut meat separation, activated carbon from saw dust, cranberry draining, copper sulfate leaching, desalting sea sand, and the Caban-Chapman process of mercury recovery.

### Strategy of Task Selection

Having established the chemistry of processing, outlined the flow of material through the process, and obtained an understanding of the general means of separation, the students are prepared for the study of the heuristic principles of task selection. We examine the ways in which separations ought to be performed to achieve efficient processing.

Techniques are presented for examining the ordered lists of physical and chemical properties of materials to detect the best plan of separation. Table 1 shows the species present in the reactor effluent in the Sinclair-Koppers 500 million pounds per year light olefin process; the species ordering is according to volatility, the property to be exploited to separate the methane and hydrogen for use as fuel, the ethylene and the propylene as products, the ethane and propane for recycle, and the heavies for processing into motor fuels. What principles lead to the discovery of a sequence of distillations to accomplish the separation?

Table 1. Reactor Effluent Ranked According to Volatility. (Sinclair-Koppers 500 million lbs/yr ethylene process)

Species	Amount	Boiling point	Boiling point difference
Hydrogen $\text{H}_2$	18%	-253°C	92°C
Methane $\text{C}_1$	15	-161	57
Ethylene $\text{C}_2$	24	-104	15
Ethane $\text{C}_2$	15	-89	41
Propylene $\text{C}_3$	14	-48	6
Propane $\text{C}_3$	6	-42	42
Heavies $\text{C}_4^+$	8	70	

To be separated into: 1-Hydrogen-methane; 2-Ethylene; 3-Propylene; 4-Ethane-propane; 5-Heavies.

In this chapter we establish the following general principles

1. Of the many differences which may exist between the source and destination of a stream, differences involving composition dominate. Select the separation tasks first. This heuristic is based on the idea that attention should not focus on differences in

pressure, size, temperature, and other bulk properties until after the means of separation has been established.

2. **When possible reduce the separation load by stream splitting and blending.** Here we reduce as much as possible the amount of separation to be performed, as is done in the blending of gasolines to each desired product specifications.
3. **All other things being equal, aim to separate the more plentiful components early.** This reduces the load on the down stream units.
4. **Remove the corrosive and hazardous material early.** The remaining separations can then be done in less elaborate equipment.
5. **The difficult separations are best saved for last.** The extremely expensive separations should not be performed in the presence of material which need not be there.
6. **All other things being equal, shy away from separations which require the use of species not normally present in the processing.** This favors separations driven by the addition or removal of energy, such as distillation, over those driven by the addition and removal of material not normally present in the processing, such as extraction.
7. **Avoid excursions in temperature and pressure, but aim high rather than low. In distillation favor the removal one-by-one of the more volatile components.** This rule derives from the high costs of low temperature and low pressure operation compared to pressure and temperature operation.
8. **Favor the removal of products from the least harsh environment.** For example, the final products in a distillation sequence ought to come from the top of the towers, rather than the bottoms where degradation may occur.

The application of these heuristics to a large extent identifies the separation sections of industrial processes. For example, the student examining Table 1 would arrive at these conclusions.

- a) the boiling points of propane ( $42^{\circ}\text{C}$ ) and propylene ( $48^{\circ}\text{C}$ ) are very close, as are the boiling points of ethane ( $89^{\circ}\text{C}$ ) and ethylene ( $104^{\circ}\text{C}$ ). Thus the  $\text{C}_2$  splitter and the  $\text{C}_3$  splitter ought to be last to place the most difficult separations in that position.
- b) to get at the  $\text{C}_2$  and  $\text{C}_3$  fractions species more volatile and less volatile must be removed. We favor the removal of the more volatile methane and hydrogen to raise the temperature of coolant needed to drive subsequent distillations. This will reduce utilities costs substantially.
- c) the ethylene and propylene ought to be tower top products to insure the removal of degradation products.

These heuristics explain the gross features of the Sinclair-Koppers process the flow sheet of which is shown in Figure 2.

This kind of heuristic reasoning leads to an understanding of the separation sections of a wide variety of processes.

