

CHE

chemical engineering education

VOLUME XXII

NUMBER 2

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CHEMICAL ENGINEERING DIVISION OF AMERICAN SOCIETY FOR ENGINEERING EDUCATION

James E. Bailey *of Caltech*



The Mystique of Entropy
KYLE

Flow Sheet is Process Language
FEHR

A Course on Presenting Technical Talks
FELDER

Discrete-Event Simulation in Chemical Engineering
SCHULTHEISZ, SOMMERFELD

Safety and Loss Prevention in the Undergraduate Curriculum
CROWL, LOUVAR

A Pilot-Scale Heat Recovery System for Computer Process Control
CALLAGHAN, LEE, NEWELL

Engineering Management: Minimizing Functional Handicaps of Graduates
ELLINGTON

Levels of Simplification: Using Assumptions, Restrictions, and Constraints in Engineering Analysis
WHITAKER

and ChE at the

ILLINOIS INSTITUTE OF TECHNOLOGY

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Chemical Engineering Education

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JAMES E. BAILEY

of Caltech

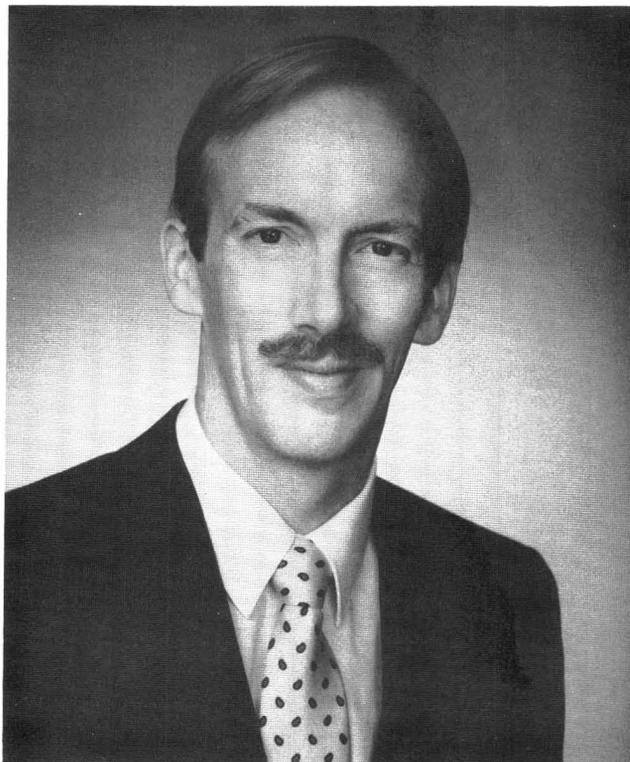
ROBERT FINN

*California Institute of Technology
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HIS COLLEAGUES describe James E. (Jay) Bailey as a man open to new ideas. Trained as a classical chemical engineer (Bailey did his doctoral work on chemical reactor theory, optimization theory, and non-linear mathematics) he soon developed an interest in the relatively young field of biochemical engineering. Lately, Jay has turned even more biological in his approach, pioneering a brand new field he calls metabolic engineering. His graduate students, who have joined in this odyssey, are well prepared to combine the techniques of molecular biology with more traditional engineering methods in the chemical engineering problem-solving armamentarium.

Jay ascribes many of the twists and turns of this intellectual odyssey to fortunate encounters with bright students and interesting colleagues. One of these chance encounters took place at the University of Houston in 1972 when Jay, then on the UH faculty, happened to meet biochemical engineer David Ollis. (Ollis was at Princeton University at that time; he is now Distinguished Professor of Chemical Engineering at North Carolina State University.) As Jay recalls it, "I was really impressed by the breadth of Dave's knowledge in biochemical engineering. I didn't know what a protein was in those days, but after a 30-minute conversation and a couple of phone calls, we decided to write a textbook."

The result was *Biochemical Engineering Fundamentals*, which has by now become the required text in almost every biochemical engineering course in the United States and in much of the rest of the world. It is now in its second edition. "Writing the first edition of this text was a tremendous learning experience," Jay recalls. "I didn't know much biochemistry, microbiology, or biochemical engineering at that time. I read texts and review articles, and I went to Elmer Gaden's short course. All this convinced me that we had to emphasize the background material in biochemistry, physiology, and genetics that differen-



tiates biochemical engineering from chemical engineering. A lot of other texts assume that you know what a protein is, what a bacterium is, what a gene is. We decided to define those terms, and others, very explicitly. I think that my entry into the field as a beginner made the text suitable for other beginners. The second edition, prepared after I had been heavily involved in biochemical engineering research for more than a decade, provided an opportunity to inject some personal perspectives into the text, in addition to improving its organization and updating its content."

Jay's own education as a chemical engineer was typical enough. He did both his undergraduate and graduate work at Rice University, earning his doctorate working on reactor theory and optimization with Fritz Horn. After a two-year stint with Shell Development in Emeryville, California, Jay established his own laboratory in the Department of Chemical Engineering at the University of Houston. It was there that he first let himself be nudged in the direction of biochemical engineering.

"In the late 1960s and the early 1970s, the National Science Foundation sponsored a major effort in en-

Trained as a classical chemical engineer, [Jay] soon developed an interest in the relatively young field of biochemical engineering. Lately, he has turned even more biological in his approach, pioneering a brand new field he calls metabolic engineering. His graduate students, who have joined in this odyssey . . . combine the techniques of molecular biology with more traditional engineering methods . . .

zyme engineering," Jay notes. "I was doing computational and theoretical work on immobilized enzyme catalysis and on some diffusion-reaction problems with unusual properties. Two of my graduate students at UH had interesting backgrounds—Mike Cho had a background in biochemistry, and Jila Fazel-Madjlessi had a background in microbial fermentation. They helped me start experimental programs in those areas."

With Cho, for example, Bailey made major theoretical and practical advances in the area of immobilized enzymes. Their work involved the first application of the carbodiimide-mediated covalent attachment of enzymes to activated carbon. Using this approach they constructed hybrid catalysts that combined an enzyme's activity with the catalytic action of the support surface. Specifically, they looked at the oxidation of glucose by the enzyme glucose oxidase. A byproduct of this reaction is hydrogen peroxide, which tends to deactivate the enzyme. Bailey and Cho discovered that activated carbon decomposes the peroxide and also assists in the supply of oxygen to the enzyme sites within the porous catalyst. They also discovered, however, that loading too much enzyme onto the support compromises its efficiency in deactivating peroxide, and they were able to characterize the tradeoff between higher enzyme loading and peroxide decomposition in some detail.

Jay's experimental work on immobilized enzymes continues to this day. One of his most significant discoveries was accomplished in collaboration with Ph.D. student Doug Clark (now an assistant professor and NSF Presidential Young Investigator at the University of California, Berkeley). Clark and Bailey combined classical activity studies with electron paramagnetic spin resonance measurements of spin-labeled immobilized enzymes. Using this technique, they were able to establish direct evidence of active site modification caused by immobilization and to show the relationship between the degree of modification and the activity of the enzyme.

Bailey's collaboration with Clark characterizes Jay's philosophy of graduate education. He firmly believes that graduate students should participate heavily in their research projects and in formulating strategies for solving their problems. He observes, "Graduate students are here to learn how to do research—not just how to do experiments or calcula-



Jay enjoys weekly group seminars to discuss progress and problems in the lab.

tions, but how to identify a particular problem within an important general area. I encourage them to consider the method of accomplishing a solution and its feasibility as well as the ultimate impact that the solution will have. Besides, since I've been fortunate to work with many excellent students, it would be foolish of me to presume that I have all the necessary ideas and knowledge. I depend on my students to contribute substantially to all aspects of their projects. On many occasions, including Doug Clark's work, my students have transformed my vague suggestions into highly original and productive research."

Jay's work on periodic processes and biochemical engineering during nine years on the faculty of the University of Houston was recognized in 1979 by the Allan P. Colburn Award of the American Institute of Chemical Engineers. He came to Caltech in 1980. According to John Seinfeld, a close friend of Bailey's and Caltech's Louis E. Nohl Professor and Professor of Chemical Engineering, "I first met Jay about twelve years ago at an AIChE meeting and we became friends. Around 1979 I realized that Jay might consider moving. He was quickly establishing himself as one of the leading people in biochemical engineering in the United States."

Jay has been good for Caltech, and the intimacy and informality of the Caltech environment have apparently been very good for him as well. "The biggest qualitative change in my work came after I arrived at Caltech. Here my students and I can learn from and

interact with some of the top people in biochemistry, molecular biology, and cell biology, not to mention chemical engineering. Cross-disciplinary collaboration happens almost automatically at Caltech."

It was at Caltech that the techniques of genetic engineering began influencing Jay's work. The revolution in recombinant DNA technology that began in the late 1970s has been widely seen as the biologist's show. But Bailey realized that if these techniques were to realize their commercial potential, chemical engineers would have to get intimately involved.

He also realized that modeling concepts from traditional chemical reaction engineering could be effectively applied in a new context—viewing a single cell



A sophisticated flow cytometer-cell sorter, here operated by Dane Wittrup and Elaine Meilhoc, has supported many PhD projects in Bailey's laboratory.

as a complex chemical reactor and transport apparatus. Working in Jay's group, Sun Bok Lee (now at the Korea Advanced Institute for Science and Technology) and Steve Peretti (currently an assistant professor at North Carolina State University) formulated powerful new mathematical models that included genetic level regulation.

Another consequence of Jay's interest in genetic engineering was his collaboration with Caltech's Judith Campbell, associate professor of chemistry and biology, who studies basic mechanisms of DNA replication in yeast. Genetic engineers often use the technique of inserting recombinant "plasmids" into yeast cells to get them to produce desired proteins in quantity. Plasmids are relatively small, circular segments of DNA that contain regulatory genes and genes that code for proteins. There is one important problem with foreign plasmids, however: As the recombinant yeast cells divide, they tend to lose their plasmids generation by generation, gradually becoming less and less productive.

Bailey and Campbell have made a concerted effort to understand this process using flow cytometry measurements to provide unprecedented detail on single-

cell plasmid content in recombinant populations. In flow cytometry individual cells are sent past a laser beam, one by one, but very rapidly. In a process that takes about one millisecond per cell, flow cytometry permits determinations of cell size, shape, internal structure, and the concentration of specific compounds in individual cells. Many graduate students and post-doctoral fellows have contributed to a growing body of flow cytometry research in Jay's lab, and several of these collaborators, including Friedrich Sreenc at Minnesota and Jin-Ho Seo at Purdue, are now extending these methods in their research labs.

Some of Jay's work in progress involves sharpening the focus of the genetic engineering studies to more subtle and interesting problems. For example, he's gotten interested in the details of what exactly happens to a protein after synthesis. There are essentially three possibilities: The protein can be degraded, it can be exported from the cell, or it can remain in the cell in solution or in an aggregate. If genetic engineering is to fulfil its economic promise, these alternatives must be understood and the factors that control protein targeting must be better characterized in quantitative terms.

Typically, genetic engineers concern themselves with attempts to make cells produce certain proteins in quantity. But chemical engineers are well aware of the fact that proteins are not the only compounds of economic importance made by cells. Realizing this, Jay's group is concentrating on a brand new field that Jay calls metabolic engineering. "Metabolic engineering involves the application of genetic engineering techniques to alter or enhance the metabolism of cells," Jay explains. "The goal is to overproduce specific amino acids, acetone, vitamins, certain biopolymers, or other important chemicals made in cells. Metabolic engineering requires a lot better understanding of what a cell is doing.

"First, we must understand all the pathways available to an organism for producing the target compound and determine what additional pathways we could make possible by introducing new enzyme activities into that organism. Then, it's important to judge which regulatory points along the pathway are most important, since these determine the rate and the selectivity for the target compound. After determining the most promising target enzymes, we must clone the gene for that enzyme, attach the gene to a suitable vector, and insert it into the organism. Then, of course, we must investigate the effects of our genetic manipulations on the production of the target compound and its intermediates."

Jay's group has made significant advances in all

steps of this process. In terms of understanding metabolic pathways in detail, Alex Seressiotis, a former student of his who's now at Columbia University, developed a computer program called MPS (Metabolic Pathway Synthesis). The program contains a database system that stores enzyme and substance descriptions. "MPS can be used on a qualitative basis to examine the effects of adding or deleting enzyme activities to or from the cellular environment, to classify pathways with respect to cellular objectives, and to extract information about metabolic regulation," Jay says. In an illustration of the power of MPS, Seressiotis and Bailey had it consider the conversion of pyruvate to the amino acid L-alanine. MPS came up with a route to L-alanine that does not incorporate the enzyme alanine aminotransferase, which is commonly assumed to be a required step for alanine biosynthesis.

Jay's lab has the distinction of being one of the first chemical engineering labs in the world with full cloning facilities. "The traditional way of producing strains of an organism with desired properties was to use a mutagenesis program," notes Bailey. This involves exposing the cells to radiation or other mutagens and assaying the resulting organisms for the property in question. "But this is a very random, time consuming, and sloppy technique. By using recombinant DNA technology we can make the whole process far more rational. Furthermore, students with cloning experience are more equipped to consider genetic as well as process solutions to engineering problems. And they'll be far better prepared to interact productively with molecular biologists in the future."

To investigate the effects of genetic manipulations made in his lab, Jay's group has recently developed novel data analysis methods for use with his new, 300 megahertz, wide-bore NMR. These methods allow important measurements to be accomplished simultaneously from a group of living cells. In a single experiment, Jay's students can estimate intracellular pH, the concentration of several key sugar phosphate metabolic intermediates, and the concentrations of adenosine di- and triphosphate (ADP and ATP).

At present, Bailey's lab is working on three projects in metabolic engineering. In the first of these projects, the lab is attempting to enhance the uptake of the sugar hexose in the yeast *Saccharomyces cerevisiae*. Hexose uptake is the rate-limiting step for growth in this economically important organism, which is used for ethanol production and in the genetically engineered production of other compounds. The second project involves engineering the bacterium *Escherichia coli* to produce ethanol by inserting genes



Jay explored the crater of Mt. Bromo in Java, Indonesia, in April 1987.

for pyruvate decarboxylase and alcohol dehydrogenase. In a third project, the group is trying to improve production of ATP (the cell's energy currency) in *E. coli*.

Not all chemical engineers agree with the direction Bailey's research has taken. According to John Seinfeld, there are still a few diehards out there who express skepticism about chemical engineers who get involved with essentially biological techniques. But, Seinfeld says, there are fewer and fewer naysayers. "I think biochemical engineering is going to mature. People are recognizing that it will take its place as a firm field in chemical engineering and, in a sense, settle down. It is difficult for biochemical engineering to be as rigorous as some other fields of chemical engineering that are closer to physics. That level of rigor is being supplied by people like Jay Bailey. There will be more biology in the education of future chemical engineers as a result of his work."

The education of chemical engineers is a subject that's important to Bailey. He's particularly proud of the fact that many of his former graduate students have become faculty members at important universities around the world. Frances Arnold, assistant professor of chemical engineering at Caltech and Bailey's wife says, "Jay takes a personal interest in each of his students. He's always willing to sit down with them and tell them the 'facts of life' of the chemical engineering profession. His students show a lot of loyalty as a result of his interest in them."

Important institutions to Jay's group of students and postdocs are Friday afternoon group seminars and, following that, the traditional "Ho-Ho" in the Rathskeller of the Athenaeum, Caltech's faculty club. "Gathering outside the lab for conversation and a few

Continued on page 102.



Chemical engineering offices and laboratories are located in Perlstein Hall.

ILLINOIS INSTITUTE OF TECHNOLOGY

SATISH J. PARULEKAR

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THE DEPARTMENT OF Chemical Engineering at the Illinois Institute of Technology (IIT), formally established in 1904, is one of the oldest chemical engineering departments in the nation. The development of the department in the pre-1971 period was previously described in this journal [1]. Dramatic changes have occurred in the department since that time in terms of faculty, undergraduate and graduate programs, and research. All current chemical engineering faculty, with the exception of one member, were added after 1974. Since then, there has been a significant expansion in research activities and research areas pursued, with the current faculty having expertise in traditional as well as emerging areas in

chemical engineering. This is also reflected in the undergraduate and graduate curricula, which have changed significantly to meet the changing needs of the profession.

IIT's main campus, internationally recognized as an architectural landmark and located three miles south of Chicago's downtown area and a mile west of Lake Michigan, was designed in the 1940s by Ludwig Mies van der Rohe, one of this century's most influential architects. The current university population on the main campus includes about 6500 undergraduate and graduate students and about 500 faculty. The other campuses of IIT are located in downtown Chicago and in the western suburbs of Chicago in DuPage County. Chicago, one of the largest cities in the world and a national and international center of business and industry, offers students an exceptionally wide variety of professional and cultural resources. The close proximity of several chemical, food, and allied industry research centers and production

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Since engineering is largely a team effort, we believe that development of the individual's ability to work effectively as part of a team is important. To accomplish this, the laboratory courses and the design courses involve teams of students . . . laboratory sections are small and a high level of personal contact between students and instructor is maintained . . .

plants provides for the IIT community an invaluable source of close interaction with industry.

THE DEPARTMENT

The chemical engineering offices and laboratories are located in Perlstein Hall. Presently, about 150 full-time undergraduate students and 60 full-time graduate students are enrolled in the department. In addition, there are about 40 part-time undergraduate students and 50 part-time graduate students. Three graduate degrees are offered by the Chemical Engineering Department: Master of Science (MS), Master of Chemical Engineering (MChE), and Doctor of Philosophy (PhD). The department annually awards nearly 40 Bachelor of Science, 10 MS, 10 MChE, and 8 PhD degrees.

Over the years, the department has graduated many competent engineers, a number of whom have obtained significant national prominence in their professional careers. Several of our alumni have held national office in the American Institute of Chemical Engineers. Although a majority of our alumni have pursued professional careers in industry, we are proud that, over the years, a significant number have joined chemical engineering faculties at major institutions.

RESEARCH

The research areas pursued in the pre-1971 period were chemical reaction engineering, separation processes, thermodynamics, and transport and interfacial phenomena [1]. In recent years, many additional areas of research have been initiated and strengthened. They include biochemical engineering, biomedical engineering, combustion, energy technology, enhanced gas and oil recovery, and process dynamics and control. Interdisciplinary research has been a strong tradition at IIT and several joint initiatives with other departments have evolved to address problems in the critical emerging areas. Some of the faculty have cooperative research activities with the Institute of Gas Technology, IIT Research Institute, and Argonne National Laboratory. All such interactions provide an intellectually stimulating environment for the graduate students. The development of IIT's very strong research and educational center in food technology at the Moffett Technical Center (located in the Chicago area) will be completed this summer.

Some of the chemical engineering faculty will be closely associated with this center.

It is interesting to look at the current faculty in chronological order of joining the chemical engineering department at IIT in order to trace the growth of our program in recent years.

Darsh Wasan, currently acting Dean of the Armour College of Engineering, is the oldest faculty member in terms of service, having joined IIT in 1964. He served as department chairman from 1971 to 1987. His research deals with interfacial and colloidal phenomena, enhanced oil recovery, and separation processes. Darsh and his research team are developing experimental techniques to accurately measure surface and interfacial rheological properties. This research has significant utility in control of a variety of dispersed phase systems and in study of the mechanisms of oil bank formation and propagation in chemical flooding processes involving surfactants and alkaline agents, foams, emulsions, and polymers for mobility control. Research in separations is concentrated on separation of fine particles from non-aqueous media based on electrokinetic phenomena, emulsification/demulsification processes and thin liquid film phenomena. Darsh is a recipient of the Western Electric Fund Award of the ASEE, the Hausner Award of the Fine Particle Society, and the Special Creativity Award of the National Science Foundation.

The mid-1970s saw the addition of two of the current faculty members, Rob Selman and Dimitri Gidaspow. **Rob Selman**, currently acting chairman of the department, joined the faculty in 1975. His research interests are electrochemistry and electrochemical engineering with a special emphasis on high-temperature processes. Rob and his students are currently investigating the formation, growth, and corrosion of dendritic metal deposits, a problem common in the charging of zinc-based aqueous batteries which are being developed for electric vehicles and load leveling. Other current research projects deal with fundamental aspects of molten carbonate fuel cells and development of porous-electrode models for these fuel cells. The characterization of micro-emulsions by AC impedance is being investigated to assess the effectiveness of electrochemical oxidation as a means of breaking micro-emulsions. Other research projects under Rob's direction deal with molten salt processes involving

carbon cathodes and amorphous metal deposition from molten salts.

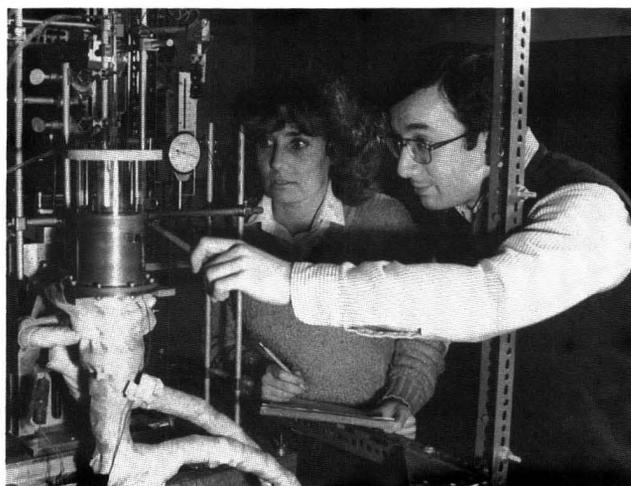
Dimitri Gidaspow joined the faculty in 1977. Dimitri's research interests are in the areas of mathematical modeling and analysis of various energy conversion processes. His current research involves studies of the hydrodynamic theories of fluidization and gas-solids transport. Generalizations of Navier-Stokes' equations are being solved using supercomputers to predict phenomena such as cluster formations in risers and bubble motion in fluidized beds. In collaboration with Darsh Wasan, he also conducts research in the areas of separation of colloidal particles and electrostatic desulfurization of coal. Dimitri has been recognized for his research through the Donald Q. Kern Award of the AIChE and the Special Creativity Award of the National Science Foundation.