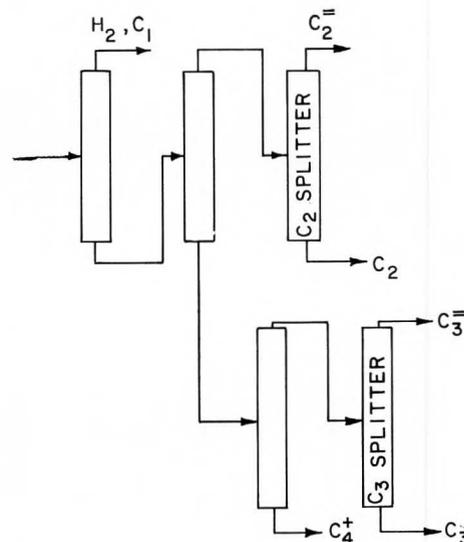


Fig. 2. Sinclair-Koppers Separation Flowsheet.

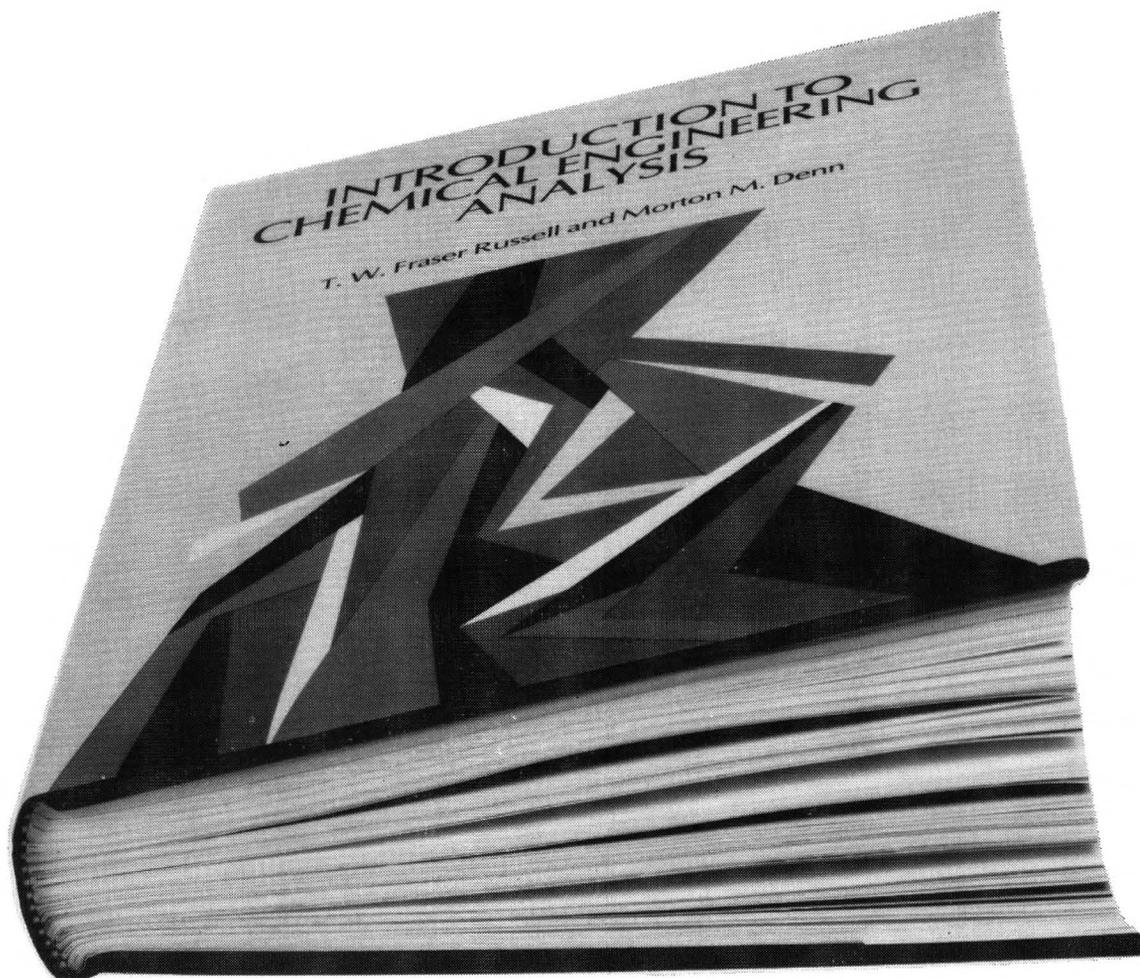
Typical home work problems involve the processing of cheese whey, crushed rock screening, high purity beryllium from the oxide, detergent manufacture, allyl chloride production, the development of screening circuits and an examination of many other industrial processes.