The bulk of the present faculty members arrived on the scene in the 1980s. **Richard Beissinger** joined the chemical engineering department in 1981.



Taha Alkhamis and Richard Beissinger working with a Weissenberg rheogoniometer for blood viscosity measurement.

Richard's research is concerned with transport phenomena in biological systems. His current research activities are in blood-artificial surface interactions, biorheology, and development of artificial red blood cells. He also conducts research in the development of implantable drug infusion systems and in pharmacokinetics. Some of his current research projects are: augmented mass transport in sheared suspensions; macromolecular adsorption to solid surfaces; liposome-encapsulated hemoglobin and hemoglobin-in-oil-in-water multiple emulsion droplets as red blood substitutes; and the effects of red blood cells on platelet adhesion and aggregation in laminar shear



Jill Weldon and Selim Senkan discussing experiments with a flat flame burner in the combustion research laboratory.

flow. Rich is also directing development of the interdisciplinary Polymer Science and Engineering program.

Ali Cinar, who arrived in 1982, conducts research in process control and dynamics. Control strategies for multivariable chemical processes are being developed and tested using experimental systems and real-time microcomputers. One of his research projects deals with developing methods for selecting robust operating configurations and improved control strategies using a pilot plant consisting of two catalytic tubular reactor beds with internal heat exchange and a feed-effluent heat exchanger. Ali and some of his graduate students are also investigating forced periodic operation of chemical reactors using the vibrational control approach. Their work is focused on stabilization of exothermic continuous stirred tank reactors and tubular packed bed reactors as well as on improvement in selectivity and yield of complex reactions. Another of Ali's research projects deals with development of expert systems for fault-tolerant computer control of complex processes, such as multi-bed autothermal reactors.

Selim Senkan joined IIT in 1982. His research is in the areas of combustion and high-temperature chemical reaction engineering as applied to problems in energy conversion, propulsion, and environmental protection. One of his research projects deals with experimental and theoretical investigation of oxidation and pyrolysis of chlorinated hydrocarbons (CHCs) using model compounds. In the experimental program, stationary flames of selected CHCs are probed for the determination of species and species profiles

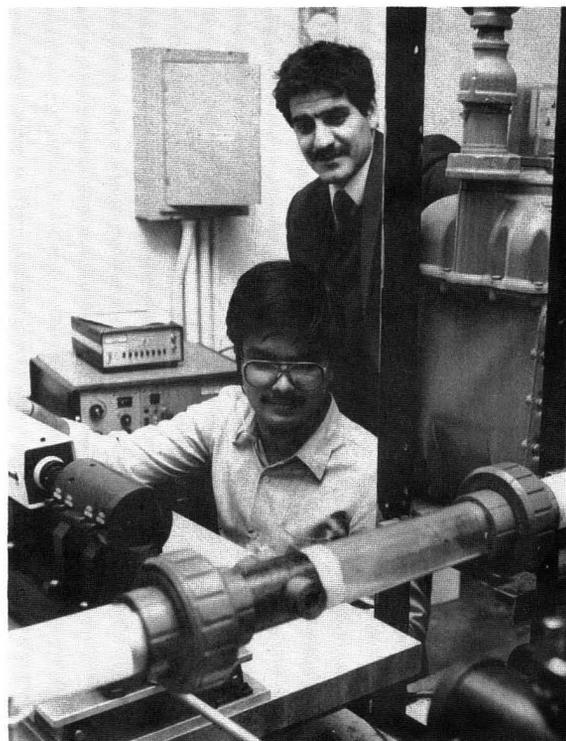
using supersonic jet sampling coupled with on-line molecular beam mass spectroscopy (MBMS). An outcome of this research is the recently patented, economic process for conversion of methane into acetylene and ethylene. Because of low NO_x pollutant emissions, catalytic combustion is an attractive alternative to flame combustion when very high temperatures are not required. Selim and his group are also involved in the study of the impact of halogens on catalyst development, reaction rates, and selectivity in catalytic combustion processes.

William Weigand joined the IIT faculty in 1983. His research interests are biochemical engineering and process control. Bill and his research group are involved in kinetic modeling of cell growth and product formation for microorganisms which produce primary and secondary metabolites. The optimal operating procedures are then derived and examined with the aid of computer simulations and experiments carried out with highly-instrumented, computer-coupled fermentors. Bill is also interested in development of new sensors and the use of estimation techniques which permit optimal operation in the absence of complete variable measurement. In the area of process control, techniques for control in the presence of modeling error, for changing system dynamics, and for nonlinear interacting systems are being developed.

Hamid Arastoopour and **Satish Parulekar** joined the department in the fall of 1985. **Hamid Arastoopour** has research interests in the areas of multiphase flow, flow in porous media and unconventional gas reserves, and fossil fuel conversion processes. Current research projects being investigated by Hamid and his graduate students are hydrodynamic analysis of pneumatic conveying of solids, numerical analysis of single and multiphase flow in unconventional reserves, analysis and measurement of the agglomeration of sticky particles and heat transfer in fluidized beds, and analysis and measurement of transient gas and condensate flow in gas transmission and distribution systems.

Satish Parulekar conducts research in biochemical engineering and chemical reaction engineering. His research in biochemical engineering deals with production of extracellular and intracellular enzymes/proteins by recombinant and wild-type microorganisms and production of biochemicals using immobilized cell reactors. The research with recombinant organisms is aimed at gaining a fundamental understanding of host-plasmid interactions in these species and the effect of these interactions on plasmid stability, cell growth and product gene expression. The research with wild-type microorganisms is di-

rected towards understanding the mechanism of synthesis of extracellular enzymes such as amylases and proteases. The research dealing with immobilized cell reactors is focused on study of alteration in cellular metabolism due to immobilization and implications of such alteration in design of these reactors. His research in chemical reaction engineering is concerned with identification of optimal reactor structures for



Prasad Davuluri and Hamid Arastoopour studying transient gas transport with a Laser Doppler velocimeter.

complex reaction networks and experimental and theoretical investigation of forced periodic operation of continuous flow (CSTR and tubular) reactors.

Henry Linden joined the faculty in the spring of 1987 as the F. W. Gunsaulus Distinguished Professor of Chemical Engineering. Henry has had an exceptionally illustrious career in research in fuel technology at both the Institute of Gas Technology and the Gas Research Institute and was president of each of these institutions for several years. His distinguished career has led to membership in the National Academy of Engineering, as well as to numerous honors and awards such as the Distinguished Service Award from the American Gas Association. Having Henry on board will give us the benefit of his wide-ranging experience and insight in energy-related research.

UNDERGRADUATE PROGRAM

The mission of the undergraduate program in chemical engineering at IIT is to prepare our students for their professional careers and to enable them to develop the technology of the future. There is enough flexibility in the program for each student to tailor an individualized curriculum to satisfy his or her particular scientific or technical interests. The first two years are devoted to the fundamental sciences, mathematics, and engineering sciences and are particularly concerned with the development of professional skills. In addition to developing engineering competence, the program examines the economic and societal implications of chemical engineering. The required courses are material and energy balances, and unit operations-I in the sophomore year; thermodynamics, transport phenomena, unit operations-II, and chemical engineering laboratory-I in the junior year; and chemical reaction engineering, process control, chemical process design (two semesters), and chemical engineering laboratory-II in the senior year.

In addition, there are elective courses in bioengineering, computer applications in chemical engineering, colloidal and interfacial phenomena, electrochemistry, energy technology, food technology, microelectronics fabrication, and polymer processing. Students interested in gaining professional specialization may include some of these courses in their curriculum to earn a specialized minor in one of the following areas: biotechnology, computers in chemical engineering, energy technology, food technology, and polymer engineering.

Since engineering is largely a team effort, we believe that development of the individual's ability to work effectively as part of a team is important. To accomplish this, the laboratory courses and the design courses involve teams of students. Since individual instruction is so important to students' growth, laboratory sections are small and a high level of personal contact between student and instructor is maintained. Some of our best students also choose to work on independent research projects during their junior and/or senior years, which prepare them for graduate research.

GRADUATE PROGRAM

The coursework for MS and MChE degrees must include at least four of the following six core courses: chemical reaction engineering, fluid mechanics, heat transfer, mass transfer, process control, and thermodynamics. For a PhD degree, coursework in all six areas is required so that the students will be equipped

At IIT we are developing courses to integrate these emerging areas into our curricula while, at the same time, leaving the emphasis on science and engineering fundamentals unchanged.

to apply advanced principles from the entire spectrum of chemical engineering irrespective of their research specialization. A student pursuing an MS must complete eight credit hours in research and thesis work. The MChE is a professionally-oriented degree program which permits a concentration in engineering practice. The requirements are the same as those for the MS degree, except that additional courses and/or a project replace the eight credit hours of thesis. Every prospective PhD candidate must take a qualifying examination to determine fitness and aptitude for further graduate study. Research qualities are judged during the oral comprehensive examination over the student's dissertation proposal, taken some time after admission to candidacy. After successfully clearing this examination, the candidate pursues the selected research program in consultation with the research adviser and advisory committee.

In addition to the core courses, IIT offers a wide variety of elective graduate courses which in the past three years have included biochemical engineering, catalysis, computational techniques, electrochemical engineering, polymer processing, reservoir engineering, separation processes and transport phenomena in living systems. Many of the graduate courses, particularly the core courses, are televised through the IIT/V network. Remote centers for reception of these telecasts are located near several of the industrial centers within a fifty-mile radius from the IIT campus for the benefit of part-time students.

THE FUTURE

As the chemical engineering profession changes and adapts to the technology needs of the next decade and the next century, so must chemical engineering education. In the coming years, the curriculum content will be modified to accommodate new technology areas in chemical engineering. At IIT, we are developing courses to integrate these emerging areas into our curricula while, at the same time, leaving the emphasis on science and engineering fundamentals unchanged. As in the past, thorough training of the undergraduate as well as graduate students will continue to receive the highest priority.

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AICHE JOURNAL

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A M E R I C A N I N S T I T U T E O F C H E M I C A L E N G I N E E R S

A PILOT-SCALE HEAT RECOVERY SYSTEM FOR COMPUTER PROCESS CONTROL TEACHING AND RESEARCH

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IN THE LAST two decades efficient energy utilization and process integration have become increasingly important to chemical plant economics. Plant design for these factors has meant higher levels of process interaction, often with positive feedback, which require improved control. A typical example is the heat recovery circuit in reactor or distillation systems.

Process equipment used in the laboratory to investigate the control problems created by tighter process integration is more convenient. This can be summarized as

- Lower cost of pilot-scale equipment, and
- Loss of production and or product quality are not issues during process experimentation.

However, instrumentation and control equipment is "off the shelf" as is found in industry and hence is a significant cost factor. The aim in building process control rigs for undergraduate teaching and graduate

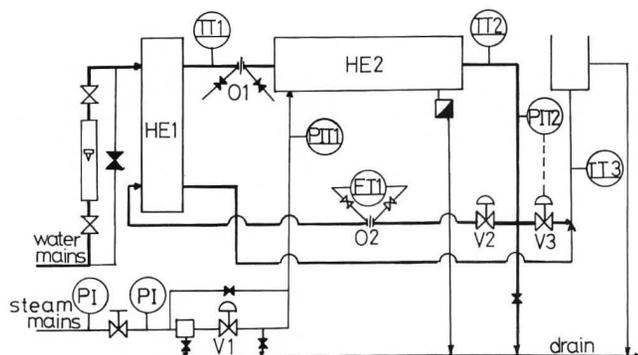


FIGURE 1. Schematic diagram of pilot-scale heat recovery circuit.

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The pilot-scale heat recovery system is a valuable teaching and research tool. It is sufficiently flexible to demonstrate basic principles and yet sufficiently complex to demonstrate common process control problems such as nonlinearities and interactions between variables.

research is to create rigs that are

- Flexible enough to demonstrate a number of basic principles
- Sufficiently complex to demonstrate common process control problems such as nonlinearities and interactions between variables
- Economical

Due to the important role of real time computing in process control, it is essential to provide teaching and demonstration facilities of such techniques. In addition, most advanced control strategies require the use of process control computers for successful implementation.

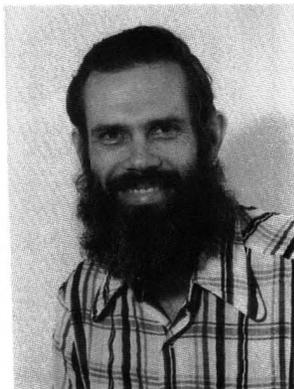
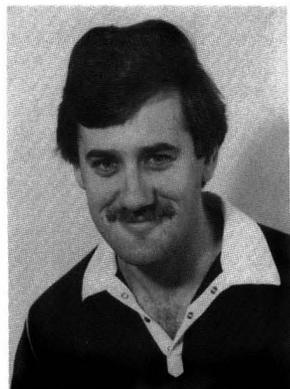
**TABLE 1
Equipment Details**

Valves V1 and V2	Fisher Control Valves, size 34 and 30 respectively
Valve V3	Badger Meter Inc, size B
Double pipe exchanger	2.43m long, 13mm diameter copper pipe, 38mm diameter copper jacket
Plate heat exchanger	Alpha Laval P20-HB
Rotameter	Metric Series 18 with S.S. plug
dp Cell	Taylor Instruments, 0-5"H ₂ O
Pressure transmitter PIT1	Beckman, 0-500 kPa
Steam supply pressure to experimental apparatus	0.2MPa
Pressure transmitter PIT2	Honeywell, 0-500 kPa

PILOT-SCALE HEAT RECOVERY CIRCUIT

A schematic diagram of the laboratory rig is shown in Figure 1. Mains water is preheated in a pre-heat plate heat exchanger, HE1. After preheating it flows through a steam heated double pipe heat exchanger, HE2. After the double pipe exchanger the water splits either to be used in the preheat plate heat exchanger or to bypass the heat exchanger. When the streams rejoin they are fed to a constant head drain. A control valve, V3, is installed in the bypass line and may be used to regulate the bypass flowrate. Equipment details are given in Table 1.

There are two manipulated variables in the system: a control valve in the steam line, V1, and a control valve, V2, in the hot line after the double pipe exchanger leading to the preheat plate exchanger. They can be used to control any of the dependent variables, but typically the final mixed temperature, TT3,



P. J. Callaghan received his BEChem and his MEngSci degrees from the University of Queensland in 1984 and 1986. His Master's programme centered on the development and use of a predictive control algorithm for the heat exchange system described in this paper. He is currently employed by Akoa Ltd. as a control engineer. (Not pictured)

P. L. Lee received his BEChem from RMIT in Melbourne and his PhD from Monash University in 1980. He worked in the design and commissioning of computer control systems for both continuous and batch plants for three years before coming to Queensland. His early research was on the control of the unstable steady state in an exothermic CSTR. His interests include multivariable self-tuning and adaptive control of fermentation and heat recovery systems. (L)

R. B. Newell received his BScApp and BEChem from Queensland and his PhD from the University of Alberta. He also has a DipEd in Tertiary Education from Monash. He joined the staff at Monash University in 1974 and moved to Queensland in 1980. His early research was in the multivariable control of a pilot plant evaporator, unstable steady state control in a CSTR, and multilevel hierarchical optimization. Current interests include optimization of the Australian oil refinery and transportation system, combined fuzzy and deterministic control, and self-tuning and adaptive control of heat recovery systems. (R)

and the temperature out of the double pipe exchanger, TT2, are used. A standard differential-pressure bypass control loop is usually implemented to maintain the pressure drop across the plate heat exchanger constant.

PROCESS-CONTROL SYSTEM INTERFACE

An interface box between the process instrumentation and the control system is located on the rig. This box displays all rig variables, both manipulated and controlled, *i.e.*, the steam pressure, the hot side water flowrate to the plate heat exchanger, and the three temperature measurements and the valve positions. The interface box is supplied with 240V AC power and supplies 24V DC for instruments and transducers. Standard signals are 0-5V for control signals and 1-5V for measurements. The interface box also has the facility to switch the manipulated variables from remote to local, by interrupting the signal from the control system and supplying a manual signal.

Figure 2 shows the responses in the exit tempera-

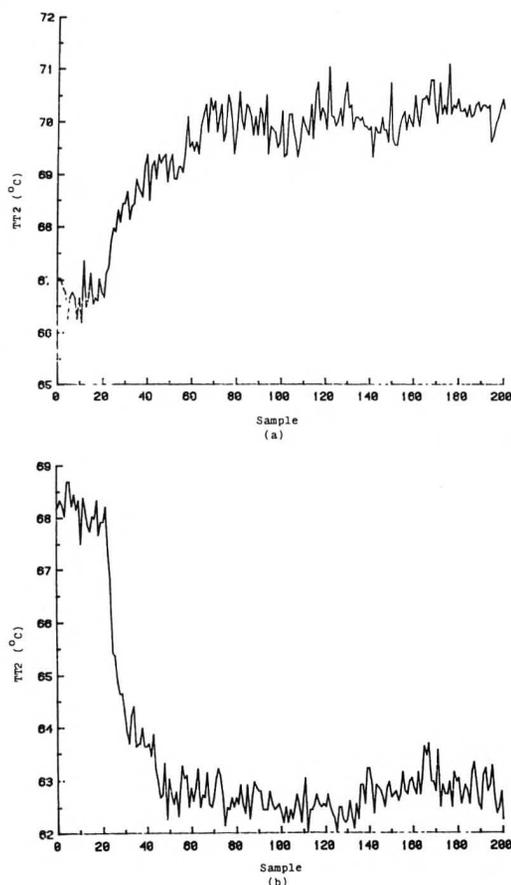


FIGURE 2. Step test responses for TT2 due to a 10% step (a) up and (b) down in V1 after sample 20.

ture to 10% step changes up and down in the steam. The sample time during the collection of this data was five seconds. Note that both magnitude and shape of responses differ, illustrating non-linear behaviour. Also the need for filtering is apparent from this raw data.

CONTROL SYSTEM EQUIPMENT

Basic Data Collection and Regulatory Control

The control system used to monitor and control the pilot-scale apparatus is arranged as shown in Figure 3. This equipment is arranged in a hierarchical manner, consisting of two layers: a primary data collection and regulatory control level, and an advanced control level.

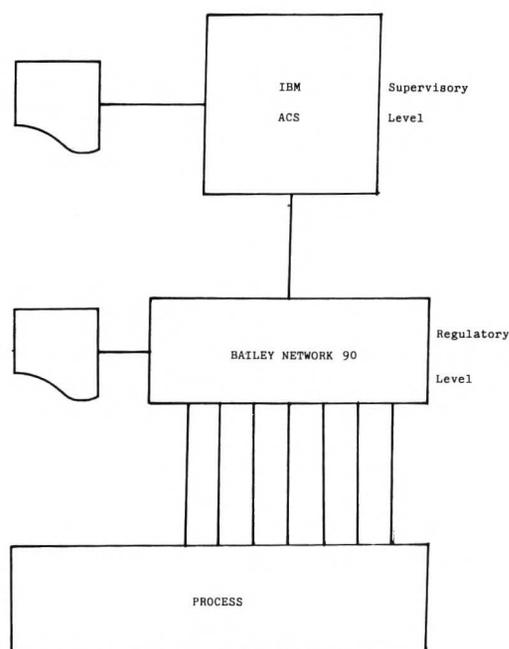


FIGURE 3. Control system equipment.

The primary data collection and regulatory control functions are performed using a Bailey Network 90 distributed control system. The heart of the system is a "multi-function controller," which is a micro-processor based controller. It performs all of the regulatory control functions and coordinates the operation of the analog-to-digital input and digital-to-analog output cards. Operator interface is provided by means of a color CRT display. This display is capable of showing schematic representations of the pilot-scale equipment with measurement data displayed, controller faceplate displays, trend plots of measurement inputs, and combinations of the above types of displays.

Advanced Control Function

The advanced control functions, such as implementing multivariable predictive controllers are performed using the IBM Advanced Control System (ACS) previously described in this journal by Koppel and Sullivan [1]. However, this application uses ACS in a real-time environment.

The University of Queensland installation consists of an IBM 4341-2 mainframe with 8 Mbytes of memory, 12 terminals and 2 printers in two clusters, line-printer, 1.8 Gbytes of disc storage, a tape drive and a Series/1 minicomputer with direct process I/O and connections to the Bailey Network 90 system.

UNDERGRADUATE COMPUTER-BASED PROCESS CONTROL INSTRUCTION

The experimental rig has a number of interesting characteristics that make it particularly suitable for teaching real-time process control:

- **Non-linear behaviour.** This is shown in Figure 2, which illustrates the different time constants for a step increase and a step decrease in the steam supply valve V1. The time constants are approximately 96 and 45 seconds respectively.
- **Interacting behaviour.** This is illustrated by examination of the relative gain array for this process shown in Table 2.
- **The inherent noise in the measurements,** again illustrated in Figure 2.

The following teaching experiments utilize this rig:

1. **Examination of digital filtering.** Students are asked to examine the effects of different filter bandwidths and different filter types (exponential, Butterworth, union). This short experiment is used in teaching real-time computing and would be expected to take one hour of laboratory time.

2. **A cascade loop controls the double pipe exit temperature with a slave loop controlling the pressure in the steam jacket via the steam valve.** This experiment only utilizes the Bailey Network 90 system and students are expected to complete this experiment in one and a half hours.

3. **Feedforward control.** A feedforward controller compensates for disturbances in the feed flowrate by adjusting both the steam and water valves. This experiment, combined with a model identification exercise usually takes about three hours of laboratory time.

4. **Decoupling control.** Two feedback loops or two interacting feedback loops are used as a basis for in-

roducing the concept of process interactions. The students are then expected to design and implement a decoupled controller using lead-lag compensators. This experiment normally takes six to nine hours to complete.

5. **Adaptive control.** An adaptive single loop controller adjusts the steam valve to control the exit temperature. This experiment, used in a fourth-year elective control course, makes use of the ACS system and would normally involve fifteen hours of laboratory time.