### Task Integration

The skelton of the process has been discovered when the processing tasks were defined in the previous chapters. Many of these tasks involve the addition and removal of energy, and these are costly operations. The last subproblem of process synthesis introduced is task integration where we free the process as much as possible from the purchase of heating and cooling service. We seek to have one task in the process drive other tasks, by the integration of their operation.

Before task integration can be attempted, the elementary principles of energy balancing must be presented. We show how the heat energy added to a system and the work done by a system are related to the enthalpy changes which occur in the material passing through the system. Then, methods of estimating the enthalpy change caused by temperature change, phase change, and chemical change are presented. This gives the quantitative background required for the understanding of the energy management principles to be discussed.

We show how energy management principles are used to supply heat to endothermic reactions, to remove heat from exothermic reaction, and to utilize the energy of product recovery. For example, the endothermic reaction of calcining limestone can be driven by matching it with an exothermic reaction, the combustion of coal: the be-



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ginner can calculate how much coal is needed per ton of limestone processed, obtaining a more complete picture of raw material costs in lime production.

The synthesis of networks of heat exchangers to recover sensible energy is discussed using the simple but approximate criteria of avoiding heating and cooling with external sources of these expensive utilities.

Typical problems include freezing of fish fillets, gas desulfurization, energy storage in checker brick regenerators, cost of sugar evaporator operation, and processing of junk cars by freeze milling.

### Fresh Water by Freezing

The scope of each of the preceding chapters was limited in turn to a specific aspect of process synthesis. Such limitations are necessary and desirable to present a compact package of knowledge which can be digested without too much difficulty. In practice no field is as clean and orderly as textbooks tend to describe it to be. This is certainly true of the field of process synthesis.

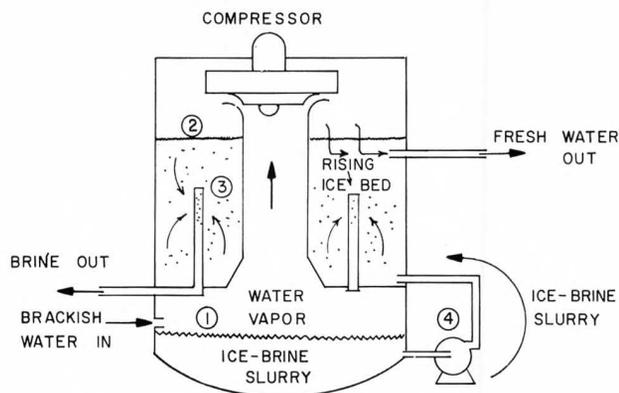
For one thing, few, if any, real problems are equally balanced among the several topics presented in the earlier chapters. Some problems are dominated by the chemistry, others by task sequencing still others by a critical separation, and many by the integration of energy and material use. Further, an experimental program usually parallels process synthesis for rarely is sufficient information to be found in the literature on phenomena to be exploited in a new area of processing. Finally, the early discovery stages of engineering are not sufficiently detailed to arrive at just one process, and several alternatives survive to undergo the detailed engineering studies necessary to determine economic and engineering feasibility.

These things are now brought into focus by tracing the development of a process to obtain fresh water from brackish water. We risk the appearance of contrived spontaneity by condensing the years of work of a number of engineers into a scenario of process discovery. However, it is important for the reader to come close to the act of discovery, even if the discovery is only one simulated by the authors.

This chapter begins with the observation that the *ice crystals formed in brackish water are salt free*, and ends with processes now commercially available for the production of fresh water. This engineering problem is dominated by task integration problems, for it is the cost of energy which dominates the water cost. Figure 3 is a schematic drawing of the vacuum freezing-vapor compression process, the synthesis of which is a problem in task integration discussed in this chapter.