POSTGRADUATE PROCESS CONTROL RESEARCH

Current research utilizing the rig is on a predictive control design technique described by Maurath, *et al.* [2]. The basic predictive control algorithm uses a model to predict the output for a number of future moves due to the previous inputs. An error is formed by subtracting the prediction of the output from the setpoint. This error vector is then used to calculate a change in the manipulated variables. The design technique being tested is to use a singular value decomposition to condition the Dynamic Matrix [2] of step responses. Results from this study are reported elsewhere [3].

Future work on the rig will include fuzzy identification and control. A model-based controller designed around a fuzzy model of the process will be used to control the rig. Fuzzy identification techniques will be used off-line to derive an initial model, and on-line to provide continuous updating of the model. The on-line use of fuzzy identification turns the model-based controller into a fuzzy adaptive controller [4, 5, 6].

A reactor heat recovery system is a possible extension to the current rig. This is achievable by using an exponential function on the exit temperature of the double pipe exchanger to move the steam valve. This allows for simulation of variable heats of reaction without the danger and cost of reactants. In this mode only one manipulated variable is possible, i.e., the water valve (V2).

CONCLUSIONS AND SIGNIFICANCE

The pilot-scale heat recovery system is a valuable teaching and research tool. It is sufficiently flexible to

TABLE 2
Relative Gain Array

	TT2	TT3
V1	0.22	0.78
V2	0.78	0.22

demonstrate basic principles and yet sufficiently complex to demonstrate common process control problems such as nonlinearities and interactions between variables.

The process control system equipment allows students to obtain experience in real time computing, at several process control functional levels.

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ChE letters

UPDATED REFERENCES

Dear Editor:

In a recent paper, "A Course in Mass Transfer with Chemical Reaction," *Chem. Eng. Ed.*, **21**, No. 4, 164 (Fall 1987), W. J. Decoursey refers to *Gas Liquid Reactions* by P. V. Danckwerts as a source in English for the seminal papers by S. Hatta which were published in Japanese [*Technol. Repts. Tokoku University*, **8**, 1 (1929); **10**, 613,630 (1931); and **11**, 365, (1932)]. Complete translations of the latter articles have been published in *International Chemical Engineering*, **18**, 443-475 (1978). The readers of this article may also be interested to know that a translation of the closely related pioneering paper by G. Damkohler, "The Influence of Diffusion, Fluid Flow and Heat Transport on the Yield in Chemical Reactors," *Der Chemie-Ingenieur*, **3**, Part I (1937), has recently been published in *International Chemical Engineering*, **28**, 132-198 (1988).

Stuart W. Churchill
University of Pennsylvania

In Memoriam

James J. Christensen 1931-1987



Dr. James J. Christensen's life was devoted to service: service to wife and family; service to his profession in chemical engineering and to the field of thermodynamics; service to his university, the Brigham Young University and to his students, both graduate and undergraduate; and service to his church and community. This life of service was brought to a close by a sudden heart attack on September 5, 1987.

Jim's worldwide recognition as an outstanding thermodynamicist and a developer and builder of state-of-the-art calorimeters gave him and his wife a great opportunity to travel around the world. An outstanding feature of the family room of their home is a large map with the continents shown in bas-relief cut from plywood. The map is studded with pins, indicating the many places they have gone where they had the privilege of meeting new people and of teaching his methods to many. Jim and Virginia shared each other's life in this way as well as in taking dance classes together and in participating in the great books program over the last 28 years. He was dedicated to his four sons and a daughter and spent many hours with them in such activities as hiking. One of his sons followed him into the chemical engineering profession. Although Jim loved his professional career, he loved service to his family equally well.

Jim's service to the profession in the field of calorimetry and thermodynamics is unparalleled. He received a BS degree in 1953 and an MS degree in 1955 in chemical engineering from the University of Utah. He then went on to complete his formal education with a doctor's degree from Carnegie-Mellon in 1958. Part of his research work involved heat transfer to coils which later showed up in the design of the first-class calorimeters which he built. These

calorimeters have been developed commercially, are sold around the world, and are a standard for making precise calorimetry measurements. One of Jim's early ambitions was to build a calorimeter precise enough to measure the germination of a single seed but his designs greatly exceeded this. The early designs were crude compared with the later designs, but still required corrections for the energy input from a stirrer motor. His latest design was a calorimeter which would measure the heat of mixing at high pressure and high temperature.

Professor Christensen was also a prolific author. He has written or edited twelve books and co-authored fifteen major review articles. He has also published over 250 research articles in a wide variety of journals. He was instrumental in the founding of international conferences dealing with the chemistry of macro-cyclic molecules. He has been recognized by his peers, who selected him for the Sigma Xi annual lecture, a Blue Key lecture, and the Distinguished Faculty Annual Lecture at Brigham Young University. He also received the Maiser Outstanding Research Award and the Huffman Memorial Award as an outstanding thermochemist. Last August he was asked by the Chemical Engineering Division of the American Society of Engineering Education to give the 3M lecture which is based on outstanding research and contribution to the profession. (This lecture is scheduled for publication in a future issue of *CEE*).

Jim had a genuine love for his students, both graduate and undergraduate, and they returned that love through extra effort. He was recognized three times by the students as being the outstanding lecturer in the department, and he was recognized by the college as the outstanding teacher with the university's Maesar Outstanding Teaching Award (which is the counterpart of the outstanding research award.)

Jim took great delight in collecting "toys" which demonstrated the principles of thermodynamics and used them continually to interest the students. They included the familiar bird dunking its beak into water, rotating pinwheels, and his latest acquisition, a motor which worked by dipping one end in hot water. Jim's favorite courses were thermodynamics and creativity, and he exhibited creativity in teaching. He taught the students new ways of approaching old problems. He was dynamic in his presentations and gave an animated demonstration of the energy content of gas molecules by running back and forth, twirling and jumping up and down, colliding with students and walls. Almost every year during the student banquet, this little demonstration was repeated by the students as a sign of their regard. His annual backpacking trip

to the Uintah mountains with the graduate students was a highlight of each year.

He also served his community and church, the Church of Jesus Christ of Latter-Day Saints, in many ways. He was active in the education of his children and in the processes by which parents can contribute (P.T.A., *etc.*). He participated in great book discussion groups, he was a cub master for eight years, and demonstrated his love of teaching by teaching adult priesthood groups.

Jim's life of personal service has concluded. But his influence will continue to be felt in the lives of his family, his students, and his friends for many years to come.

Dee H. Barker

Roland Andrew Ragatz 1898-1987



Roland Andrew Ragatz, Professor Emeritus of Chemical Engineering at the University of Wisconsin, was born in Prairie du Sac, Wisconsin, in 1898, and died in Madison, Wisconsin, on May 30, 1987, at the age of 88. He is survived by his wife Nancy, who he married in 1930, a son Andrew (Ellen), a daughter Karen Roberts (Burnell), and seven grandchildren.

Professor Ragatz graduated from Prairie du Sac High School in 1915. He completed his studies for a BS degree (in the then new discipline of chemical engineering) in 1920 at the University of Wisconsin, Madison, and was immediately appointed instructor in chemical engineering. He remained on the teaching staff at Wisconsin until his retirement in 1969, except for a one-year leave of absence in 1929-30. While serving as a full time instructor, Professor Ragatz earned his MS degree in 1923 and his PhD degree in 1931, also in chemical engineering. He served as department chairman during three periods, totalling sixteen

years, and as associate chairman for five years thereafter.

Professor Ragatz' 49-year period of service to the University is one of the longest on record. He contributed significantly to his college and department and to his students during the important early period when the developing field of chemical engineering was emerging from an empirical discipline and evolving into a more scientifically based study. Basically devoted to teaching, Roland's areas of interest followed the needs of the department and its students in preparing them for industrial careers in a variety of often traditional manufacturing enterprises. In 1920 he began the development of introductory and advanced metallography courses, including laboratory studies related to the microscopic structures of metals, with emphasis on materials of construction. When instruction in this area was transferred to the Department of Mining and Metallurgy in 1948, Professor Ragatz turned his interest in materials to developing courses in plastics, again including a laboratory program. This early attention to materials science established the foundation on which the department's current strong program is based.

Starting in 1935, Professor Ragatz joined the late Olaf A. Hougen (and, during the 1940s, Kenneth M. Watson) in giving courses in material and energy balances and in thermodynamics for chemical engineers and participated in rewriting the corresponding parts (I and II) of the text *Chemical Process Principles*, which long has been a standard work in chemical engineering.

During his extended service as department chairman, Roland alternated with Olaf Hougen, and, in the words of Professor Hougen, "he assembled a staff well balanced in special talents for teaching and research, for undergraduate and graduate instruction, for variety in engineering and scientific interests, and with balance in laboratory and classroom instruction."

Roland also served long and efficiently as chairman of the College of Engineering committee on fellowships and scholarships, as well as on numerous other committees. He was a long-time member of the ASEE, serving on its Council, as chairman of its Chemical Engineering Division, and as organizer of the important Summer School for Teachers of Chemical Engineering (at Madison in 1948).

Professor Ragatz exemplified the ideals of the faculty of the University of Wisconsin: scholarship, research, public service, and above all, teaching.

Roger J. Altpeter
Wayne K. Neill
Charles C. Watson

SAFETY AND LOSS PREVENTION IN THE UNDERGRADUATE CURRICULUM

A Dual Perspective

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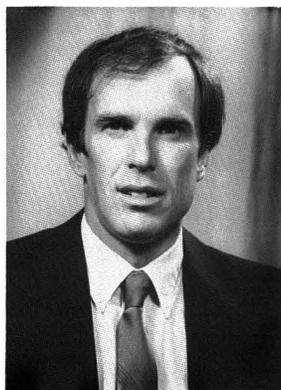
RECENT CHEMICAL PLANT accidents in India and in Switzerland have increased public and industry-wide concern and awareness of safety and loss prevention. This is in spite of the fact that the chemical process industries are safer than most other industries [1]. However, due to the potential for a serious plant accident, both the public and industry recognize that safety must be increased.

The AIChE is taking considerable steps to improve safety. First, it has formed a Center for Chemical Process Safety with the charge to "address the concerns about the handling of toxic or reactive materials and the safety of plant operating procedures" [2]. Second, it has formed the Design Institute for Emergency Relief Systems (DIERS) User Group to continue the cooperative industrial activities to extend the DIERS technology [3]. And third, a Task Force on Safety and Health in the Undergraduate Curriculum has been formed under the Safety and Health Division of the AIChE with the major objective to "identify the key concepts of loss prevention, safety, and health which should be considered essential for accreditation of the curriculum by 1990" [4]. As a result of this new awareness and concern for safety, it is apparent that safety and loss prevention will become a part of the future undergraduate chemical engineering curriculum.

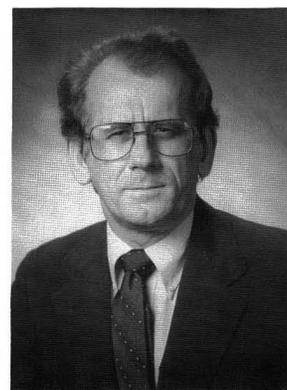
Most undergraduate chemical engineering curricula in the United States contain little in the way of safety and loss prevention. In fact, university laboratories are, typically, serious safety offenders.

Great Britain has had an ambitious safety and loss prevention program in their undergraduate curriculum for some years now. This is a result of a substantial chemical process accident that occurred at Flixborough, England, in 1974 [1]. All British chemical, engineering curricula are presently required to contain a significant amount of safety related content for accreditation. This is achieved through a combination of dedicated courses or by demonstrating a certain fraction of safety related content in the existing courses.

This article will provide a dual perspective on the need for more emphasis on safety in our chemical engineering undergraduate curricula. Both the academic



Daniel A. Crowl is an associate professor of chemical engineering at Wayne State University. He received his BS degree in fuel science from the Pennsylvania State University and his MS and PhD in chemical engineering from the University of Illinois. After graduation he spent two years as a senior process control engineer for St. Regis Paper Company before returning to academic work. His present research interests are in chemical process safety, process simulation, and the application of CAD techniques to process design. (L)



Joseph F. Louvar is director of the Chemical Engineering Department (Research and Development) of BASF Corporation, Wyandotte, MI. A member of AIChE's Loss Prevention Committee, he also teaches experimental statistics at Wayne State University. He received a PhD in chemical engineering from Wayne State University, an MSChE from Carnegie-Mellon University, and a BSChE from the University of Missouri (Rolla). (R)

This article provides[s] a dual perspective on the need for more emphasis on safety in our . . . undergraduate curricula. Both the academic and industrial viewpoints [are] presented. We . . . also discuss a unique safety related course development effort being undertaken at Wayne State and Michigan Tech Universities . . .

and industrial viewpoints will be presented. We will also discuss a unique safety related course development effort being undertaken at Wayne State University and Michigan Technological University, with substantial technical assistance from BASF Corporation. This program is being supported by the National Science Foundation under its University/Industry/Government (UIG) program.

THE UNIVERSITY PERSPECTIVE

Dan Crowl

In the summer of 1986 I had an opportunity to spend a few months at BASF Corporation working on a computer simulation project. One day I was visited by Joe Louvar, Director of Chemical Engineering, who asked me if I was interested in working on a few safety related projects. In total ignorance I replied, "You mean hard hats and safety shoes?" Joe went on to explain some of the more fundamental aspects of safety, including reactor dynamics, two-phase flow during reactor venting, gas dispersion models, and so forth. It had never occurred to me that safety had a fundamental aspect! I had always assumed safety was simply a set of rules developed as a result of practical experience.

During the remainder of my stay at BASF, I observed how safety was practiced in an industrial environment. It became apparent to me that practicing chemical engineers spend a considerable amount of time on safety related activities. In spite of all my years of academic training, I felt woefully inadequate with respect to safety. I could indeed understand pieces of the fundamental components, but using those pieces in the practical application and management of safety seemed a mystery to me.

Despite a continuing feeling of inadequacy, I was now aware of safety. I began to look at my past academic experiences and at the experiences we are providing for our present students. I found little in the way of safety instruction. Many of you will argue that the academic experience is designed to provide only a fundamental knowledge, with practical application being the responsibility of industry. But safety is a systems science, involving the application of a broad range of fundamental skills strongly coupled with practical application. Why not adjust the fundamental skills taught to our undergraduates to strengthen the

safety aspect? Can the academic community continue to neglect an area that is already very important to the industrial community?

As an undergraduate I learned that process design is motivated by savings in material usage and capital investment. In the 1970's energy also became an important driving force in design. Now, safety considerations are becoming just as important.

The academic community is in a difficult position with respect to safety. First, most faculty have little safety experience. This is either a result of little industrial experience or of participation in industry during a time when safety was a lower priority and was practiced in a different fashion than it is today. Second, we have inadequate equipment and facilities for demonstrating safety. Finally, our curricula are already at their practical maximums. Where can we find room to add a safety component?

One possibility is to add safety instruction throughout all of the chemical engineering courses. Safety is practiced in every aspect of the industrial experience, so why not practice it throughout the entire undergraduate course sequence? I agree with this approach. However, a final capstone course is necessary to culminate the course sequence. One can teach reactor safety (runaway reactors) in the kinetics and reactor design course, but a capstone course is essential for the teaching of safety reviews, hazard identification, risk assessment, and other topics that are special to safety.

I recently attended the International Symposium on Preventing Major Chemical Accidents, organized by the Center for Chemical Process Safety of the AIChE. This symposium was held in Washington, DC, during the week of February 3, 1987. Of the over four hundred participants, less than five were from academia. This was surprising since the papers presented were as fundamental and research-oriented as those presented at academic conferences. I believe that safety can become an important academic area if faculty become aware of 1) the potentially fundamental nature of safety, and 2) the opportunities for research and funding. Safety is an excellent area for industry/academic research collaboration since most of the industrial proprietary barriers dissolve.

Safety is an essential part of the industrial experience, more now than some of the traditional fundamental chemical engineering areas. I believe it is time

to include safety as an important part of the undergraduate chemical engineering experience as well.

THE INDUSTRIAL PERSPECTIVE

Joe Louvar

All of my safety knowledge has been acquired in an industrial setting. It came in bits and pieces, and it took several years to really appreciate the significance, the subtlety, and the technical complexity of chemical process safety. In hindsight, I recognize that during those formative years I made many serious safety errors. It was only the result of pure chance

that I escaped having serious accidents and/or injuries.

Using today's standards, most of my past errors would have been identified and corrected by supervision or by the safety review process which is used very effectively within industry. Unfortunately, I am convinced that the self-motivation necessary to take on the responsibility for safety (responsibility of every engineer), and to learn the technology of safety, still requires years within an industrial setting.

From a management standpoint I have also recognized that supervision has a serious handicap when working with fresh graduates. Although they have an

TABLE 1
Course Outline

- | | |
|--|---|
| <ol style="list-style-type: none"> 1. <i>Introduction</i> <ol style="list-style-type: none"> A. Course syllabus B. Introduction C. Accident and loss statistics D. The accident process E. Three significant disasters F. Personal and management responsibilities G. Legislative responsibilities H. Employee and community "right to know" 2. <i>Fundamentals of Safety</i> <ol style="list-style-type: none"> A. Toxicology, industrial hygiene and exposure control <ol style="list-style-type: none"> 1. Toxicology <ul style="list-style-type: none"> • History • Dose vs response • How the body responds to exposure • Determining safe working levels 2. Industrial hygiene and exposure control <ul style="list-style-type: none"> • Types of exposure • Methods for exposure control • Administrative and engineering methods • Personal protection B. Fires <ol style="list-style-type: none"> 1. Flammability of vapors and liquids 2. Minimum oxygen concentration 3. Inerting 4. Autoignition temperature 5. Auto-oxidation 6. Adiabatic compression 7. Effects of sprays and mists C. Explosions <ol style="list-style-type: none"> 1. Definitions: Explosion, detonation, deflagration, confined and unconfined vapor explosion, BLEVE 2. The nature of the explosion process 3. Effects of explosions 4. Calculations relating to explosions D. Liquid and Vapor releases <ol style="list-style-type: none"> 1. Gaussian distribution 2. Gaussian plume model 3. Gaussian puff model | <ol style="list-style-type: none"> 4. Spill models 5. Inhalation exposure: spills or from vessels 6. Inhalation exposure: filling containers <ol style="list-style-type: none"> 3. <i>Applications for safety</i> <ol style="list-style-type: none"> A. Introduction B. Designing for safety <ol style="list-style-type: none"> 1. Intrinsic design 2. Extrinsic design 3. Maintenance C. Engineering to Prevent Fires and Explosions <ol style="list-style-type: none"> 1. The Fire Triangle 2. Passive Protection Methods <ul style="list-style-type: none"> • Types of environments • Eliminating sources of ignition • Atmospheric control, including inerting and purging • Plant siting 3. Active Protection Methods <ul style="list-style-type: none"> • Shutoff and check valves • Combustible gas monitors • Emergency material transfer • Sprinkler systems • Water vs. foams for fire control D. Engineering to Prevent Toxic Release <ol style="list-style-type: none"> 1. Relief systems 2. Design and selection of relief valves 3. Flares, vents and scrubbers E. Process hazards identification and risk assessment <ol style="list-style-type: none"> 1. Hazards identification <ul style="list-style-type: none"> • Hazards surveys, including the Dow Index • HAZOP • FMECA 2. Risk Assessment <ul style="list-style-type: none"> • Event trees • Fault trees • Consequences analysis • Limitations to risk assessment 3. Safety reviews <ol style="list-style-type: none"> 4. <i>Accident Investigations</i> 5. <i>Case histories</i> |
|--|---|

excellent foundation in the traditional chemical engineering fundamentals, the concepts of safety are foreign to them. In fact, they perceive safety to be unimportant because the subject is hardly mentioned during their schooling. In some universities, safety practices are totally neglected. Consequently, industry starts with graduates who need a basic improve-

TABLE 2
Video Session 1

INTRODUCTION

1. Introduction
2. Brief description of five video sessions
3. BASF Corporation's safety program
 - a. Policy
 - b. Commitments
 - c. Training
 - d. Activities
 - e. Audits
4. Introduction to safety terminology and principles
 - a. XP vs. non-XP
 - b. Relief vs. rupture disc
 - c. Runaway reaction
 - d. Two phase flow
 - e. Design Institute for Emergency Relief Systems (DIERS)

TABLE 3
Video Session 2

BASIC SAFETY EQUIPMENT AND PROCEDURES

1. Introduction
2. Personal protection equipment
 - a. Motivation
 - b. Face and eye protection: glasses, goggles, face shield
 - c. Clothing: aprons, gloves, suits
 - d. Respirators: dust, cartridge, canister, air-line
 - e. Miscellaneous: hats and shoes
3. Sources of toxicity and safety information
 - a. Material Safety Data Sheets (MSDS)
 - b. Vendor information
4. Safety procedures
 - a. Hot work permits
 - b. Lock - Tag - Try
 - c. Vessel entry
 - d. Grounding and bonding
 - e. Fail safe
 - f. Safety reviews
5. Safety features
 - a. Sprinklers
 - b. Alarms
 - c. Showers
 - d. Color indicator tubes
 - e. Extinguishers

ment in attitude prior to addressing the more complex features of safety.

The chemical industry is entering an era where processes will be even more complex. To prepare our future engineers for this era, I believe we must begin to educate them on the principles of safety. This education must begin at the university, with an emphasis equal to heat transfer, mass transfer, thermodynamics, *etc.*, and should be given during the same period as the core courses. This would be an effective way of emphasizing the importance of safety.