### Detergents from Petroleum

In this chapter we apply the principles of process synthesis to the development of part of the technology to convert crude oil into detergents. No new ideas are presented, we apply what we already know. Our attention

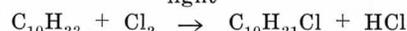


1. Vaporization of sea water at triple point causes ice formation.
2. Vapor condenses on clean ice surface to form fresh water.
3. 5% of fresh water used to wash rising piston of ice.
4. Ice-brine slurry pumped to bottom of ice wash column.

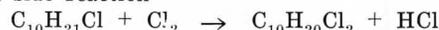
Fig. 3. Vacuum Freezing—Vapor Compression Process.

is focused on the problem of converting a kerosene fraction of the crude oil into an intermediate material, a chlorinated hydrocarbon, which then fits into the large campaign of detergent production.

Given fragmentary conversion data on these reactions



with the side reaction



We seek the technology to produce monochlorodecane economically on a commercial scale. Dominating this process synthesis problem are problems in species allocation and task selection.

To give some idea of the tenor of this chapter, we sketch out part of the development of the final process flow sheets. Figure 4 shows five ways of separating the reactor effluents shown in Table 2 into an HCl waste,  $\text{Cl}_2$ -decane recycle, monochlorodecane product, and dichlorodecane waste. How might the beginning student select among these?

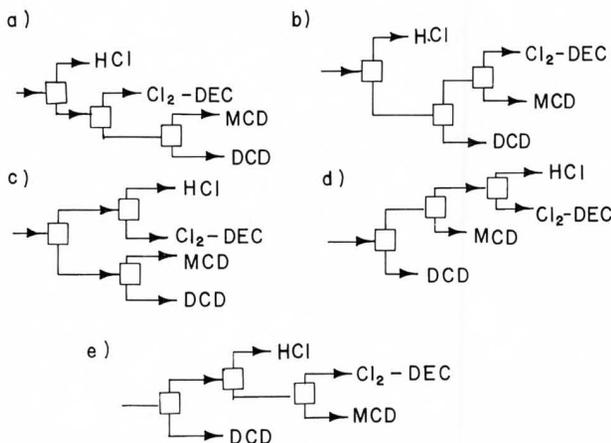


Fig. 4. Alternative Separations.

The dominance of science oriented courses in undergraduate education is caused by the very important role analysis has in engineering . . . The absence of the organizing influence of basic principles of synthesis is possibly the major reason why analysis tended to dominate education.

Table 2. Effluent from Photochlorination Reactor

Species		Moles	Boiling point
Monochlorodecane	MCD	0.95	215°C
Dichlorodecane	DCD	0.05	241
Decane	DEC	4.0	174
Chlorine	Cl <sub>2</sub>	trace	-34
Hydrogen chloride	HCl	1.05	-85

Applying the task selection heuristics

Plans a and c lead to low amounts of material processed

Plans a and b lead to low cooling costs by the early removal of volatile material

Plans a and c reduce processing costs by minimizing the amount of material processed during the most costly separation.

Plans a and b reduce costs by removing corrosive materials early

Plans a and c remove the MCD on a distillate rather than bottoms product

Hence, by applying these simple rules it appears that structure a is favored for a number of reasons. However, much more synthesis must be performed to develop better processing alternatives.

Figure 5 shows eight flowsheets which are synthesized using the principles developed in this early course. Figure 6 shows the economic analysis against which these processes are compared.

Flowsheet 2, which has the separation sequence for the last two columns in Flowsheet 1 reversed, is less attractive than 1 for all values of conversion. The decane is the largest component in the reactor effluent, and is also the lowest boiling component leaving the phase separator. The failure to remove decane early causes the increased cost in this case.

Flowsheet 3 involves the use of decane as a solvent to remove chlorine from the vapors leaving the phase separator. Since the chlorine not converted in the reactor is re-

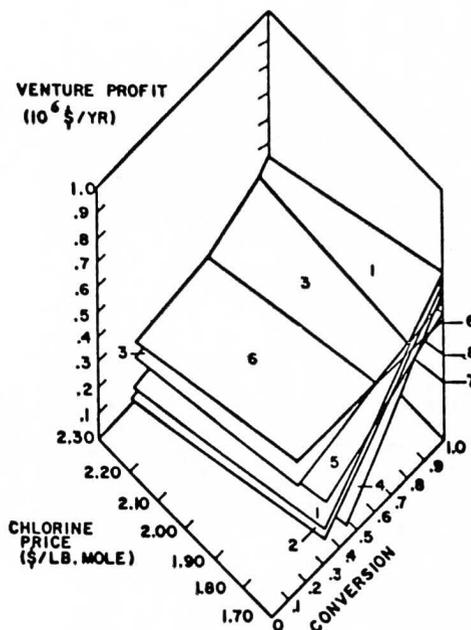


Fig. 6. Venture Profit Surfaces for Monochlorodecane Processes.

cycled, this flowsheet is not nearly as sensitive to conversion or chlorine cost as are Flowsheets 1 and 2. The maximum profit for Flowsheet 3 is not as high as the optimum for Flowsheet 1, but it is much less sensitive to the level of conversion. If uncertainty in the reactor design is large, the selection of Flowsheet 3 may be wise. The addition of a separator to recover unconverted chlorine adds to the equipment and operating costs but gives much greater flexibility in operation.

Flowsheet 4, which utilizes the reverse separation sequence of Flowsheet 1, is decidedly less attractive. The repeated processing of the low boiling components, par-

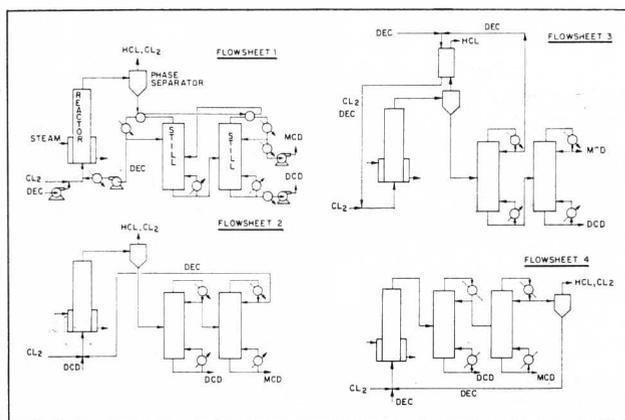
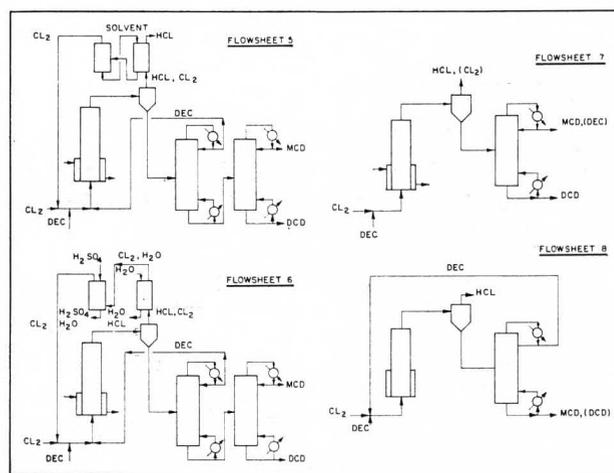


Fig. 5. Flowsheets synthesized using the principles. (Reproduced by permission of Chem. Eng. Prog. 68, No. 9, pp. 91-92, 1972)



ticularly HCl, causes very high equipment and utility costs. The loss of chlorine, as in Flowsheets 1 and 2 makes the profit for this process dependent on reactor conversion and chlorine cost.

Flowsheet 5 shows the same independence of conversion as Flowsheet 3. The profit is less due to solvent costs and the additional separator.

A profit nearly as high as that for Flowsheet 3 is obtained for Flowsheet 6. Flowsheet 6 utilizes water to remove hydrogen chloride from the vapors leaving the phase separator. Wet chlorine returning to the reactor inlet is dried by contacting concentrated sulfuric acid. The low cost of the solvent, water, and the fact that the water need not be regenerated make this alternative very attractive. However, the corrosive nature of the hydrogen chloride-water mixture and the sulfuric acid-water mixture require more expensive materials of construction. The danger of water entering the reactor must also be considered. If the reactor and separators are constructed of carbon steel, any traces of water in the presence of the hydrogen chloride reaction product would lead to rapid failure of these units due to corrosion.

Flowsheet 6 has a higher profit than Flowsheet 3 at low conversion. This because of the large amounts of decane solvent required in Flowsheet 3 for low chlorine conversions.