I believe that there should be a three-hour course during the third year which is dedicated to safety. Some educators believe that safety should be a part of every course, and I agree. But the more technically complex areas of safety need more time and attention than could possibly be allotted in core courses. The following subjects could only be adequately covered in a separate safety course:

- Dispersion studies
- Relief valve sizing (including 2-phase flow)
- Safety reviews and hazard identification
- Flammability of chemicals
- Toxicity of chemicals

The benefits of teaching safety in the university exceed those mentioned above. An important spin-off of safety courses could be the development of more interest in initiating safety-oriented research. In a review of university research (PhD dissertations), it is apparent that there is very little research devoted to safety. Topics which could be fruitfully addressed by universities include:

- Advanced adaptive reactor control methods for hazardous reactions
- Expert systems for monitoring reactor and/or plant safety
- Expert systems to improve the reliability of fault analysis
- Advanced relief methods for runaway two-phase flow systems

From my perspective, the chemical industry will continue to stress faster reactions, more complex reaction systems, and a more complex utilization of investments via multiple product reactor systems. The success of these complex processes will depend upon our ability to design modern systems with the safety features demanded by both industry and the public. To meet these challenges of the future, we must give more attention, concern, and respect to safety.

NEW COURSE DEVELOPMENT

We have developed a senior level course entitled "Safety in the Chemical Process Industries." This development effort was supported by the National Science Foundation under their UIG program. The unique feature of the course was that it included five two-hour lectures, broadcast live from the chemical pilot plant facilities at BASF Corporation in Wyandotte, MI. The format supported interactive questioning between the students in the classroom and the practicing chemical engineering professionals in the pilot plant. The broadcasts were uplinked to a satellite for downlinking at both Wayne State University in Detroit and Michigan Technological University in the upper peninsula. The course was taught simultaneously at both locations during the fall of 1987.

The course provided a rare opportunity for students to see safety being practiced by professional chemical engineers in an actual chemical plant environment. Demonstrations were provided using actual equipment and safety situations that could never be shown in the classroom or laboratory. The video lectures were in addition to a series of 25 one and one-half hour classroom lectures. These lectures presented the fundamental and theoretical features of safety, subjects requiring problem solving and discussion within the classroom environment.

TABLE 4
Video Session 3

INSPECTION OF LABORATORY AND PROCESS AREA

1. Introduction
2. Inspection concepts
3. Review film on Stop - Observe - Act - Report (SOAR)
4. Inspection of laboratory (several examples of poor safety practices will be staged)
 - a. Storage of solvents
 - b. Storage of glass equipment
 - c. Safety equipment and operation
 - d. Principles of using hoods
5. Inspection of Process Development (PD) area (several examples of poor safety practices will be staged)
 - a. Reliefs and rupture discs
 - b. Nitrogen vented in room
 - c. Non-XP in XP room
 - d. Poor grounds
 - e. Belts not guarded
 - f. Bad drum vent
 - g. Incorrect tools
 - h. Poor ventilation
 - i. No double block and bleed (show correct configuration via glass system)
 - j. No hot-work permit

A total of four industrial and seven academic contributors were involved with the effort. The BASF Corporation industrial participants were: G. W. Boicourt, M. Capraro, J. F. Louvar, and J. Strickland. Their effort was directed mostly towards the video lecture material and scripts. J. F. Louvar also contributed towards the development of lecture material. The academic participants were D. A. Crowl and R. W. Powitz from Wayne State University and M. Banks, B. A. Barna, E. R. Fisher, N. K. Kim, and D. G. Leddy from Michigan Technological University. The major focus of the academic group was toward

TABLE 5
Video Session 4

EXPERIMENTS FOR SAFETY

1. Introduction
2. Vent Sizing Package (VSP) for sizing reliefs
 - a. Show features of equipment
 - b. Show types of data collected
 - c. Illustrate specific tests for various objectives
 - d. Introduce relief valve sizing concepts
3. Characterizing dusts
 - a. Deflagration index
 - b. Illustrate features of equipment
 - c. Describe test procedures
 - d. Describe data from tests
 - e. Introduce relief sizing concepts
4. Flammability limits
 - a. Illustrate features of equipment
 - b. Describe test procedures
 - c. Describe data from tests
 - d. Introduce relief sizing concepts

TABLE 6
Video Session 5

SAFETY REVIEWS

1. Introduction
2. Informal safety review in laboratory
 - a. Describe phosgenation system
 - b. Analyze procedures relevant to safety
 - c. Progressively make improvements via team dialogue concept
3. Formal safety review
 - a. Introduction
 - b. Safety Review Meeting
 - c. Equipment inspection
 - d. Wrap-up meeting and development of Action Plan
4. Wrap-up of video sessions
 - a. Summary remarks
 - b. Open questions and answers

development of the lecture materials. The overall project was managed by D. A. Crowl.

The course outline is shown in Table 1. It is divided into two major parts. The first part presents the fundamentals of safety and includes discussions of toxicology, fire, explosion, and toxic release. The second part deals with using those fundamentals in practice and includes a discussion of "designing for safety" and using various safety review procedures (such as hazards and operability studies). The course also includes a discussion on case histories and accident investigations.

The outlines for the five video lectures are shown in Tables 2 through 6. Except for video session 4, the videos are not dependent on the lecture material. The emphasis of the videos was to show the students how safety is practiced on real process equipment. The fourth video lecture on "Experiments for Safety" required some fundamental lecture material prior to broadcast.

ChE book reviews

INTRODUCTION TO POLYMER VISCOELASTICITY, Second Edition

by John J. Aklonis, William J. MacKnight
John Wiley & Sons, Somerset, NJ 08873; \$39.95 (1983)

Reviewed by Albert Co
University of Maine

This book introduces various fundamental concepts in studying the viscoelastic behavior of polymers, with an emphasis on the molecular approach. The book consists of nine chapters.

Chapter 1 introduces the reader to several experiments that display the viscoelastic nature of polymers. In Chapter 2, viscoelastic material properties in transient and oscillatory experiments are defined and are illustrated clearly with simple experiments. The Boltzmann superposition principle is stated; its applications in relating the creep compliance and the stress relaxation modulus and in relating transient and oscillatory properties are demonstrated.

In Chapter 3 the regions of viscoelastic behavior are described and the effects of molecular weight, crystallinity, and plasticizing agents are explained. The concept of time-temperature superposition, the master curves, and the WLF equation are then presented. In Chapter 4, the phenomenon of glass transition is examined, and explanations based on free volume, thermodynamics, and kinetic theories are presented. The effects of structural parameters on glass

SUMMARY

This paper has presented both the industrial and university perspectives regarding the need for teaching safety in the chemical engineering undergraduate curriculum. We have also presented one approach to teaching safety and loss prevention. As a result of NSF support we had a unique opportunity to bring the students into an operating chemical pilot plant, through the use of live TV.

We hope that this approach, and others, will improve the engineers of the future and result in safer chemical process plants.

REFERENCES

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2. Anonymous, *AIChE Environmental Division Newsletter*, February, 1986.
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4. Glass, Arnold J., Letter of February 2, 1986. □

transition temperature and the relaxation occurring in the glassy state are rationalized in terms of molecular motion and chain mobility. In preparing the reader for subsequent chapters, the statistics of a polymer chain are reviewed in Chapter 5.

In Chapter 6, various treatments of rubber elasticity and the structural factors that affect rubber elasticity are discussed. In Chapter 7, the behavior of typical mechanical models is analyzed and the Rouse-Zimm molecular theories for polymer solutions are discussed. Extensions of these molecular theories to bulk polymers are then considered and the reptation theories are briefly described. In Chapters 8 and 9, the phenomena of dielectric relaxation and chemical stress relaxation are examined, respectively.

Throughout the book, the mathematical treatments are maintained at a level comfortable for undergraduates. Advanced mathematics required for the discussion of a subject matter are elaborated in the corresponding appendices. The problems at the end of each chapter range from simple calculations to advanced problems requiring a certain degree of mathematical sophistication. Readers will find the solutions located at the end of the book to be helpful.

Overall, this book is an excellent introduction to polymer viscoelasticity. However, the treatise is restricted to amorphous polymers. The treatment on crystalline polymers is very limited, and topics such as solution behavior, melt rheology, and birefringence are not covered. Nevertheless, it is a good choice as a textbook for one of a series of courses on polymer viscoelasticity. □

ENGINEERING MANAGEMENT

A Course to Minimize Functional Handicaps of Graduates

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THE INDUSTRIAL ECONOMY in the U. S. has undergone significant changes since 1982. Some of the changes have been initiated by recent intensive overseas competition, some by the drop in oil prices, and some by mergers. In the 'right sizing,' or downsizing, that has taken place in most companies in this decade in order to maintain competitiveness, whole layers of management have been expunged. Other changes resulted from technological developments in the late 1970s and in the first half of this decade. Developments in computer workstations and software have added such power to the individual engineer that companies in chemical processing and the engineering companies serving them will never again need as many engineers of any discipline for the same volume of business as they needed in the 1975 era. As a consequence, there has been a reduction in hiring by most



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companies, with the result that many students have not been able to find jobs even months after graduation. Competition for the available jobs has become intense, and many young engineers have had to go into fields where they may never be able to use their hard-won training. The purpose of this paper is to review a course, "Engineering Management," that has been developed at the University of Oklahoma to improve the students' ability to get jobs and to perform better in any company.

Important technical consequences of the industrial changes which were described in a recent article in this journal [1] agree with my own observations as a senior manager that

- A smaller percentage of all engineers, especially in larger companies, will be able to move into management.
- All engineers will have to be more competent technically and to remain competent longer before they can become managers.
- While they practice their specialty, engineers will have to function more effectively in a company environment to have job security.
- Engineers will need far greater organization- and people-skills than past graduates possessed.

The needs represented by the last item have been voiced by every industrial advisory group that I have known or been a part of in the last twenty years.

As soon as recruiters identify a lack of understanding of the industrial environment and an obvious lack of people-skills in interviewees, they lose interest. These graduates may never get an engineering job, or they may be shuffled aside at an early date. As recently as April 1987, senior managers advising our department told about students who were essentially unemployable, no matter what their GPA, because of their obvious lack of people-skills. The student needs to understand how the industrial world operates and should develop people-skills before leaving college so he/she can function effectively immediately after being hired. Costs are simply too high for businesses

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to tolerate a one-year shakedown period for new engineers, as they did in the past.

Another educational need is based on the conviction of most senior managers that learning to manage is a lifetime job. This learning process must be started very early by engineers in order to meet the greater competition for managerial positions or they will be left behind, and business majors will skim off an even larger share of the top jobs in the future.

CHANGING THE CURRICULUM

C. T. Sciance [1] cites a significant need to augment the technical content of the chemical engineering curriculum, but it could be even more important to improve people-skills and knowledge of how industry functions. Many students gravitate toward engineering because their natural aptitudes lie more in math and science and less in communication and interpersonal relations. Throughout their engineering study this unevenness in skills probably increases. Students are shocked to find, while being interviewed or upon being hired, that the practice of engineering is a very people-oriented profession. They soon realize they are woefully unprepared in many areas that could affect career achievement even more than their calculation ability. A serious gap in their education soon becomes apparent.

The effects of the new employment environment have only lately reached the universities in the form of reduced job opportunities, but few changes have been made in the educational program in response to the needs of those now graduating and to the next generation of students. Why has the gap in organizational know-how not been filled? Many professors have no industrial experience, or it was of such short duration, or at such a junior level, that they do not know what is really involved and are uncomfortable trying to teach such material. They may agree with the need, but they lack the tools to deal with it.

An effort has been underway at the University of Oklahoma to develop a local solution to the problem for students willing to devote three semester hours to the effort, and to draft a text which could be used by other faculties. Further, we hope that the text might ultimately become a desktop reference which will be consulted more frequently than many technical references.

COURSE SPECIFICS

Ideas for this course have gestated for more than a decade, through thousands of goal-settings, performance reviews, hirings, firings, and many mistakes

The course then becomes one of high student-participation. Basic value systems are discussed to help the student understand why others react to life's inputs differently than the student himself does.

by the author. They came from fellow executives of all ages who urged that students be made aware of the things that cause so much difficulty in industry and handicap so many careers. Time and time again, the root causes of those difficulties are poor communication and lack of interpersonal relation ability, inadequate knowledge of company workings, or distorted concepts of management. Lately, new ideas have come as feedback from recent graduates.

This is a course in what life is really like "out there." Many of the rough edges have been ground off. Attendance has been interdisciplinary, and the first results have been good. Feedback and requests from earlier graduates have resulted in the development of a text. Graduates have already reported on more comfort in working in team situations, a greater ability to determine supervisors' needs by quickly determining how an organization works, and less fear of moving into project work immediately. These results suggest that the effort is moving in the right direction.

The first draft of the text was developed to meet classroom needs and it is outlined in Table 1. The first part of the course is very important for the student and new graduate. It starts with a brief perspective of the entire course and then presents a view of the types of behavior and functioning expected of all employees. The characteristics of effective employees and good supervisors are discussed. There are numerous "horrible examples" to awaken the student to things that can happen which develop a bad reputation. The intent is to open the student's mind to the concepts that lead to being an effective person.

The course then becomes one of high student-participation. Basic value systems are discussed to help the student understand why others react to life's inputs differently than the student himself does. In the main, students seek the company of peers and cliques with whom they are comfortable. It is often a shock for them to realize that they may have to get along and work with people who see life differently. The value system is a convenient mechanism for identifying differences in reaction to one's environment.

Next, attention turns to getting a job—the right job for the individual. The student is taught how to take full, personal charge of job-finding. Careful assessment of the student's attributes leads to the de-

velopment of lists of job opportunities, location of target companies, investment of significant time on company research, and improved communication in resumes and interviews. Effort is expended to heighten the student's awareness of his/her impact on recruiters, interviewers, and other people during plant trips.

Then, important things that the newly employed engineer should consider in order to get the best possible start on the job are reviewed. These are obvious truisms, but they are often overlooked or ignored.

It is necessary to develop a different frame of mind in the students in order to attack the deficiency in communication ability which is mentioned by nearly all supervisors.

Some of the most important areas concern the study of personal ethics, business ethics, technical and intellectual property of a company, liability problems (to give the student perspective regarding what must be protected), and obligations during and after employment. Then they examine one problem all of them will encounter some day in some way: whistle blowing. Moral obligations are analyzed in detail.

It is necessary to develop a different frame of mind in the students in order to attack the deficiency in communication ability which is mentioned by nearly all supervisors. Communication theory is examined briefly to learn why some of the best intentions go awry in speaking and writing. Throughout the course there are opportunities to make brief formal presentations, and each is critiqued by the class for its organization and delivery. At least one presentation is repeated several times in order to force the individual to revise and improve it. Written assignments are required frequently. The student is taught to observe audience awareness, whatever the occasion.

The true function of management is examined next and it proves to be a revelation for many students. As a result, some students are less anxious to become managers, but at the same time they develop a better appreciation of the needs of supervisors and managers. To help the student understand his/her new environment, subjects such as types of company organization, job descriptions, job evaluations, goal setting for individuals, performance reviews, and merit budgeting are taken up. Leadership types are examined in some detail so that young employees can better characterize the behavior of supervisors and work with individuals more effectively. Equal employment opportunity requirements are carefully dis-

cussed to help people avoid problems and/or to insure that their rights are observed.

The added awareness provided by these subjects makes the student a better employee. People who have had the course seem to get a faster start on the job and to have an edge on the competition—befitting the adage, "If at first you don't succeed, you may never." They are more aware of the importance of fitting into group activities, have greater empathy for a supervisor's needs, and are able to develop a personal program for advancement at an early date. The rate of return for the time and money invested in this part of the course appears to be very high.

MODERN TECHNOLOGY EMPHASIZED

The middle section of the course deals with modern methods of modeling, planning, and analysis. Techniques and sophistication vary widely from company to company, so the treatment provides a look at the utility of these tools without taking a course in operations research or a business course in modeling. Each method is examined from a management rather than a program writer's viewpoint, to show how the analyst and manager must work together and how model computer outputs or "decisions" are used. General economics and spreadsheets are reviewed quickly to provide the basis for economic decisions. Reading and analysis of company financial reports is stressed as an ability that every young engineer should have. The linear programming, which is one of the most widely-used optimization aids—from refinery operation to vegetable planting—is taken through graphical interpretation, matrix methods, analysis of computer outputs, and sensitivity studies. Study of integer programming provides the basis for analyzing supply, transportation, and other networks. Among these are the critical path and PERT techniques. Next, the student is presented with the structural basis for making decisions on a more rational basis. Decision theory considers the different paths electable in solving a problem and deals with the probable cost or consequence of picking each. Several types of business examples are used.

Reliability analysis is a field which the Japanese have adopted more widely than we have in the U.S. for a number of years. Failure, reparability, maintainability, and availability are taken up in terms of process plant units and design for reliability. This leads to consideration of risk analysis, fault trees, and failure mode and effect analysis. The fact that the rigor of the methods clarifies thinking is immediately clear. Results of these analyses do no good in the files,

however, and emphasis is placed on continued thinking by those involved in operations in order to prevent future catastrophes such as those which have occurred in the last decade.

By this time, students realize the limitations of deterministic inputs to models. Distributions are considered for input values, and Monte Carlo methods are applied to such things as cost estimates and sequential operation simulations. This section of the course provides a new awareness and perspective of tools most engineering students have not seen before. With this awareness comes the ability to help supervisors through the use of tools lacking in other engineers and the ability to sharpshoot with further study when the time comes.

PROJECT MANAGEMENT TOOLS TAUGHT

Since so many tasks in business and engineering are of a project nature, the third part of the course treats management of projects from beginning to end. Few young engineers know how projects get started; therefore, design bases, requests for proposals, proposals, contracts, and agreements are carefully re-

TABLE 1
Table of Contents

PART I. Functioning with People in Organizations

1. Introduction
2. Value Systems
3. Getting the Correct Job
4. Ethics, Technical Property and Legal Issues
5. Getting Along on the Job
6. Communication
7. Functions of Management
8. Company Organization
9. Managing People

PART II. Planning and Analysis Methods

10. General Economics
11. Linear Programming
12. Integer Programming and Networks
13. Decision Theory
14. Reliability, Fault Trees, FMEA
15. Probabilistic and Simulation Models

PART III. Work Management (Project Basis)

Glossary

16. Project Initiation
 17. Project Organization/Kickoff
 18. Engineering and Detailed Design
 19. Equipment and Material Procurement
 20. Time and Money control
 21. Quality Assurance
 22. Construction and Manufacture
 23. Project Completion
-

viewed and discussed to show that projects don't "just happen." A typical project is organized and engineering and detailed design activities are defined. Project activities and individual engineering discipline activities are related to total project progress curves, with emphasis on the interrelationship of activities. Probability of success on any project is related to the amount of planning, to the handling of details, and to the accuracy of measurements that go into it. All procurement activities (spec sheets, inquiries, bids, bid tabs, vendor selection, expediting, inspection, vendor data acquisition, and transport) are put into time perspective. Time and money control discussions involve activity definition, loading of effort on activities, critical path analysis, time and cost estimates, and cost control. Emphasis is placed on the need to measure progress in the same terms as the original estimate for accurate progress reporting. Product and service quality assurance needed for better reliability, maximum productivity, and lower costs in the face of overseas competition, provide background for treatment of construction or manufacturing and project completion.

At the end of this section, many students understand the unusual characteristics of good project engineers. Although they may not want to enter this specialty, they can function much more effectively on any project and realize the benefit of a project-manage-approach to their own lives.

CONCLUSIONS

Obviously, many topics are treated quickly, and not all are treated every semester. But the objective is perspective and development of the "big picture" viewpoint. With this, the young engineer knows where to dig when the need for details of a given method or topic arises. Over the years, the author has found that the engineer who has this perspective is most often the one who defines the problem correctly and comes up with the needed solution at the right time, *i.e.*, is the most promotable individual.

The chapter listing for the text is given in Table 1. Comments and ideas from educators or industrialists are always welcome. As a veteran project manager, the author's primary interest is improving the product and serving the customer (the student and the employer).

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A COURSE ON PRESENTING TECHNICAL TALKS

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IN THE ONGOING debate about what should be put in and taken out of the chemical engineering curriculum, one of the few points of universal agreement is that oral communication skills are essential for all practicing engineers and not enough is done to develop them in most engineering curricula.

Like many other departments, we used to have a senior seminar course in which each student presented a single 30-45 minute talk sometime during the semester. The results were not particularly impressive: the students whom you would have expected to give good talks gave them; the other talks ranged from poor to average; evaluations were superficial; and the one-shot nature of the talks provided little opportunity for individual improvement. Also, the worst of the talks, being as long as 45 minutes, were excruciating experiences for everyone involved.

When Harold Hopfenberg became Department Head eight years ago, one of the first changes he introduced was a complete reorganization of the seminar course. Under the new system the senior class is divided into groups of six to eight students and a faculty member is assigned to each group. The groups meet once a week for most of the semester. Each faculty member runs the seminar in any way he or she chooses; the next section describes a structure that has worked particularly well for the author.

COURSE STRUCTURE

Each student prepares and delivers two talks during the course. Talks in the first round are each fifteen

... one of the first changes [Harold Hopfenberg] introduced was a complete reorganization of the seminar course. Under the new system the senior class is divided into groups of six to eight students and a faculty member is assigned to each group.



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minutes long for a 50-minute class period and twenty minutes long for a 75-minute period. Talks in the second round are ten minutes long.

The first meeting is organizational. The instructor explains the course structure and hands out and reviews a list of suggestions for good presentations (to be given subsequently in this paper). He then lists all of the dates on which the course will meet and requests volunteers for the first two presentations, to be given two weeks from the current date. If there are volunteers the rest of the calendar can usually be filled in on a voluntary basis; if not, a lottery is used to assign presentation dates.

In the second period the instructor delivers an illustrative seminar. He begins by explaining that he has been giving technical talks for a long time and the students should not expect to be able to duplicate his skill at this stage of the game. He adds that even experienced speakers can find room for improvement, and he requests that the students take notes on things that might be improved in the presentation. He then

He provides no real introduction but launches directly into a long monologue read verbatim from notes. He shows a crudely drawn flow chart with no units or streams labeled; several data plots with no apparent relationship to anything; and one transparency that looks like a facsimile of the Dead Sea Scrolls . . . no eyecontact is made; and gum is chewed continuously and ostentatiously.

proceeds to give the worst talk he can possibly give. He provides no real introduction but launches directly into a long monologue read verbatim from notes. He shows a crudely drawn flow chart with no units or streams labeled; several data plots with no apparent relationship to anything; and one transparency that looks like a facsimile of the Dead Sea Scrolls, filled from top to bottom with handwritten equations in tiny print. The talk is crammed with undefined technical jargon; no eye contact is ever made; and gum is chewed continuously and ostentatiously. The speaker concludes by fumbling around with his transparencies and then muttering, "Well, I guess that's about it."