Flowsheets 7 and 8 are the special cases when conversion is complete. Flowsheet 7 has the advantage of only requiring two separators and no recycle. The high conversions using stoichiometric feed ratios lead however, to the production of large amounts of DCD. Hence, the profit for this alternative is low.

Flowsheet 8 represents the situation when large excesses of decane are utilized. Complete conversion of chlorine is achieved, hence no separation is required for its recycle. A small amount of DCD appears in the product. These advantages are offset by the costs associated with the separation and recycling of large amounts of decane.

In summary, three regions exist when comparing the eight flowsheets over wide ranges of conversion. At low conversions process Flowsheet 6, which utilizes water as a means to separate HCl and chlorine, is best. At intermediate conversion levels, process Flowsheet 3 is best. Process 3 utilizes the feed and recycle decane as a solvent for absorbing chlorine from the waste hydrogen chloride stream. For high levels of conversion, process Flowsheet 1, which discards unconverted chlorine, is optimal.

## CONCLUSION

An essential difference between the aims of education in science and in engineering ought not be lost. Herbert A. Simon states in the *Sciences of the Artificial*

Historically and traditionally, it has been the task of the science disciplines to teach about natural things: how they are and how they work. It has been the task of the engineering schools to teach about artificial things: how to make artifacts that have the desired properties and how to design. . . . Everyone designs who devises courses of action aimed at changing situations into preferred ones.

Science aims to *analyse* natural phenomena, and engineering aims *synthesize* from natural phenomena preferred situations. For example, while it may be sufficient for a scientist to develop an understanding of the phenomena of ice formation, the engineer ought to be concerned with use of his knowledge in the development, say, of an artifact which economically can produce fresh water from the sea by freezing.

The dominance of science oriented courses in undergraduate education is caused by the very important role analysis has in engineering, and is also caused by the availability of well organized and carefully planned text material in these areas. The natural organization of methods of analysis lends itself to course development and text preparation.

The absence of the organizing influence of basic principles of synthesis is possibly the major reason why analysis tended to dominate education. It remains to be seen if the course described will bring the proper balance between analysis and synthesis in engineering education. □

## LETTERS: (Continued from page 3)

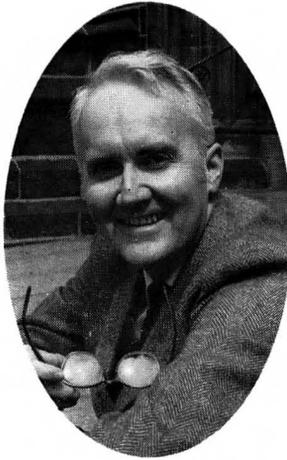
A little checking has revealed that the non-zero value is the result of a reformulation of steam table data published by the ASME in 1967.<sup>1</sup> Recognizing that a stable liquid-vapor equilibrium can't exist below the triple point temperature of 32.018°F, the reference conditions were changed so as to assign the value zero to the entropy and *internal energy* of the saturated liquid phase at the triple point. This, of course, forces the associated enthalpy to be (Pv) units greater or about 0.0003 Btu/lb<sub>m</sub>. One can certainly estimate the conditions for the metastable vapor-liquid equilibrium at precisely 32°F through simple extrapolation and obtain values of about -0.0181 Btu/lb<sub>m</sub> and -0.0178 Btu/lb<sub>m</sub>, respectively, for the internal energy and enthalpy of the liquid phase. The error in the Combustion Engineering tables, then, is the omission of the minus sign together, perhaps, with out spelling out the convention not stating (as does the reference above) that the first entry in the saturation table corresponds rigorously to a metastable state. At least one recently published text<sup>2</sup> on chemical engineering thermodynamics has copied this error, but the new edition of "Steam Tables" by Keenan, Keyes, et al,<sup>3</sup> does note both the negative values and metastability below the triple point.

Kenneth R. Jolls  
Iowa State University

1. "Thermodynamic and Transport Properties of Steam," American Society of Mechanical Engineers (1967).

2. Balzhiser, R. E., M. R. Samuels and J. D. Eliassen, "Chemical Engineering Thermodynamics," Prentice-Hall, Inc (1972).

3. Keenan, J. H., F. G. Keyes, P. G. Hill and J. G. Moore, "Steam Tables," John Wiley & sons, Inc. (1969).



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