The talk lasts for approximately eight minutes and by the end of it the students have all caught on to what is happening. The class then brainstorms the things that were wrong about the talk and what should have been done differently. The instructor subsequently gives a coherent version of the same talk, complete with introduction, body, summary, and intelligible transparencies, and the class briefly discusses the things that made a difference relative to the first presentation.

At least one week before students are scheduled to present their talk they are required to submit a topic. They may talk about published papers or about work they did on projects or summer jobs; the only ground rule is that the talks should be reasonably heavy in technical content at a level appropriate for chemical engineering seniors. The instructor reviews the chosen topics and tells the students either to go ahead with them or to find alternatives with more technical content. During the week before the presentation the students write, duplicate, and hand out seminar announcements and abstracts to the instructor and to all group members.

A typical class session begins with the presentation of the first talk. During the talk the class members jot down questions about the content and comments on the presentation. A five-minute questioning period follows the talk. The students and instructor then fill out a checklist rating various aspects of the talk (introduction, body, and summary; level of the material presented; use of time; quality of transparencies; clarity of presentation; speaking style; strong and weak points of the talk). Finally, the students and the instructor each present brief oral critiques. The

checklists are given to the speaker to review and are handed in to the instructor at the following class session. The procedure is then repeated for the second speaker.

Since the course was last offered the department has acquired a videotaping facility. In the future, each talk will be taped and the students will be requested to view their presentations and critique themselves.

SUGGESTIONS TO SPEAKERS

Preparation and Organization

- Know the technical background of your audience and gear your talk to that level. Do not use a lot of unexplained technical jargon unless you are sure the audience already knows what it means, and don't explain what a material balance is to a group of chemical engineering seniors.
- Make sure your talk has a distinct introduction (outline what you are going to say and why it might be important or interesting to your audience), a body, and a summary (repeat what you particularly want your audience to retain from the talk).
- Use overhead transparencies or slides to present main points and provide explanatory details in the talk. Transparencies work well for informal seminars, and you can easily make them yourself. Slides are more difficult to produce, but they are often more convenient for short tightly-timed presentations and they are required at some national and regional conferences.
- Never present a large body of information orally without summarizing its main points on a transparency.
- Do not present more than about eight lines on a single transparency. Transparencies crowded with information are useless. It should take about two minutes to go through a single transparency in the talk.
- Use large type on transparencies—a label maker or the Orator ball on a Selectric typewriter or a word processing program with variable type size. Ordinary size type doesn't look good. If you handwrite the transparency, use large block lettering with horizontal guidelines to keep your lines straight. Never use script unless you're Octave Levenspiel.
- If you show a process flow chart, make sure the units and streams are labeled. A bunch of unlabeled boxes and lines with arrows is worthless to the audience.
- Try to avoid complex equations, which can rarely be explained intelligibly in the amount of time available. If you are talking about a mathematical model, focus on what it does (input and output variables, assumptions) and provide, at most, qualitative summaries of the mathematical and computational details. (If listeners want more de-

tails they can ask you for them in the question period.)

- If you show data plots be sure the axes are clearly labeled.
- Rehearse your talk several times with a friend or in front of your mirror, and make sure the time it takes is within one minute of the time allotted for the talk. Running long can be a disaster in a formal presentation and running short may not win you any friends if you're at a meeting where consecutive talks are scheduled at set times.

Presentation

- Never read directly from prepared text—there is nothing more deadly to an audience.
- Make frequent eye contact with your audience throughout the talk. Do not stare at your notes or at the screen.
- Sound enthusiastic about your subject, or at least interested in it. Do not speak in a monotone. Gesture occasionally. If you seem bored by your material you can be guaranteed your audience will follow your lead.
- Make sure your watch is visible and check it occasionally to see how the time is running. If you see you are running short or long, try to adjust the speed of your presentation to compensate.

DISCUSSION

The improvements in the student presentations as the semester progresses are clear and frequently dramatic. Almost invariably poor speakers become adequate, adequate speakers become good, and good speakers become better. During the past six years a student from our department has won the regional AIChE student chapter paper award competition three times. We can't prove it, but we are convinced that the seminar course has a lot to do with this record.

The oral critiques are a valuable and interesting part of the course. The natural student tendency is to be excessively polite, to avoid criticizing harshly lest they themselves come in for the same treatment when it's their turn to speak. As a result, in the first few sessions the principal burden of criticism falls on the instructor. However, as the semester progresses the student criticisms become more and more germane and incisive, although courtesy is always appropriately retained. (We are Southern here, after all.) By the end of the semester the instructor is almost redundant: the points he is prepared to make in his critique are usually made first by the students.

Requiring each student to give a fifteen- or twenty-minute talk and subsequently a ten-minute talk seems to work very well. It is usually difficult (even for seasoned professionals) to present a significant body of technical material in twenty minutes;

having to do so provides the students with excellent practice in preparing technical seminars such as those at national AIChE meetings. Cutting the material down to ten minutes presents a whole different set of problems, as the students quickly discover. The latter exercise is good preparation for, say, company staff meetings at which many people must summarize their work in a relatively short time.

Finally, it is critically important for the course instructor to remember that the students taking the course are particularly vulnerable: they are nervous about public speaking in general and they are especially not used to being publicly critiqued. If the criticism is destructive or unduly harsh, or seemingly arbitrary and unfair, the course has the potential of doing much more harm than good. However, as long as the instructor establishes firm ground rules about criticism and takes the lead himself in creating a supportive environment, the course can be among the most positive and rewarding educational experiences the students experience in their academic careers. □

ChE book reviews

CATALYST DESIGN: PROGRESS AND PERSPECTIVES

by *L.L. Hegedus, A.T. Bell, N.Y. Chen, W.O. Haag, J. Wei, R. Aris, M. Boudart, B.C. Gates, and G.B. Somorjai*

John Wiley & Sons, Somerset, NJ 08873; 288 pages, \$47.50 (1987)

**Reviewed by
R. J. Gorte
University of Pennsylvania**

While there are a number of books on catalysis, it is very difficult to find a book which gives a balanced presentation of the many topics in this field. The problem is that everyone working in catalysis has a different view of what the subject is and what is important. People working in surface physics view catalysts as adsorption on single crystals in ultra-high vacuum, mathematical modellers view it as concentration and temperature gradients across a catalyst pellet, and traditional workers in catalysis view it as the turnover number or selectivity for a reaction carried out over a fixed bed. While not written specifically as a textbook, *Catalyst Design: Progress and Perspectives* has tried to give an overview of work carried out by

all types of catalyst researchers by bringing together leaders from several of the important areas in the field and having each write a brief review of the important aspects of their particular area.

The book itself is a series of short review articles, each written by a different author. The first chapter, written by L.L. Hegedus, very briefly discusses the continued importance of heterogeneous catalysis to industrial practice and lists the applications which utilize the largest quantities of catalysts.

A microscopic viewpoint of catalysis on single-crystal, metal surfaces is presented by G.A. Somorjai in Chapter 2. The work cited is mainly from Professor Somorjai's own research and discusses the results of reaction and adsorption studies on single crystals, including topics such as the importance of crystallographic structure for reactions on metals and the influence of surface modifiers on several example reactions. It should be noted, however, that some of the conclusions reached in this chapter are still controversial within the surface science community.

The third chapter provides a discussion of supported, organometallic clusters by B.C. Gates. The chapter begins with a review of catalysis by transition metal clusters and continues with a discussion of work carried out to anchor these compounds to a support. This second part reviews the synthesis of supported complexes and concentrates on the spectroscopic techniques which have been utilized in characterizing these catalysts. Following the section on synthesis and characterization is a discussion of the catalytic properties for several example catalytic systems.

Chapter 4, by A.T. Bell, is a review of supported metal catalysis, with an emphasis on the effect that the support can have on the metal. The chapter reviews a wide range of topics, including support acidity, preparation procedures for introducing metals onto a support, and the influence that a support can have on a metal's adsorption and reaction properties. Most of this last section involves a discussion of the unusual properties which can be observed with titania supported metals. It should be noted that Professor Bell presents certain conclusions concerning the role of titania which are still being debated in the literature.

A discussion of reaction kinetics and the design of catalytic cycles is given in Chapter 5 by M. Boudart. Since most reactions involve several elementary steps, Professor Boudart suggests ways for logically designing catalysts assuming that the intermediate

steps can be selectively altered by judicious choice of catalyst or operating conditions.

W.O. Haag and N.Y. Chen have written a review of acid catalysis by zeolites in Chapter 6. Their chapter starts by describing what zeolites are, followed by a discussion of zeolite properties including sorption behavior, diffusional phenomena, and catalytic activity. The chapter includes a concise introduction to preparation methods for zeolites, to techniques for characterization of the acid sites, and to methods for changing zeolite acidity. Following this introduction, the role of zeolites in several commercial processes is described, with a particular emphasis on the importance of molecular shape selectivity in those processes. The chapter ends with an overview of the design principles which were incorporated into the development of the first zeolite hydrocarbon cracking catalysts.

The section on mathematical modelling of transport properties in catalysis, Chapter 7, was written by R. Aris. The chapter begins with the history behind calculations of catalyst effectiveness and follows with a tutorial on how to determine the influence of catalyst geometry, reaction kinetics, and other factors on the observed reaction rates. The chapter includes a short section on methods for controlling the distribution of catalytic activity within a catalyst pellet and concludes with a discussion of rate multiplicities and stabilities.

The final chapter, written by J. Wei, presents the design considerations used for hydrodemetallation catalysts. The chapter begins by introducing the reader to the complex structure of metal-containing molecules which are present in petroleum. The rest of the chapter reviews the problems associated with hydrodemetallation in the presence of hydrodesulfurization and discusses the principles used to design catalysts which have a high activity for long periods of time.

Over all, this book provides a good review of a wide range of topics in heterogeneous catalysis. While the book could be used as a text for a course in catalysis, it would be necessary to provide supplementary materials to provide background on the different techniques which are discussed. As with any book on topics for which research is ongoing, one should not consider any of the chapters as being the final word. However, each section does provide a good beginning for the interested reader. There is clearly a need for a book of this type. □

FLOW SHEET IS PROCESS LANGUAGE

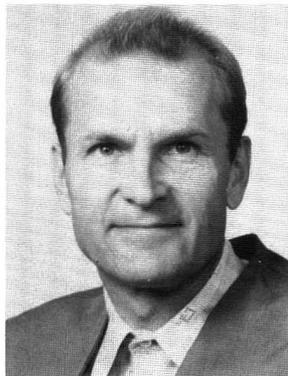
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TEXTBOOKS WRITTEN FOR chemical engineering core courses do not generally provide links between the theory presented and industrial practice of process engineering. Many surprises are waiting for students in the plant environment. We have found that this situation can be considerably improved by incorporating flow sheet conception into the lecture program, mainly in unit operations and design courses. The flow sheet forces the student to consider a particular piece of equipment in its true industrial context where it ties in with utilities and basic control strategy. The method not only motivates students to participate creatively, but it also generates questions on process engineering logic that are a welcome enrichment of class activity. This paper will illustrate with examples how students can be induced to ask these questions and to find answers to them.

FIRST HEAT EXCHANGER EXAMPLE

To illustrate the calculations for heat transfer to jacketed tank reactors, we went through an example solved in a well-known textbook [1]. Knowing the heat



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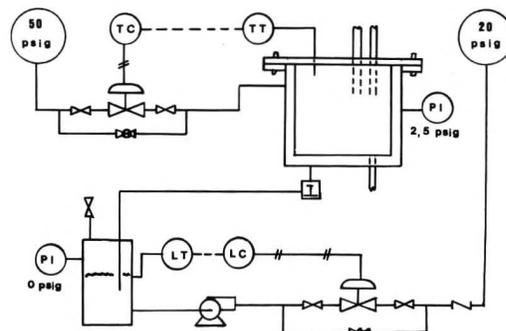
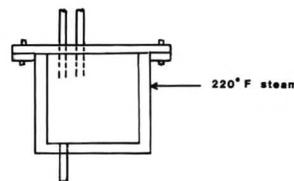


FIGURE 1. Steam supply to reactor jacket. Above: book approach. Below: flow sheet approach.

load and the available surface, the steam temperature required in the jacket is found to be 220°F. The subject matter of the book goes this far, but thinking that this was not a real challenge to my students, I went on to speak some process language: our plant has two steam headers, 50 psig and 150 psig, and a condensate return header at 20 psig. I asked the students to prepare a flow sheet with enough details to show exactly how steam flows from which of the supply headers through the jacket and back into the return header. The jacketed reactor then acquires its true identity as part of the processing unit. This is process language. Some quite common “nonsense situations” were submitted from which a lot could be learned about the logic of process engineering. Can you imagine a pump at the jacket exit that simply pulls the steam through from the supply header? Figure 1 shows a workable solution. It also depicts the difference between a book approach and a flow sheet approach to the problem.

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SECOND HEAT EXCHANGER EXAMPLE

When studying the thermal design of shell and tube exchangers, we went through an example solved in another well-known textbook [2] which states that "atmospheric pressure steam condenses on the shell side." Nobody objected to this as long as we were busy figuring the number of tubes and passes. The surprise came when I again asked for the flow sheet. Only then did it become clear that book language is not process language. Even the simplest steam trap requires a pressure drop to function, which means that in addition to the equipment shown in Figure 1, it will be necessary to pull a vacuum on the condensate collection tank in order to make the steam flow at all. What is more, this vacuum has to be monitored if a pressure of 1.00 atm. abs. is to prevail in the shell. The flow sheet question helped integrate the exchanger into the processing environment, and it became evident that atmospheric pressure was a poor choice for the shell.

EVAPORATOR EXAMPLE

The typical textbook evaporator calculation [3] will state the pressure in the last effect to have a certain value, such as 100 mm Hg absolute or 26 in Hg vacuum. All calculations are based on this number, although no effort is made to explain its source. In addition, our school is located 3500 feet above sea level where 26 in Hg is considered perfect vacuum. This is another excellent situation to be explored with process language. I got surprised looks when I asked, "Would you please supply a flow sheet?" and, "What would you do if some day you were asked to operate at 23 in Hg vacuum?" The problem statement in the book did not require that the student think this far ahead. Many misconceptions about vacuum equipment can be dispelled by simple confrontation of sense and nonsense on the flow sheet. Can you imagine a pump that sucks out all the vapor produced in the last effect? The surprised looks disappeared as the answers slowly took shape. A workable solution is presented in Figure 2. Again, the figure compares book approach to flow sheet approach to show the enrichment obtained through process language.

DISTILLATION PRESSURE EXAMPLE

An uncommon situation appeared in the study of the conversion of fermented beer into 96 volume % ethanol in two distillation towers. The equilibrium conditions are such that no reflux is required in the first column. The overhead vapor containing 24 mol %

The method not only motivates students to participate creatively, but it also generates questions on process engineering logic that are a welcome enrichment of class activity. This paper will illustrate . . . how students can be induced to ask these questions and to find answers . . .

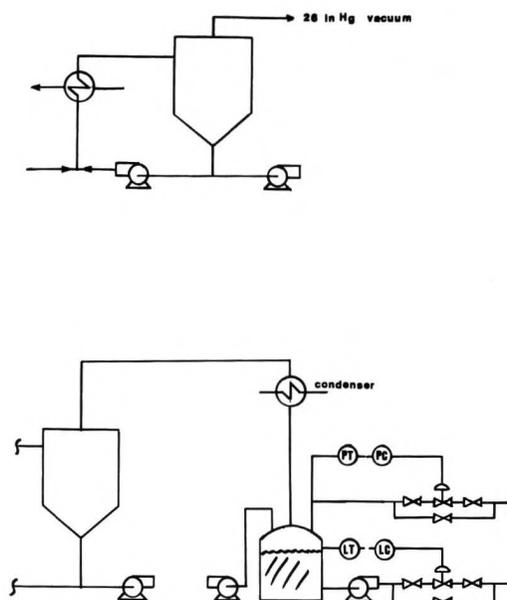


FIGURE 2. Condensate collection from evaporator. Above: book approach. Below: flow sheet approach.

ethanol is fed directly to the appropriate plate of the second column. On paper, the two columns looked like any column depicted in textbooks, with the number of plates determined by the method of McCabe-Thiele and the feed plates chosen accordingly. Mass and heat balances closed with the correct amount of open steam at the bottoms and the correct amount of cooling water in the second column condenser. There was but one little problem: At the start, on deciding the operating pressure, there was no reason for it to be much different from atmospheric. A distilling company was consulted and the information obtained that the first column runs at 3 psig, which confirmed our reasoning. Consequently, the design proceeded with this pressure. When the time came to provide a flow sheet, there was no variable available for manipulation to control the first column pressure. Textbooks were consulted but no answer was found. On combining the flow sheets of the two towers and after a brainstorming session, the fact slowly emerged that the first column pressure in this scheme is not an inde-

pendent variable as it is in standard reflux columns discussed in the books. The second column pressure has to be controlled at the condensate drum, and the first column pressure would then find its own equilibrium value, much like it does in a double effect evaporator. Had the problem been terminated at the textbook stage, this "discovery" would have been lost.

CONCLUSIONS

Flow sheet is process language. Process language is exciting. Process language transforms book examples into process plant examples. Process language resorts to the use of utilities to vitalize unit operations teaching. Process language is a stimulating teaching tool.

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ChE book reviews

DISTILLATION TRAY FUNDAMENTALS

by M. J. Lockett

Cambridge University Press, Cambridge and New York, 1986. 224 + xxiii pp. \$54.50

Reviewed by

James R. Fair

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The distillation column continues to be the principal separation device for the chemical and petroleum processing industries. For many years it was characterized as a vertical, cylindrical column containing plates or trays upon which rising vapor and descending liquid were brought into intimate contact, for purposes of effective mass transfer. In recent years designers of distillation columns have shifted some attention to the use of structured (as opposed to random) packings as vehicles for effecting intimate phase contacting. However, such packings are considerably more expensive than trays, and their cost is often justified only when their lower pressure drop carries an economic advantage, as in some vacuum distillations. Thus, the tray column remains as the standard and basic device for vapor-liquid contacting.

Despite the title, this book deals not only with

trays for distillation services but also covers applications in absorption and stripping. It covers all of the important aspects of tray design, those of a more hydrodynamic nature as well as those relating directly to the mass transfer propensity of the two-phase mixture on the tray. Considerable space is devoted to the characterization of this mixture: foam, emulsion, froth, spray, and so on. The overall coverage is quite complete, with no detail of design left unaddressed. Such important topics as phase flow distribution, capacity limits, pressure drop and interphase mass transport are dealt with on quantitative bases. A commendable effort has been made by the author to consider all historical approaches (mostly empirical) that deal with the various design parameters. The literature coverage is near exhaustive, and the reader will not find elsewhere as complete a bibliography on the distillation tray as is provided here. For each design consideration, a method with some fundamental and mechanistic support is provided—and for practitioners of distillation system design this is a welcome advance from the art and empiricism that have often prevailed.

There are some limitations to the treatment that should be mentioned. First, the author has not always found it possible to make a forthright recommendation when several alternate models or procedures are available for a particular design step. The reader must then make his own choice. Also, despite the title, all tray-type contacting devices are not considered. There is very little on valve trays, essentially nothing on bubble-cap trays, and complete silence on dualflow trays (those without downcomers). Emphasis is clearly on crossflow sieve trays, but this is not all bad. While there are still many bubble-cap tray columns in operation, very few new ones have been designed during the last few decades. The valve-tray is really a proprietary contactor, with design often left up to the proprietor. The dualflow tray is a rather specialized device (and tricky to design), used mostly for fouling services. On the other hand, the sieve tray is an efficient and relatively inexpensive non-proprietary device that has been the object of many basic studies, and its simple geometry (in effect, one or more sheets of perforated metal, joined to a downcomer for handling liquid passage) makes it reasonably amenable to fundamental modeling. Still, the title might have read "Distillation Sieve Tray Fundamentals."

The book might have been improved by the inclusion of some worked-out design examples, some advice on laboratory or pilot plant scaleup procedures, and an author index. Still, the development of rational, fundamental-based approaches to the handling

of complex two-phase mixtures, as are found on trays, is refreshing and encouraging. The author has an extensive background in the research, testing and modeling of distillation devices, and his authoritative text reads very well. There is no equal to the book presently on the market. Anyone concerned with the design or analysis of distillation, absorption or stripping columns of the tray type will want to take advantage of the modern approaches presented in this book. □

GAS SEPARATION BY ADSORPTION PROCESSES

by *Ralph T. Yang*

Butterworth Publishers,

80 Montvale Avenue, Stoneham, MA 02180;

352 pages, \$52.95 (1986)

Reviewed by

D. M. Ruthven

University of New Brunswick

The importance of adsorption as a separation process in the chemical and petroleum industries has increased dramatically in recent years, but the subject is still not covered in any significant way in most chemical engineering curricula. There have been three recent books on the subject: *Principles of Adsorption and Adsorption Processes*, by this reviewer, published by Wiley in 1984; *Large Scale Adsorption and Chromatography*, by P. C. Wankat, published by CRC Press in 1986; and the present volume by Ralph Yang, published by Butterworth Publishers in 1987. None of these is really a textbook in the formal sense, but any of them could be used as the basis for a graduate level (or possibly a final year elective) course on the subject.

The coverage of the present volume is broadly similar to that of *Principles of Adsorption and Adsorption Processes*, and there is considerable overlap, which is probably inevitable since many of the source references are common. The emphasis is, however, different—reflecting the different areas of interest and expertise of the authors. The book provides a coherent and comprehensive account of the subject, including the basic physico-chemical principles as well as process technology. Although the title is *Gas Separation by Adsorption Processes* (and this is indeed the main focus), liquid phase separation processes such as the "Sorbex Process" and parametric pumping are also covered briefly. As with its predecessors, the emphasis is on fundamentals rather than on technological details, and the level of background knowledge which is assumed is also similar.

The book is divided into eight chapters: 1. Intro-

duction; 2. Adsorbents and Adsorption Isotherms; 3. Equilibrium Adsorption of Gas Mixtures; 4. Rate Processes in Adsorbents; 5. Adsorber Dynamics—Bed Profiles and Breakthrough Curves; 6. Cyclic Gas Separation Processes; 7. Pressure Swing Adsorption—Principles and Processes; 8. Pressure Swing Adsorption—Models and Experiments.

It is not a book for the undergraduate, but it should be easily understood by graduate students and those with some experience in research and development. Since most adsorption processes operate under transient conditions, some familiarity with partial differential equations is needed to follow the sections dealing with column dynamics and process modeling (Chapters 5 and 8). I found Chapter 3, which contains a good review of the various approaches to the correlation and prediction of multicomponent adsorption equilibria, and Chapters 7 and 8, which provide an authoritative summary of PSA technology and modeling, to be most useful.

There is no discussion of membrane separation processes which compete directly with pressure swing adsorption in a number of applications. While membrane separations may not be included within the narrower definition of adsorption processes, some such discussion would have been useful to allow the reader to assess the relative merits of either approach, particularly in view of the publisher's claim that this is a "complete treatise covering all aspects of adsorption processes . . ."

Inevitably in a book which covers such a wide range of subjects, one can expect controversy over the treatment of certain topics. For example, in the discussion of surface diffusion and intracrystalline diffusion in zeolites (pp. 113-121) it should probably have been pointed out that the kinetic treatment (which is emphasized) and the quasi-thermodynamic treatment (which is criticized) are not necessarily in conflict, but merely represent different ways of looking at the same phenomenon. The advantage of the quasi-thermodynamic treatment is that it allows meaningful transport co-efficients to be derived without knowledge of the detailed diffusion mechanism. This may not be obvious to the casual reader. Such criticisms are, however, minor, and any lack of balance is more than offset by the advantages in the presentation of coherent perspective.

Taken as a whole, the book presents a concise and readable summary of the voluminous literature of the subject. It will no doubt become required reading for those working in this area, both in universities and in industry. At US \$52.95 it is (just about) within the affordable price range for individuals. □

THE MYSTIQUE OF ENTROPY

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STUDENTS OF thermodynamics soon learn to appreciate the utility of entropy in making various calculations involving process heat and work effects. These are direct applications found in engineering and physical science. However, in addition to these quantitative applications, one finds qualitative and metaphoric uses of entropy in a wide diversity of fields. The extent to which the concept of entropy has suffused contemporary thought is well illustrated by Lord C. P. Snow's assertion that any definition of culture should include a technical component and that an understanding of the second law of thermodynamics is the cultural equivalent of a familiarity with the works of Shakespeare [1].

Igoring incidental uses, a few examples will be presented here in which the concept of entropy is central to the development of a theme or is thought to provide insight. The intent is to illustrate the pervasiveness of the fascination evoked by the entropy concept—the entropy mystique.

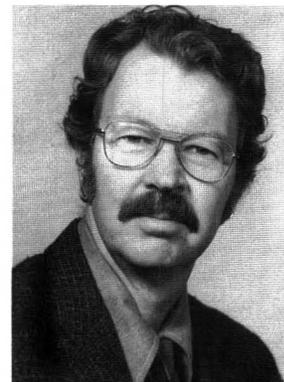
COSMOLOGY

Of the many formulations of the laws of thermodynamics, the boldest and most provocative was advanced in 1865 by Rudolf Clausius:

- The energy of the universe remains constant.
- The entropy of the universe tends to a maximum.

Here Clausius has taken concepts arising from limited, earth-bound experience and with a great leap of imagination has vested them with cosmic significance. While both statements are daring, the second-law statement has sparked the most interest and con-

... a few examples will be presented in which the concept of entropy is central to the development of a theme or is thought to provide insight. The intent is to illustrate the pervasiveness of the fascination evoked by the entropy concept—the entropy mystique.



Benjamin G. Kyle is professor of chemical engineering at Kansas State University and is enjoying his thirtieth year of teaching. He holds a BS from the Georgia Institute of Technology and a PhD from the University of Florida. He has not outgrown an early fascination with thermodynamics and is interested in practically all aspects of the subject. He is the author of a recently published (Prentice-Hall) thermodynamics textbook.

troverly because it leads to speculations regarding the birth and death of the universe.

Birth and Death of the Universe

By definition, the universe must be a closed system, and the uncritical extrapolation of our terrestrial experience would suggest that its entropy is increasing toward a maximum. Because an increase in entropy is associated with a decreased ability to perform work, the second law implies that the universe will ultimately reach a dead state referred to as thermal death. This dead state is an equilibrium state in which all thermodynamic potentials have been leveled and processes yielding work are no longer possible.

If one accepts Clausius' statement of the second law with its implication of thermal death, then by the following simple argument one can show that the universe had a beginning. A maximum is characterized by a first derivative of zero. However, the derivative, or rate of change, is finite until the maximum is reached. Thus, if the entropy of the universe is tending to a maximum, it is doing so at a finite rate and will reach its goal in a finite time. A universe of infi-

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nite age would have already reached its equilibrium state of maximum entropy, and since this is not the case, the universe must have a finite age. Thus, the universe had a beginning and we have a position that is at least congenial to the inference of creation and a creator. Undoubtedly, the inclination to draw this inference is strengthened by a scientifically more acceptable theory originated by Lemaitre in 1927 and more recently popularized [2] as the "Big Bang" theory.

The widely published English prelate, William Inge, eagerly accepted the proof of a creator as implied by the "law of entropy" [3]. Inge used the prospect of the thermal death of the universe to argue that God the Creator could not be merely a pantheistic god found only in nature because such a god would be under an inexorable death sentence. Such would not be the fate of the transcendent god of Christianity.

It is not Christianity but modern pantheism and the myth of unending progress which are undermined by the degradation of energy.

Most notable among those espousing the creation view was Pope Pius XII, who stated that Clausius' law of entropy provides "eloquent evidence of the existence of a Necessary Being." [4]

An argument against the inference of creation from the laws of thermodynamics was advanced by the Russian physicist, I. P. Bazarov [5], based on the dialectic materialism of Engels. Identifying flaws in the thermal death argument for the existence of a creator, Bazarov points to the unfounded assumption that the laws of thermodynamics apply to the entire universe and to Engels' argument that the creation implied by the second law would be in violation of the first law. In Engels' words, those advocating the pro-creation view saw the universe as winding down and thus assumed that an initial winding up had been provided by "a stimulus from without." However, the process of winding up imparted energy to the universe and hence the total energy of the universe has not always been constant as required by Clausius' first-law statement.

It now appears that Engels' argument of a first-law violation may be vitiated by recent calculations that indicate the total of all energy in the universe is zero [6]. This is possible because energy of motion and the energy equivalent of mass are positive while energy of gravitational or electromagnetic attraction is negative. A zero energy sum would imply that creation could have occurred without an energy input and brings to mind the theological doctrine of creation *ex nihilo*.

The theory of relativity shows that time and space are part of the structure of the universe and not . . . an empty stage on which physical events are enacted. However, within this purely physical picture there remains the basic question of the direction of time.

Bazarov's criticism regarding the unwarranted extension of the laws of thermodynamics to the entire universe seems well taken. This is especially so considering that on a cosmic scale the predominant energy effects are associated with gravitation and radiation, types of energy which are usually neglected when applying thermodynamics in its usual terrestrial context. In spite of this obvious incongruity, the question is still unresolved for today one finds astrophysicists concerned with entropy changes of various cosmic processes in which quantum and relativistic effects predominate [6].

Time

Of all the basic quantities in the physical world, time is the most elusive. This is because we not only experience it as an abstraction useful in physical science, but also in a psychological sense. Because the latter lies beyond the realm of physics, any strictly physical description of time can never be entirely satisfactory.

The theory of relativity shows that time and space are part of the structure of the universe and not, as pictured by classical physics, an empty stage on which physical events are enacted. However, within this purely physical picture there remains the basic question of the direction of time. The equations of classical mechanics, quantum mechanics, and relativity theory are symmetric in time and do not preclude the reversibility of processes. On the other hand, we know that all naturally occurring processes are irreversible and hence travel only in what we have designated as the forward direction of time. For this reason the second law of thermodynamics is said to define the "arrow of time." Time increases in the direction of increasing entropy.

The problem of reconciling the reversibility of the microscopic world of colliding molecules obeying the laws of classical mechanics with the irreversible behavior of the macroscopic world was first undertaken by Boltzmann. This search for the origins of irreversibility provides an interesting chapter in the annals of science [7] and has led to the development of statistical mechanics, an area of science which has proved quite useful in the calculation of thermodynamic and transport properties. However, despite this practical suc-

cess, the origins of irreversibility have yet to be determined to the satisfaction of scientists of a philosophical bent [8].

LIFE AND EVOLUTION

At present there is disagreement among scientists as to whether living systems can be completely described by the laws that apply to inanimate matter or whether additional, but as yet undiscovered, laws applying only to living matter are also needed. However, the various identifiable physical and chemical processes occurring within living systems require no additional laws for their explication and therefore conform to the laws of thermodynamics. Additionally, it is known that the laws of thermodynamics are obeyed by each living system as it interacts with its environment. Our present societal obsession with diets and calorie counting serves as a monotonous reminder of our bondage to the first law, but the dictates of the second law are not so obvious and, in fact, may seem counter-intuitive. The conceptual difficulty appears when we regard life as a striving to maintain order and the second law as a principle of degradation. This apparent conflict is due to our failure to recognize living systems as open systems. In an open system the combined entropy of the system and surroundings must increase. Thus, a living system can maintain itself or grow, and thereby decrease its entropy, if the surroundings undergo the appropriate increase in entropy. This leads directly to the statement that life is sustained by the conversion of low-entropy resources into high-entropy wastes. The ultimate origin of low-entropy resources is the sun which drives the photosynthetic mechanism in plants whereby solar energy is converted into chemical energy and stored as carbohydrates.

Despite reconciliation of the life force with the law of entropy, there is still a persistent undercurrent of nagging doubt when the origin and evolution of life are considered. These activities imply purpose, a goal that seems totally opposed by the entropy principle. This contradiction was recognized by Teilhard de Chardin in formulating his grand scheme of evolution towards an Omega Point of pure consciousness and ecstatic union with God [9]. Because of the law of entropy with its opposing tendencies and prospect of thermal death, Teilhard postulated two classes of energy: tangential and radial. Tangential energy is simply the energy identified by physical science and subject to the laws of thermodynamics. On the other hand, radial energy is of a psychic or spiritual nature and is not subject to the laws of thermodynamics. The evolution of life toward the Omega Point is said to be

driven by radial energy and thus is free of second-law restrictions. The relationship of the two classes of energy is tenuous and is best illustrated by Teilhard's words:

To think, we must eat. But what a variety of thoughts we get out of one slice of bread! Like the letters of the alphabet, which can equally well be assembled into nonsense as into the most beautiful poem, the same calories seem as indifferent as they are necessary to the spiritual values they nourish.

Teilhard was a Jesuit priest as well as a scientist, but he wanted his work to be judged on the basis of its scientific merit. His *Phenomenon of Man* is a monumental attempt to meld science and metaphysics to provide an answer to the question of meaning. Despite his heroic effort to fuse faith and reason, science, because it recognizes only reason, could do nothing but render a negative verdict. Nevertheless, his work has wide appeal today, some thirty years after his death. Perhaps this is because the soul of a poet and mystic shows through. After all, who but a poet or mystic would dare address such questions.

SOCIAL SCIENCE

Henry Adams, the noted American historian and man of letters, was the first to view the course of civilization (*i.e.*, history) from a second-law perspective [10]. In the opening years of the twentieth century he expounded a theory of history in which the Social Energy of civilization is continually dissipated. According to Adams, the second law of thermodynamics required that, ". . . the higher powers of energy tended always to fall lower, and that this process had no known limit." In the category of energy Adams included the Vital Energy of an individual and the Social Energy of society and stated that, "The law of entropy imposes a servitude on all energies, including the mental." All this naturally resulted in a pessimistic prognosis for civilization where ". . . the ash-heap was constantly increasing in size."

According to one of its most famous practitioners, Claude Levi-Strauss, the field of anthropology could appropriately be called "entropology." Levi-Strauss [11] sees man and his civilizations as "instruments intended to create inertia, at a rate and in a proportion infinitely higher than the amount of organization they involve." He further states

Thus it is that civilization taken as a whole, can be described as an extraordinary complex mechanism, which we might be tempted to see as offering an opportunity of survival for the human world, if its function were not to produce

what physicists call entropy, that is inertia. Every verbal exchange, every line printed, establishes communication between people, thus creating an evenness of level, where before there was an information gap and consequently a greater degree of organization.

We find familiar the concept that the net result of human life is an increase in entropy, but the idea of a leveling of social organization through communication is a bit unexpected and would appear to be a metaphoric extension of the thermal death concept.

The second law of thermodynamics has been shown to provide a realistic perspective for economics [12]. According to Nicholas Georgescu-Roegen, the conventional view of economic process as circular and timeless ignores the increase in entropy accompanying every human endeavor. Georgescu-Roegen sees economic activity as turning low-entropy inputs into high-entropy outputs.

All species depend on the sun as their ultimate source of low entropy except man, who has learned also to exploit the terrestrial stores of low entropy such as minerals and fossil fuels. Life feeds on low entropy and so does economic life. Objects of economic value such as fruit, cloth, china, lumber, and copper, are highly ordered, low-entropy structures. For low entropy is the taproot of economic scarcity.

He observes that economic development as presently practiced is based on rapacious consumption of our terrestrial dowry of low-entropy materials and concludes that this can not be indefinitely sustained.

Using the entropy-conscious economic views of Georgescu-Roegen, Herman Daly [13] argues persuasively against the fallacy of perpetual growth and even suggests that growth itself may be illusory when measured by the GNP. This closely watched economic indicator includes, besides the value of goods produced and services rendered, all costs associated with production, including pollution control costs. As the richer and more accessible resources are preferentially consumed, the remaining lower-quality resources require higher production costs and thus a rise in GNP may reflect increased cost of production rather than increased level of production. This is the entropic factor largely ignored by conventional economics. As an alternative to growth, Daly has outlined in some detail the workings of a steady-state economy.

The work of Georgescu-Roegen has also inspired Jeremy Rifkin's *Entropy: A New World View* [14] in which the entropy law is credited with singlehandedly undermining the Newtonian-Cartesian mechanistic world view. Rifkin believes that a new world view based on the entropy law would expose the fallacy in

our present obsession with growth and would allow us to meet the future with awareness and acceptance of nature's constraints. This change in outlook would affect practically every area of human endeavor ranging from technology to religion and could move us toward the long-sought but ever-distant utopian dream. There is no doubt that Rifkin has overstated his case in a single-minded and over-simplified manner, but exaggeration is a forensic device which often becomes acceptable when used in passion for a worthy cause. Because the inculcation of an entropy-conscious world view is considered by many to be such a cause, perhaps Rifkin should not be judged too harshly for his excesses.

LITERATURE AND ART

Metaphoric entropic themes abound in modern fiction [15] as well as in serious science fiction [16]. Most applications are implicit, although several writers explicitly use the term entropy in their work. These writers are predominately American and include John Barth, Donald Barthelme, Saul Bellow, Stanley Elkin, Norman Mailer, Walker Percy, Thomas Pynchon, and John Updike. As expected of fertile imaginations, one finds many variations of the entropic theme whether used explicitly or implicitly. The theme has been applied to either individuals or entire societies, sometimes within the context of a closed system, with ultimate states as extreme as chaos and stagnation.

Norbert Wiener's famous book on cybernetics [17] first appeared in 1950 and was undoubtedly instrumental in popularizing the application of the entropy concept to the many aspects of the human condition as found in modern literature. Moreover, Wiener's identification of entropy as a measure of the information content of messages stimulated writers to examine the very act of writing [18]. In Wiener's words

Messages are themselves a form of pattern and organization. Indeed, it is possible to treat sets of messages as having an entropy like sets of states of the external world. Just as entropy is a measure of disorganization, the information carried by a set of messages is a measure of organization. In fact, it is possible to interpret the information carried by a message as essentially the negative of its entropy, and the negative logarithm of its probability. That is, the more probable the message, the less information it gives. Cliches, for example, are less illuminating than great poems.

The idea behind this passage is easily grasped when applied to the transmission of factual data (e.g., a seven-digit telephone number) or a coded message (e.g., one if by land, two if by sea) but quickly becomes fuzzy when considering the transmission of subtle or

One is left wondering why the entropy concept, which offers so little insight, has been so widely employed outside its narrow scientific context and why any serious artist or writer would even consider the application of scientific principles to the very act of creating. There does indeed appear to be an entropy mystique . . .

abstract ideas or the more vital aspects of communication inherent in the sender and receiver. This becomes apparent when the idea is pushed to its limit. The writer, in an attempt to counter the entropic effect of banality, looks for unexpected or improbable ways of using words and thus runs the risk of verbal chaos. The dilemma is articulated by Lewicki [12]:

In order to avoid entropy, a writer must therefore walk a narrow path between the danger of producing probable messages of low informational value (such as, for example, new versions of old themes, written in a conventional manner), and the risk of turning out incomprehensible bodies of words that would seem disorderly to the reader.

Rudolph Arnheim [19] has recognized the contradictions in information theory as applied to art:

Here order is described as the carrier of information, because information is defined as the opposite of entropy, and entropy is a measure of disorder. To transmit information means to induce order. This sounds reasonable enough. Next, since entropy grows with the probability of a state of affairs, information does the opposite: it increases with its improbability. The less likely an event is to happen, the more information does its occurrence represent. This again seems reasonable. Now what sort of sequence of events will be least predictable and therefore carry a maximum of information. Obviously a totally disordered one, since when we are confronted with chaos we can never predict what will happen next. The conclusion is that total disorder provides a maximum of information; and since information is measured by order, a maximum of order is conveyed by a maximum of disorder.

Arnheim attributes the contradiction to a failure to distinguish order from structure:

Any predictable regularity is termed redundant by the information theorist because he is committed to economy: every statement must be limited to what is needed. He shares this commitment with scientists and artists; its meaning, however, depends on whether one chops up patterns into elementary bits or whether one treats them as structures. A straight line reduced to a sequence of dots for the purpose of piecemeal analysis or transmission can be highly redundant; in the drawing of a geometrician, engineer, or artist it is not.

In explaining the creative process underlying a work of art, Arnheim sees an interplay between the anabolic tendency which establishes the structural theme and the entropic principle which is manifested both as a catabolic destruction of patterns, or disordering,

and a simplification or ordering due to tension reduction. Here we see the entropy principle invoked metaphorically and identified simultaneously with two opposing tendencies: ordering and disordering.

COMMENTARY

Of all the properties of matter, entropy is most difficult to conceptualize and seems the most contrived. It cannot be evaluated directly from an experimental measurement, but must be calculated from a somewhat arbitrary computational path and thus its existence and evaluation are closely tied to human activity. It is tainted with a human scent. Perhaps this is a reason this most anthropomorphic of all the concepts of science has fascinated the human mind.

Despite its mystique, entropy actually provides very little insight into the mysteries of nature. This can be appreciated by recalling the familiar textbook derivations. A Carnot cycle is used to define entropy and demonstrate that it is a state property. Next, an isolated system undergoing a spontaneous process is considered and a simple argument shows that an increase in entropy results. Ramifications of this result are extremely useful for the detailed calculations made by engineers and scientists, but in what way has it improved our general understanding of nature? Are not the following statements equivalent and equally enlightening?

- A. Every spontaneous process tends toward a condition of deterioration or stagnation.
- B. Entropy is the measure of deterioration or stagnation. Every spontaneous process results in an increase in entropy.

Statement A is a direct statement of experience. Statement B is expressed in the language of an empirically based science and is therefore merely an indirect but more formalized statement of experience.

The idea of things running down, which can now be proclaimed as a decree of science, has been found to be a dominant theme in ancient myths [20]. This condition also has been lamented by Hesiod, the Greek poet of the 8th century B.C., who told of the five descending ages of Man beginning with a pristine age of gold and ending in his own worldly age of iron. Also, somewhat later, we find St. Paul [21] referring to a coming time of glory when "creation itself will be set free from its bondage to decay." These may be

regarded as generalizations of statement A and appear more naive than the B-based concept of thermal death. Yet, even though we favor statement B today, let us not be deceived into thinking it more insightful than statement A.

With regard to fixing the direction of time, it is also instructive to consider two alternative statements.

- A. In the usual sense of *before* and *after*, spontaneous processes proceed in the forward direction of time.
- B. All spontaneous processes are accompanied by an increase in entropy. The forward direction of time is the direction in which the entropy increases.

While the practical person would give no advantage to statement B, many philosophers prefer something similar to it because it appears to have eliminated some of the subjective element that clings to statement A. Their object is to define time without reference to the human mind [22]. However, in this respect an obvious problem arises in the actual determination of entropy. This requires a human mind to devise a reversible path between the initial and final states which is essential to the calculation of the entropy change. There is no entropy meter and the invoking of entropy, which is itself a construct of the human mind, does little to remove the human scent from the concept of time.

To place the question of time in perspective we should recognize that it is a construct of the conscious mind. The subconscious mind, the Freudian *id*, has no awareness of time—a fact known to science and easily verified personally by recalling the particulars of our dreams. What we have done is to construct from the regular rhythms of the universe (*e.g.*, the motion of the earth about its axis or about the sun) a lifeless, linear time scale upon which we can place in monotonic order the events of our physical world. This seems so natural that it comes as something of a shock to learn that it is possible to have a valid and effective world view that does not include the concept of time. An outstanding example of this is the language of the Hopi indians of the American southwest which contains no reference to “time” either explicitly or implicitly. This language is capable of accounting for and describing correctly, in a pragmatic or operational sense, all observable phenomena in the universe without the mental construct of time [23].

The avowed aim of science is to establish the basis of physical reality. However, two different interpretations exist: external and internal. The external version is the older, traditional view in which the human mind objectively probes and observes nature and thereby discovers natural laws. Recent developments

in physics, however, have cast doubt on the concept of an objective observer independent of the system observed [24], and this has led to the view that science merely creates a set of interlocking laws which provides a consistent description of nature. This description usually involves the use of abstractions and mental constructs far removed from our everyday experience and may thus be termed a view of physical reality internal to the mind [25]. The previous discussion of time and entropy is obviously an argument for the internal view.

One is now left wondering why the entropy concept, which offers so little insight, has been so widely employed outside its narrow scientific context and why any serious artist or writer would even consider the application of scientific principles to the very act of creating. There does indeed appear to be an entropy mystique, although the reasons for it will not be explored. Perhaps the following verse is appropriate.

ENTROPY

*For thermodynamics we feel a sense of awe
And marvel at the power of those early minds
Who showed that mundane matters lead to
natural law
And boldly stated that the universe unwinds.
The second law is never denied its due
In science, belles-lettres, and philosophy.
It pales the onward-and-upward view,
For no one is consoled by entropy.
While nothing temporal eludes its iron rule
And most would take decay's decree as true,
The sage's bane can be the builder's tool
As entropy shows the best that we can do.
This useful concept prompts a primal groan:
A dread we've only named but always known.*

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DISCRETE-EVENT SIMULATION IN CHEMICAL ENGINEERING

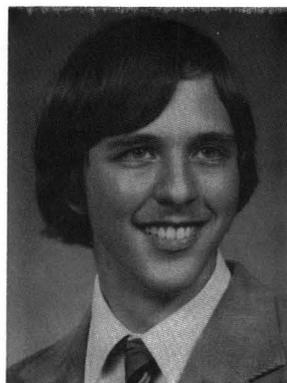
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RECENT YEARS HAVE witnessed a rapid and dramatic change in the nature of the chemical process industries in the developed countries of the world. Specifically, there has been an intense revival of commercial interest in batch chemical processes, such as those employed in the manufacture of fine and specialty chemicals, at the expense of traditional continuous steady-state processes for the manufacture of commodity chemicals. One large British chemical company reports that specialty chemicals manufactured by batch processing contributed over 30% to their total profits in 1983 as opposed to 18% in 1977 [1]. Certainly, one of the primary driving forces for this change has been the recent commissioning of many world-scale commodity chemicals plants in various developing countries.

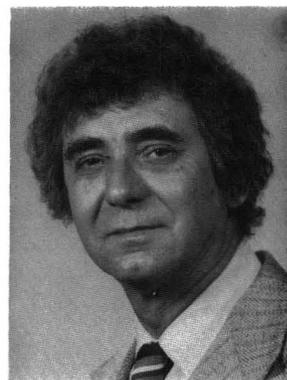
SIMULATION SYSTEMS

Concomitant with these industry changes, significant developments have occurred in the modeling and simulation of chemical processes. To be sure, usage (including academic) and development of conventional steady-state process simulators continue at an active level. Thus, the FLOWTRAN system [2] developed by the Monsanto Company was made available to chemical engineering schools in 1973 and has been extensively employed for educational purposes ever since [3]. Subsequently, newer steady-state process simulation systems such as PROCESS, ASPEN PLUS and DESIGN II became available to academic users.

Discrete-event simulators were originally developed as numerical aids to solve complex queuing theory problems which were not amenable to analytical solution. Such problems occur routinely in the field of industrial engineering . . .



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We have also witnessed the development and application of various simulators for batch chemical processes in recent years. These developments have included both discrete-event and combined (discrete + continuous) systems, as employed in the industrial engineering field. There is an unfortunate confusion in terminology here: the industrial engineering interpretation of the term 'continuous' is not the same as that associated with chemical engineering usage, namely, steady-state operation. Rather, the industrial engineering meaning of continuous should be construed by chemical engineers as dynamic or unsteady-state.

The progenitor of discrete-event simulation systems is GPSS [4], which dates back to 1959 and is still used extensively in many manufacturing sectors. Because of its easy use, availability, reliability, and efficient operation (integer arithmetic only in many versions), GPSS is a very effective tool if only discrete simulation capability is required. Other popular dis-

TABLE 1
Recent Applications of GPSS to Chemical
and Allied Processes

APPLICATION	[REF.]
Two batch reactors in parallel followed by a batch still	[7]
DDT manufacture	[8]
Chocolate manufacturing	[9]
Sequence of batch distillation columns	[10]
Large-scale poliomyelitis vaccine production	[11]
Choline chloride manufacture	[12]
Polyvinyl chloride (PVC) manufacture	[13]
Sequencing batch reactors (SBR) for wastewater treatment	[14]

crete-event simulation systems include SIMULA [5] (more prevalent in Europe) and SIMSCRIPT [6]. In general, however, there are not many published applications of discrete-event simulation systems to batch chemical processes. Morris [7], for example, has described a very simple application of GPSS to a batch process comprised of two reactors in parallel followed by a still. Other recent applications of GPSS to chemical and allied batch (or semi-continuous) processes are listed in Table 1.

DISCRETE-EVENT SIMULATION

Discrete-event simulators were originally developed as numerical aids to solve complex queuing theory problems which were not amenable to analyti-

TABLE 2
Terminology in Usage of the FLOWTRAN and
GPSS Simulators

ITEMS	FLOWTRAN (Steady-State Process Simulator)	GPSS (Discrete-Event Simulator)
Precoded functional subroutines	Blocks	Blocks
Arguments of functional subroutines	Parameters	Operands
Items moving through the model	Streams	Transactions
Numerical characteristics of moving items	Properties (e.g., temperature, composition)	Parameters
Output quantities from subroutines (other than moving items)	Retention vector contents	Standard numerical attributes

Despite their considerable differences in origin and application, there are noteworthy similarities among the various types of simulators . . . For example, FLOWTRAN and GPSS have a number of precoded functional subroutines.

cal solution. Such problems occur routinely in the field of industrial engineering and typical example applications include machine shops, customer service stations, and transportation networks.

Most discrete simulation systems have stochastic capabilities for the scheduling of time events. To support this function, most such systems also have one or more built-in random-number generators. Output from the latter is used to sample event times (or durations between time events) from various probability distributions. In GPSS, the only easy-to-use, built-in distribution is the uniform or rectangular distribution. Thus, for example, a service time can take the form, $A \pm B$, where A represents the mean value and B is the half-width, in appropriate time units, of the distribution.

SIMILARITIES IN SIMULATORS

Despite their considerable differences in origin and application, there are noteworthy similarities among the various types of simulators described above. For example, FLOWTRAN and GPSS have a number of precoded functional subroutines (generally written in FORTRAN). In both FLOWTRAN and GPSS, these functional subroutines are known as blocks.

There is a number of other similarities between these two systems, obscured only by the technical jargon employed. In conventional steady-state chemical process simulators such as FLOWTRAN and PROCESS, the items which move from one block to another in the model are known as streams. Each individual stream has a set of properties (composition, temperature, pressure) associated with it, which are typically modified as the stream passes through a block. In analogous fashion, the items which proceed from block to block in a GPSS model are known as transactions. Also in analogy with stream properties in a steady-state process simulator, GPSS transactions have associated with them various parameters (such as priority level or lifetime in the model) which can be modified by the passage of the transaction through certain blocks. In a GPSS model of a batch chemical plant, for example, transactions could represent batches of material proceeding through the process. Table 2 summarizes these similarities and terminology for the FLOWTRAN and GPSS simulators.

GPSS PROCESSOR

There are about thirty-five different blocks in GPSS, roughly the same number as in the FLOWTRAN system. A listing of these GPSS blocks is given in Table 3. It is common to construct block diagrams in the development of GPSS models. In contrast with FLOWTRAN where each block in such diagrams is represented more or less by a rectangle, each different functional block in a GPSS block diagram has its own distinctive shape (see Schriber [4]).

Some of the GPSS blocks listed in Table 3 are quite complicated and would typically be used only by more sophisticated analysts. There are others, however, which would be common to any GPSS model. Thus, GENERATE blocks are used to provide transactions to a model, much like a chemical engineer inputs feed streams to a FLOWTRAN model. Conversely, a transaction is removed from a GPSS model by a TERMINATE block.

There is a block named SPLIT in both FLOWTRAN and GPSS, but there is one fundamental difference between the two. In the FLOWTRAN system, the sum of each extensive property over all of the output streams from the block equals that property for the incoming stream. In discrete-event simulation with GPSS, however, the SPLIT block really performs a cloning operation. That is, one or more identical offspring transactions are created from the single parent transaction (which retains its existence) entering the block.

GPSS OUTPUT

As with the FLOWTRAN system which provides a summary table of the streams passing through the model and output results from each of the blocks in the model, GPSS automatically prints out a variety of output statistics at the conclusion of a simulation. These statistics pertain primarily to the various

facilities, queues, and storages in the model.

Thus, from an inspection of the facility output statistics from a GPSS simulation, an analyst might find that the average holding time per transaction for a given facility is considerably greater than the user-supplied average service time for that facility. In a chemical engineering application, for example, this could indicate that a reactor, after finishing processing of a batch (transaction), often cannot discharge the batch because of an unavailable downstream facility. The latter might correspond to a storage tank which is full or another processing unit (*e.g.*, still, centrifuge, dryer) which is engaged. The regular occurrence of such a situation would normally be accompanied by an average utilization (fraction of total time busy) approaching unity for the original upstream facility and would suggest the existence of some downstream bottleneck. The existence of similar bottleneck situations can also be deduced from the output statistics for GPSS storages. The productivity (number of batches produced) of the modelled process is, of course, related to the number of transactions passing through the GPSS model.

EXAMPLE APPLICATION

Let us consider a very simple application of GPSS to the modeling of a batch chemical process. This example is an adaptation of a problem (number 2.41.14) presented by Schriber [4]; the process flow diagram for this example is presented in Figure 1.

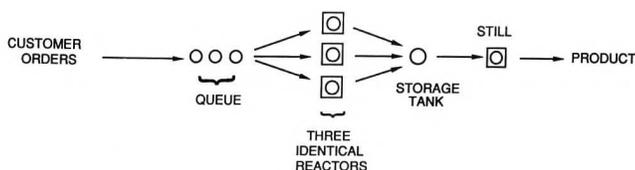


FIGURE 1. Sketch of batch process for example problem.

TABLE 3
Listing of GPSS Blocks

ADVANCE	LEAVE	RELEASE
ASSEMBLE	LINK	RETURN
ASSIGN	LOGIC	SAVEVALUE
BUFFER	LOOP	SEIZE
DEPART	MARK	SELECT
ENTER	MATCH	SPLIT
FAVAIL	MSAVEVALUE	TABULATE
FUNAVAIL	PREEMPT	TERMINATE
GATE	PRINT	TEST
GATHER	PRIORITY	TRANSFER
GENERATE	QUEUE	UNLINK

Thus, a small, single-product batch chemical plant has three identical reactors in parallel, followed by a single storage tank and a batch still. Customer orders (batches) to be filled (which begin with processing in the reactor) occur every 115 ± 30 minutes, uniformly distributed. The reaction time in a given reactor is 335 ± 60 minutes, and the distillation time in the still is 110 ± 25 minutes, both times uniformly distributed. The holding capacity of the storage tank is exactly one batch. Hence, the storage tank must be empty for a given reactor to discharge its batch; if not, the reactor cannot begin processing a new batch until the storage

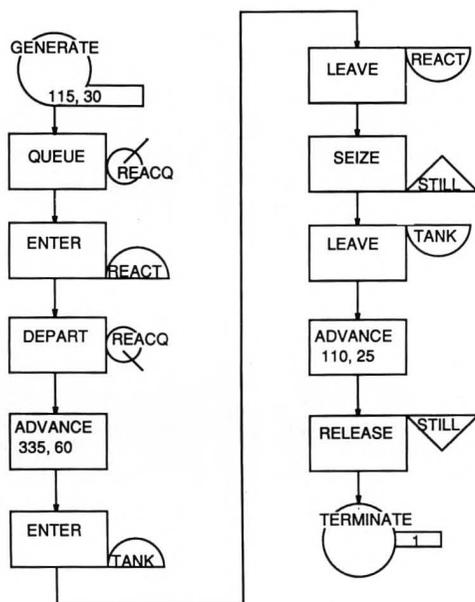


FIGURE 2. GPSS block diagram for example problem.

tank becomes empty. The simulation is to be run for 100 batches. The model should have the capability to collect waiting line statistics for the queue immediately upstream of the reactor.

The GPSS block diagram for this example model is shown in Figure 2. Note the distinctive shapes for each of the blocks employed. The first executable block is the GENERATE block, which creates transactions representing customer orders (batches). These transactions immediately queue up and attempt to capture an available reactor via the ENTER block. After capturing a reactor, a batch leaves the reactor queue through the DEPART REACQ block, and is processed in the ADVANCE 335,60 block. The batch must first be able to enter the storage tank (ENTER TANK block) before it releases its reactor in the LEAVE REACT block. The batch then attempts to capture the single still facility in the SEIZE STILL block. Having accomplished such, the batch leaves the storage tank, is processed in the still, releases the latter, and finally leaves the model through the TERMINATE block. Selected output statistics from this simulation are summarized in Table 4.

From Table 4, one sees that the batch still was in use 91.1% of the time, and the average holding (processing) time per batch was 108 minutes. The average contents in the queue upstream of the reactors was 0.44 batch, and the average waiting time for all batches, including ones which experienced no waiting, in this queue was 50.5 minutes. The three reactors were in use 95.2% of the time, and the average holding

time for a batch in a reactor was 329 minutes. Similarly the storage tank (with a capacity of one batch) was full 41.4% of the time, and the average holding time therein was 48.6 minutes. Although not presented in Table 4, the total simulation time, to completely process 100 batches, was 11,967 minutes.

One can easily explore proposed modifications to this process. Thus, one more reactor could be added in an effort to increase productivity. One might find as a result, however, a significant increase in the average reactor holding time beyond the nominal average reaction time of 335 minutes. In this case, one could explore increasing the intermediate storage capacity (TANK) and/or improving the downstream distillation operation.

SUMMARY

This article has attempted to serve as a brief introductory tutorial on discrete-event simulation, with emphasis on chemical engineering applications. For some simple batch process applications, only discrete simulation capability is required. More complex applications would require usage of a combined (discrete plus dynamic) simulation system, but knowledge of the essential features of discrete-event simulation remains useful background in such cases.

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TABLE 4
Selected GPSS Output from Example Simulation
of a Batch Chemical Process

Facility Statistics	
(batch still, STILL):	
Average utilization	0.911
Average holding time per batch, min	108
Queue Statistics	
(reactor queue, REACQ):	
Maximum contents	3
Average contents	0.44
Average waiting time (all batches), min	50.5
Storage Statistics:	
Reactors (REACT):	
Average utilization	0.952
Average holding time per batch, min	329
Storage Tank (TANK):	
Average utilization	0.414
Average holding time per batch, min	48.6

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Continued from page 97.

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EDUCATOR: Bailey

Continued from page 61.

pitchers helps my students know each other better," Jay notes. "It also helps me maintain a friendly and open relationship with my group that's important in our work together."

Research by Bailey and his students was recognized by the Curtis W. McGraw Research Award of the American Society of Engineering Education in 1983, by Jay's election to the National Academy of Engineering in 1986, and by the AIChE Professional Progress Award in 1987.

Bailey does have interests outside of the lab. Everyone who knows him remarks on his devotion to Sean, his 18-year-old son, who's now a freshman at the University of Colorado, Boulder. Jay's an avid amateur musician—the guitar is his instrument—and he loves active sports such as tennis, racquetball, and bicycling. He and Arnold also love to travel. Says Bailey, "We went to Malaysia and Indonesia last summer and just wandered around for four weeks for absolutely no professional reason whatsoever. It was wonderful."

Frances Arnold sums up Jay Bailey's influence on his profession in the following way, "Jay stands out in the field as a pioneer in new techniques in the 8,000-year-old discipline of biochemical engineering. You won't find many new products coming out of his lab, but you will find many new ideas." □

REQUEST FOR FALL ISSUE PAPERS

Each year *Chemical Engineering Education* publishes a special fall issue devoted to graduate education. This issue consists of 1) articles on graduate courses and research, written by professors at various universities, and 2) ads placed by chemical engineering departments describing their graduate programs. Anyone interested in contributing to the editorial content of the 1988 fall issue should write to the editor, indicating the subject of the contribution and the tentative date it can be submitted. Deadline is June 1st.

ChE book reviews

CATALYST SUPPORTS AND SUPPORTED CATALYSTS

by A. B. Stiles

Published by Butterworths,

80 Montvale Ave., Stoneham, MA 02180;

270 pages, \$54.95 (1987)

Reviewed by

John B. Butt

Northwestern University

The title of this book is interesting enough since most of those who deal in catalysts, particularly of supported metals, often have an uneasy feeling that the "support" (dispersive phase, contact phase, carrier, holder—*i.e.*, any number of names) has never been given enough attention. This book is a good start in trying to rectify this situation, and Dr. Stiles has collected a good group of reviews concerned with this. I particularly enjoyed the first five chapters, devoted to alumina, oxide supports other than alumina, activated carbon, and the associated information on their preparation and properties. The surface chemistry involved in catalyst-support interaction is probably not as extensively dealt with here as in other sources, but the overall treatment considered together with preparation techniques is quite a satisfying and useful one. Chapter 7, on organic polymers, also falls into this category.

The remainder of the book sort of strays from the announced title. Khoobiar has done a good job in Chapter 9 of "Spillover," and while significant opposing points are ignored, this is still a good review. Less satisfying are chapters on the "Commercial Application of Molecular Sieve Catalysts" and "Multifunctioning Catalysts." This is all old stuff, it seems rather qualitative, and it strays far from the announced title of the volume.

The book is not very well proofread, as illustrated on page fourteen as well as many other places in the text. This makes me wonder how good the numbers

in the many tables and illustrations are. The publisher should be more careful.

In spite of these reservations, I would say that this is a book worth having. Get it, and learn about supports. □

MASS TRANSFER WITH CHEMICAL REACTION IN MULTIPHASE SYSTEMS

Vol I: Two-Phase Systems (679 pages)

Vol II: Three-Phase Systems (399 pages)

Edited by E. Alper; Martinus Nijhoff Publishers, The Hague, Netherlands, 1983. \$140

Reviewed by

Arvind Varma

University of Notre Dame

This two-volume book constitutes the proceedings of a NATO Advanced Study Institute held in Turkey in 1981. It includes thirty papers, primarily of a review type, by twelve invited lecturers, and nine other contributions. Various topics in the area of mass transfer with chemical reaction in gas-liquid, liquid-liquid, and gas-liquid-solid systems are covered. These topics arise in the context of either separation processes or reaction engineering. Some of the papers treat the general problem of multiphase contacting and reactor design. Others deal with the modeling of specific types of contactors or reactors, and include methods for obtaining or estimating physicochemical and other data. Finally, some papers deal with a specific application, *e.g.*, facilitated transport, bioreactors, or reactors for coal conversion technology.

The invited lecturers are experts in the area (mostly from Europe) who have written other reviews as well. The material is somewhat dated by now, and other more recent reviews and books have appeared in print. Nevertheless, these volumes constitute a rich source of information for this relatively narrow but important area, and they should prove quite useful to those involved with multiphase chemically reacting systems.

The volumes were printed from camera-ready copy. For this type of production, the cost of the book is high. □

LEVELS OF SIMPLIFICATION

THE USE OF ASSUMPTIONS, RESTRICTIONS, AND CONSTRAINTS IN ENGINEERING ANALYSIS

STEPHEN WHITAKER
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The Navier-Stokes equations

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p + \rho \mathbf{g} + \mu \nabla^2 \mathbf{v} \quad (1)$$

are exceedingly difficult to solve in their general form. Thus there is great motivation to search for plausible simplifications. One of these simplifications takes the form: **convective inertial effects are negligible**. This allows us to extract the linear version of Eq. (1) which is given by

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} \right) = -\nabla p + \rho \mathbf{g} + \mu \nabla^2 \mathbf{v} \quad (2)$$

One could express this simplification as an equation, and there is some advantage in identifying it as a Level I *assumption* and expressing the idea as

$$\text{Level I: } \rho \mathbf{v} \cdot \nabla \mathbf{v} = 0 \quad (3)$$

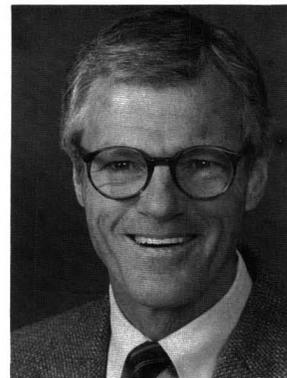
This type of statement indicates precisely what is being done in a mathematical sense, but it provides no basis for the action. For an engineer, it is more attractive to make a statement of the type: **convective inertial effects are small compared to viscous effects**. This leads to a Level II *restriction* of the form

$$\text{Level II: } \rho \mathbf{v} \cdot \nabla \mathbf{v} \ll \mu \nabla^2 \mathbf{v} \quad (4)$$

In writing inequalities of this type it is understood that the comparison is being made between the absolute values of the terms under consideration.

Equation (4) has very definite advantages over Eq. (3) since a comment concerning the physics of the process under consideration has been made. While Eq. (4) tells the reader what must occur in order that Eq. (2) be valid, it does not indicate, in terms of the parameters of the problem, when it will occur. In order to determine this, one must be able to estimate the magnitude of the terms in Eq. (4). The treatment here

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Steve Whitaker received his undergraduate degree in chemical engineering from the University of California at Berkeley and his PhD from the University of Delaware. He is the author of three books: *Introduction to Fluid Mechanics*, *Elementary Heat Transfer Analysis*, and *Fundamental Principles of Heat Transfer*, and he is the co-editor (with Alberto Cassano) of *Concepts and Design of Chemical Reactors*. His research deals with problems of multiphase transport phenomena, and he has taught at U.C. Davis, Northwestern University, and the University of Houston.

will be brief since the details are given elsewhere [1]. We begin by expressing the velocity in terms of its magnitude and a unit tangent vector

$$\mathbf{v} = v \boldsymbol{\lambda} \quad (5)$$

so that the convective inertial terms take the form

$$\mathbf{v} \cdot \nabla \mathbf{v} = v \boldsymbol{\lambda} \cdot \nabla \mathbf{v} \quad (6)$$

Since $\boldsymbol{\lambda}$ is a unit tangent vector to a streamline, we have

$$\mathbf{v} \cdot \nabla \mathbf{v} = v \frac{d\mathbf{v}}{ds} \quad (7)$$

where s is the arclength measured along a streamline. The derivative in Eq. (7) is estimated as [2, Sec. 2.9]

$$\frac{d\mathbf{v}}{ds} = \frac{\Delta \mathbf{v}}{L_p} \quad (8)$$

in which $\Delta \mathbf{v}$ represents the change in \mathbf{v} that occurs along a streamline over the inertial length L_p . Use of Eq. (8) in Eq. (7) leads to an estimate of the convective inertial terms given by

$$\rho \mathbf{v} \cdot \nabla \mathbf{v} = \mathbf{0} \left(\frac{\rho v \Delta v}{L \rho} \right) \quad (9)$$

It should be clear that a successful use of this estimate requires a reasonably good knowledge of the flow field. The viscous terms in Eq. (1) can be expressed as

$$\nabla^2 \mathbf{v} = \frac{\partial^2 \mathbf{v}}{\partial x^2} + \frac{\partial^2 \mathbf{v}}{\partial y^2} + \frac{\partial^2 \mathbf{v}}{\partial z^2} \quad (10)$$

and the associated order of magnitude is given by

$$\nabla^2 \mathbf{v} = \mathbf{0} \left(\frac{\Delta v|_x}{L_x^2}, \frac{\Delta v|_y}{L_y^2}, \frac{\Delta v|_z}{L_z^2} \right) \quad (11)$$

Here $\Delta v|_x$ represents the change of v that occurs in the x -direction over the distance L_x , and the meaning of $\Delta v|_y$ and $\Delta v|_z$ is analogous for the y and z -directions. We represent the largest of the three terms on the right hand side of Eq. (11) as $\Delta v/L_\mu^2$ and our estimate of the viscous terms takes the form

$$\nabla^2 \mathbf{v} = \mathbf{0} \left(\frac{\Delta v}{L_\mu^2} \right) \quad (12)$$

Here L_μ is referred to as the viscous length. For many cases the value of Δv in Eq. (12) is comparable to the value in Eq. (9) and this allows us to substitute Eqs. (9) and (12) into the inequality given by Eq. (4) in order to obtain

$$\frac{\rho v L_\mu^2}{\mu L} \ll 1 \quad (13)$$

Traditionally the Reynolds number is defined in terms of a length that is comparable to L_μ . Thus we use

$$\text{Re} = \frac{\rho v L}{\mu} \quad (14)$$

so that Eq. (13) takes the form

$$\text{Level III: } \text{Re} \left(\frac{L}{L_\mu} \right) \ll 1 \quad (15)$$

Obviously this Level III constraint has a great deal more utility than the Level I assumption given by Eq. (3) for it allows one to decide *a priori* whether the analysis is applicable to a particular problem. When simplifying the Navier-Stokes equations on the basis of Eq. (15), one must remember Birkhoff's warning concerning the plausible intuitive hypothesis that "small causes produce small effects" [3].

While the route to Eq. (15) is straightforward, it is important to keep in mind that it is a *scalar* constraint associated with the magnitude of *vectors* and it must be used with care. In addition, it is crucial to understand that Eq. (15) has nothing to do with di-

My thoughts concerning the various levels of simplification began to develop several years ago, and while the origin remains diffuse, I might place it in the early stages of an undergraduate heat transfer course.

mensional analysis, but is based entirely on the process of estimating the derivatives of the velocity that appear in Eq. (4). When the flow is turbulent, Eq. (1) must be time-averaged and Eq. (15) then applies to the time-averaged inertial and viscous terms. Estimating the Reynolds stress, $\overline{\rho \mathbf{v}' \cdot \nabla \mathbf{v}'}$, is more difficult than estimating $\rho \bar{\mathbf{v}} \cdot \nabla \bar{\mathbf{v}}$ since a knowledge of the magnitude of \mathbf{v}' and the turbulent length scale is required.

Often it is difficult to develop Level III constraints for complex problems (think about the "perfectly mixed" stirred tank reactor), and one must settle for the type of simplification indicated by Eq. (3) in order to meet deadlines and complete required course material. From my point of view, the clearly stated Level I assumption is an acceptable simplification for it tells you what is being done and it reminds you that Level II restrictions and Level III constraints are waiting to be found. In addition, it should remind you that the analysis has an unspecified range of validity and that experiments and further analysis are in order.

SCENE

My thoughts concerning the various levels of simplification began to develop several years ago, and while the origin remains diffuse, I might place it in the early stages of an undergraduate heat transfer course. Because the subject under consideration was heat conduction, I began a lecture with $\mathbf{v} = 0$ and quickly discarded radiant energy transport to arrive at

$$\rho c_p \frac{\partial T}{\partial t} = - \nabla \cdot \mathbf{q} \quad (16)$$

Since the assigned chapter and homework problems dealt with steady, one-dimensional heat conduction, we quickly moved to the following boundary value problem:

$$0 = \frac{d}{dx} \left(k \frac{dT}{dx} \right) \quad (17)$$

$$\text{B.C.1: } T = T_0, \quad x = 0 \quad (18)$$

$$\text{B.C.2: } T = T_1, \quad x = L \quad (19)$$

With the comment that "we can treat the thermal conductivity as constant," I was on the verge of present-

ing the classical result given by

$$T = T_0 + (T_1 - T_0) \left(\frac{x}{L} \right) \quad (20)$$

However, there was a flaw in my development. The title of the chapter under consideration indicated that we were to study the subject of steady, one-dimensional heat conduction, but it said nothing about the thermal conductivity being constant. One of the sages from the back row spotted the opening, and the traditional train of events was disrupted by the observation that "nothing is truly constant." Delighted to find that a portion of the back row was awake, I pursued Eq. (17) a bit further to arrive at

$$0 = \left(\frac{d^2 T}{dx^2} \right) + \frac{1}{k} \left(\frac{\partial k}{\partial T} \right) \left(\frac{dT}{dx} \right)^2 \quad (21)$$

Since nonlinearities can be eliminated with impunity in an undergraduate class, I was willing to assume that $\partial k / \partial T$ was zero and move on to the desired result given by Eq. (20). However, the back row was warming to the task, and one of its occupants persisted with, "But nothing is really zero is it?" A reviewer of this article suggested that I should have counter-attacked with the Kirchhoff transformation [4, Sec. 2.16] so that Eqs. (17) through (19) could be expressed as

$$0 = \frac{d^2 U}{dx^2} \quad (22)$$

$$\text{B.C. 1: } U = 0, \quad x = 0 \quad (23)$$

$$\text{B.C. 2: } U = U_1, \quad x = L \quad (24)$$

Here the transformed temperature is given by

$$U = \int_{\eta=T_0}^{\eta=T} \frac{k(\eta)}{k_0} d\eta \quad (25)$$

in which k_0 is the thermal conductivity at the temperature T_0 . This approach would have avoided making the assumption that k was constant, but it would have delayed our arrival at Eq. (20) and the physical insight that can be gained from that result. While Eqs. (22) through (25) can provide an "exact" solution to the problem posed by Eqs. (17) through (19), we usually seek "approximate" solutions and often the approximations that we make are forced on our students by the title of the chapter and the name of the textbook.

In engineering education there is a conspiracy among students and faculty to base their assumptions on the title of the chapter currently under consideration. It is a game that is played with well established rules and most often both parties are loath to depart

from the tradition. Students who are tempted to question the existence of the perfectly mixed stirred tank reactor are afraid that the instructor might plunge into a discourse on viscous dissipation, the Kolmogoroff length scale, and Damköhler numbers.* The terms of the treaty between students and faculty have been hammered out over the years, and by and large they work reasonably well. For example, can you imagine the difficulties of a study of fluid statics if it were preceded by the Level III constraints associated with

$$\rho \frac{\partial v}{\partial t} \ll \rho g, \quad \rho v \cdot \nabla v \ll \rho g, \quad \mu \nabla^2 v \ll \rho g \quad (26)$$

It is better to have a chapter entitled "Fluid Statics" so that the deck is cleared for an exploration of the pressure fields and forces associated with

$$0 = -\nabla p + \rho g \quad (27)$$

Still, the question was posed from the back row, and it deserved an answer. Furthermore, it seemed to me that Eqs. (22) through (25) were most certainly *not* the answer, for the question was, in reality: How can you justify the simplification of Eq. (21) to arrive at

$$0 = \frac{d^2 T}{dx^2} \quad (28)$$

Clearly the second term in Eq. (21) *cannot* be neglected on the basis of

$$\frac{1}{k} \left(\frac{\partial k}{\partial T} \right) \left(\frac{dT}{dx} \right)^2 \ll \frac{d^2 T}{dx^2} \quad (29)$$

but surely conditions must exist for which the variation of the thermal conductivity is "small enough" so that Eq. (21) could be replaced by Eq. (28). This raises the question of "small relative to what?" and the following problem was devised to explore this question and to help students understand what is meant by *quasi-steady*.

SAMPLE PROBLEM

We consider the boundary value problem given by

$$\rho c_p \left(\frac{\partial T}{\partial t} \right) = k \left(\frac{\partial^2 T}{\partial x^2} \right) + \left(\frac{\partial k}{\partial T} \right) \left(\frac{\partial T}{\partial x} \right)^2 \quad (30)$$

$$\text{I.C. } T = T_1, \quad t = 0 \quad (31)$$

$$\text{B.C. 1: } T = T_1 + (T_0 - T_1)g(t), \quad x = 0 \quad (32)$$

$$\text{B.C. 2: } T = T_1, \quad x = L \quad (33)$$

*It is bad enough that the material would not be available in the text, but what is worse is that it would not be covered on the final!

Here $g(t)$ is a function such that

$$g(t) = 0, \quad t = 0 \quad (34a)$$

$$g(t) = 1, \quad t = t^* \quad (34b)$$

The classic test piece in a study of separation of variables is associated with $t^* \rightarrow 0+$ and $(\partial k/\partial T) \rightarrow 0$, but in this case we should simply think of t^* as some characteristic time associated with the boundary condition at $x = 0$. Everyone knows that if t^* is "large enough" and if the variation of k with T is "small enough," the solution to this boundary value problem will yield the linear temperature profiles associated with Eq. (28). The Level I assumptions related to these conditions are

$$\text{Level Ia:} \quad \left(\frac{\partial T}{\partial t}\right) = 0 \quad (35a)$$

$$\text{Level Ib:} \quad \left(\frac{\partial k}{\partial T}\right) = 0 \quad (35b)$$

and one should be careful to identify the first of these as the *quasi-steady assumption*.

Our objective at this point is to develop the Level II and Level III restrictions and constraints that are associated with Eqs. (35a,b). Thus we seek to determine what is "large enough" and what is "small enough." If you have an idea that a satisfactory solution to Eqs. (30) through (34) might be given by*

$$T = T_1 + (T_0 - T_1)g(t) \left[1 - \left(\frac{x}{L}\right)\right] \quad (36)$$

the possibility can be explored by decomposing the temperature into the result represented by Eq. (36) and whatever else is left. One method of doing this is to arrange Eq. (30) as

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha} \left(\frac{\partial T}{\partial t}\right) - \frac{1}{k} \left(\frac{\partial k}{\partial T}\right) \left(\frac{\partial T}{\partial x}\right)^2 \quad (37)$$

and to form the indefinite integral in order to obtain

$$\frac{\partial T}{\partial x} = \frac{\partial T}{\partial x} \Big|_{x=0} + \int_{\xi=0}^{\xi=x} \left[\frac{1}{\alpha} \left(\frac{\partial T}{\partial t}\right) - \frac{1}{k} \left(\frac{\partial k}{\partial T}\right) \left(\frac{\partial T}{\partial \xi}\right)^2 \right] d\xi \quad (38)$$

Use of the definition

$$\Omega = \frac{1}{\alpha} \left(\frac{\partial T}{\partial t}\right) - \frac{1}{k} \left(\frac{\partial k}{\partial T}\right) \left(\frac{\partial T}{\partial \xi}\right)^2 \quad (39)$$

*This solution is obtained by using Eqs. (35a,b) to reduce Eq. (30) to the form given by Eq. (28). When Eq. (28) is solved subject to Eqs. (32) and (33), the solution given by Eq. (36) results.

along with a second integration leads to

$$T(x,t) = T \Big|_{x=0} + x \left(\frac{\partial T}{\partial x}\right)_{x=0} + \int_{\eta=0}^{\eta=x} \int_{\xi=0}^{\xi=\eta} \Omega d\xi d\eta \quad (40)$$

The boundary conditions given by Eqs. (32) and (33) can be used to evaluate the two constants in Eq. (40) and the general solution is given by

$$T(x,t) = T_1 + (T_0 - T_1)g(t) \left[1 - \left(\frac{x}{L}\right)\right] + \int_{\eta=0}^{\eta=x} \int_{\xi=0}^{\xi=\eta} \Omega d\xi d\eta - \left(\frac{x}{L}\right) \int_{\eta=0}^{\eta=L} \int_{\xi=0}^{\xi=\eta} \Omega d\xi d\eta \quad (41)$$

One should keep in mind that this is an exact representation for the temperature, but it is only useful when the integrals are negligible. The integrals in Eq. (41) can be estimated as

$$\int_{\eta=0}^{\eta=x} \int_{\xi=0}^{\xi=\eta} \Omega d\xi d\eta = \mathbf{0}(\Omega) \frac{x^2}{2} \quad (42a)$$

$$\int_{\eta=0}^{\eta=L} \int_{\xi=0}^{\xi=\eta} \Omega d\xi d\eta = \mathbf{0}(\Omega) \frac{L^2}{2} \quad (42b)$$

and use of these estimates in Eq. (41) leads to

$$T(x,t) = T_1 + (T_0 - T_1)g(t) \left[1 - \left(\frac{x}{L}\right)\right] + \frac{xL}{2} \left[1 - \left(\frac{x}{L}\right)\right] \mathbf{0}(\Omega) \quad (43)$$

We are now in a position to state that the solution for $T(x,t)$ is given by

$$T(x,t) = T_1 + (T_0 - T_1)g(t) \left[1 - \left(\frac{x}{L}\right)\right] \quad (44)$$

provided that the following inequality is satisfied

$$(T_0 - T_1)g(t) \gg \frac{L^2}{2} \mathbf{0}(\Omega) \quad (45)$$

This result allows us to replace the Level I assumptions given by Eqs. (35a,b) with the following Level II restrictions

$$\text{Level IIa: } (T_0 - T_1)g(t) \gg 0 \left[\frac{L^2}{\alpha} \left(\frac{\partial T}{\partial t} \right) \right] \quad (46a)$$

$$\text{Level IIb: } (T_0 - T_1)g(t) \gg 0 \left[\frac{L^2}{k} \left(\frac{\partial k}{\partial T} \right) \left(\frac{\partial T}{\partial x} \right)^2 \right] \quad (46b)$$

Here we are beginning to see how "long" one must wait before the solution becomes quasi-steady, and how "small" the variation of the thermal conductivity must be in order that the last term in Eq. (30) can be discarded.

In order to proceed further, we must be willing to estimate the derivatives that appear in Eqs. (46a,b), and in this development we will be satisfied with the rather crude estimates given by [2, Sec. 2.9].

$$\frac{\partial T}{\partial t} = 0 \left(\frac{T|_{x=0} - T|_{x=L}}{t} \right) = 0 \left(\frac{(T_0 - T_1)g(t)}{t} \right), \quad t \geq t^* \quad (47a)$$

$$\frac{\partial T}{\partial x} = 0 \left(\frac{T|_{x=0} - T|_{x=L}}{L} \right) = 0 \left(\frac{(T_0 - T_1)g(t)}{L} \right) \quad (47b)$$

This aspect of the problem could be considered more carefully by introducing the thermal boundary layer thickness; however, we are interested in knowing under what circumstances Eq. (44) is valid and the estimates given by Eqs. (47a,b) are consistent with that objective. When Eqs. (47a,b) are used in Eqs. (46a,b) we obtain the Level III constraints given by

$$\text{Level IIIa: } \frac{\alpha t}{L^2} \gg 1, \quad t \geq t^* \quad (48a)$$

$$\text{Level IIIb: } \frac{1}{k} \left(\frac{\partial k}{\partial T} \right) (T_0 - T_1)g(t) \ll 1 \quad (48b)$$

The first of these clearly indicates that the process will be quasi-steady when t^* is large compared to L^2/α and an exact solution of the boundary value problem will indicate that this is a conservative constraint. Since $g(t)$ has an upperbound of one, Eq. (48b) can be replaced by

$$\text{Level IIIb: } \frac{1}{k} \left(\frac{\partial k}{\partial T} \right) (T_0 - T_1) \ll 1 \quad (48c)$$

While the results given by Eqs. (48a,b,c) are something that "everyone knows," not everyone knows how to arrive at these constraints without solving the full boundary value problem and exploring special cases. In addition, the identification of various levels of simplification is an important concept to bring to the attention of students, for it allows us to move quickly to certain simple engineering solutions while

reminding us of our obligation to be more thorough when time permits or necessity demands. Following up on our obligations is sometimes easy to do. For example, in the typical heat transfer course transient processes are always studied, and when exact solutions are available it is easy to remind students of prior constraints that were developed on the basis of order of magnitude analysis. In the study of transient heat conduction in a flat plate one finds that Eq. (48a) can be replaced with $\alpha t/L^2 \geq 1$, thus providing a clear indication that the original estimation was overly severe. To support the result given by Eq. (48c), a homework problem associated with Eqs. (22) through (25) does rather nicely. The process of following order of magnitude estimates with exact solutions is an attractive method of encouraging students to develop their own assumptions, restrictions and constraints. As they gain confidence in this process, chapter titles become guidelines for the voyage rather than constraints for the next exam.

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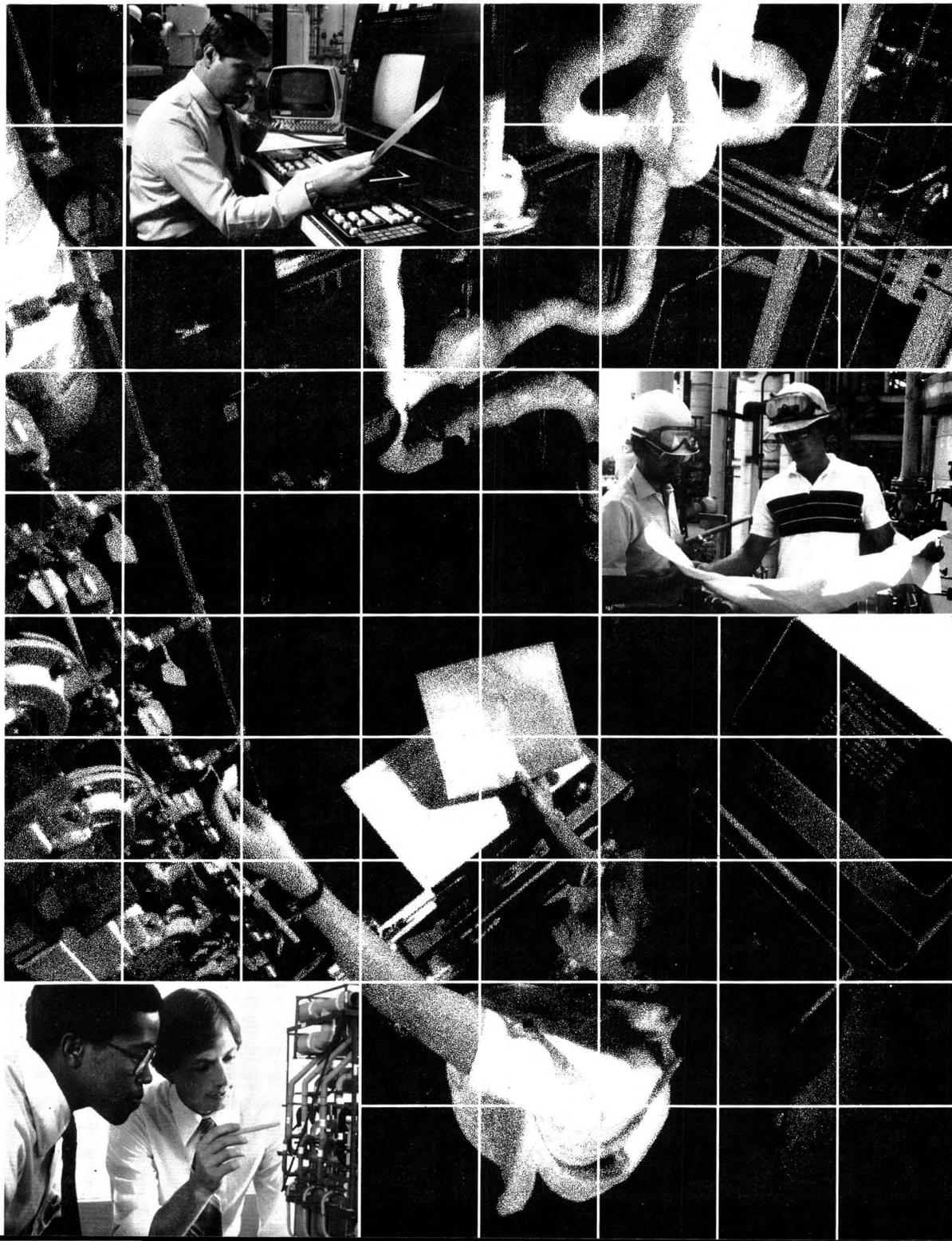
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