

CHE

chemical engineering education

VOLUME XIX

NUMBER 1

WINTER 1985



CHEMICAL ENGINEERING DIVISION OF AMERICAN SOCIETY FOR ENGINEERING EDUCATION

KLAUS TIMMERHAUS

*of the
University of Colorado*



Encouraging Creativity in Students
PRAUSNITZ

Cheating—An Ounce of Prevention
FELDER

Extended Form of the Gibbs Phase Rule
RAO

A Simple Geometrical Derivation of the Spatial Averaging Theorem
WHITAKER

Sequential Design Laboratory Experiment for Separating Particles by
Fluidization Principles
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Simulation of Simple Controlled Processes with Dead-Time
WATSON, WONG, DESHPANDE

Resource-Based Approach to ChE Education
NEWELL, LEE, LEUNG

Computer-Assisted Laboratory Stations
SNYDER, HANYAK

**AND CHE AT THE
UNIVERSITY OF MARYLAND**

U.S. Postal Service STATEMENT OF OWNERSHIP, MANAGEMENT AND CIRCULATION <i>Required by 39 U.S.C. 3685</i>		
1A. TITLE OF PUBLICATION CHEMICAL ENGINEERING EDUCATION	1B. PUBLICATION NO. 1 0 1 9 0 0	2. DATE OF FILING 9/5/84
3. FREQUENCY OF ISSUE Quarterly	3A. NO. OF ISSUES PUBLISHED ANNUALLY 4	3B. ANNUAL SUBSCRIPTION PRICE See Attached Rates
4. COMPLETE MAILING ADDRESS OF KNOWN OFFICE OF PUBLICATION (<i>Street, City, County, State and ZIP Code</i>) (<i>Not printers</i>) CHEMICAL ENGINEERING EDUCATION, Room 317, Chemical Engineering Department University of Florida, Gainesville, FL 32611		
5. COMPLETE MAILING ADDRESS OF THE HEADQUARTERS OF GENERAL BUSINESS OFFICES OF THE PUBLISHER (<i>Not printer</i>) Chemical Engineering Division, American Society for Engineering Education, 11 DuPont Circle, Washington, DC 20030		
6. FULL NAMES AND COMPLETE MAILING ADDRESS OF PUBLISHER, EDITOR, AND MANAGING EDITOR (<i>This item MUST NOT be blank</i>)		
PUBLISHER (<i>Name and Complete Mailing Address</i>) ASEE - Chemical Engineering Division, 11 DuPont Circle, Washington, DC 20030		
EDITOR (<i>Name and Complete Mailing Address</i>) Ray W. Fahien, Chemical Engineering Department, Room 319, University of Florida, Gainesville, FL 32611		
MANAGING EDITOR (<i>Name and Complete Mailing Address</i>) Carole Yocum, Chemical Engineering Department, Room 317, University of Florida, Gainesville, FL 32611		
7. OWNER (<i>If owned by a corporation, its name and address must be stated and also immediately thereunder the names and addresses of stockholders owning or holding 1 percent or more of total amount of stock. If not owned by a corporation, the names and addresses of the individual owners must be given. If owned by a partnership or other unincorporated firm, its name and address, as well as that of each individual must be given. If the publication is published by a nonprofit organization, its name and address must be stated.</i>) (<i>Item must be completed.</i>)		
FULL NAME		COMPLETE MAILING ADDRESS
Official publication of Publisher as listed above		Any mail addressed to owner should go to Editor as listed above
8. KNOWN BONDHOLDERS, MORTGAGEES, AND OTHER SECURITY HOLDERS OWNING OR HOLDING 1 PERCENT OR MORE OF TOTAL AMOUNT OF BONDS, MORTGAGES OR OTHER SECURITIES (<i>If there are none, so state</i>)		
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<input checked="" type="checkbox"/> (1) HAS NOT CHANGED DURING PRECEDING 12 MONTHS <input type="checkbox"/> (2) HAS CHANGED DURING PRECEDING 12 MONTHS (<i>If changed, publisher must submit explanation of change with this statement.</i>)		
10. EXTENT AND NATURE OF CIRCULATION	AVERAGE NO. COPIES EACH ISSUE DURING PRECEDING 12 MONTHS	ACTUAL NO. COPIES OF SINGLE ISSUE PUBLISHED NEAREST TO FILING DATE
A. TOTAL NO. COPIES (<i>Net Press Run</i>)	2410	1960
B. PAID CIRCULATION		
1. Sales through dealers and carriers, street vendors and counter sales	-0-	-0-
2. Mail Subscription	2178	1796
C. TOTAL PAID CIRCULATION (<i>Sum of 10B1 and 10B2</i>)	2178	1796
D. FREE DISTRIBUTION BY MAIL, CARRIER OR OTHER MEANS SAMPLES, COMPLIMENTARY, AND OTHER FREE COPIES	93	83
E. TOTAL DISTRIBUTION (<i>Sum of C and D</i>)	2271	1879
F. COPIES NOT DISTRIBUTED		
1. Office use, left over, unaccounted, spoiled after printing	139	81
2. Return from News Agents	-0-	-0-
G. TOTAL (<i>Sum of E, F1 and 2- should equal net press run shown in A</i>)	2410	1960
11. I certify that the statements made by me above are correct and complete	SIGNATURE AND TITLE OF EDITOR, PUBLISHER, BUSINESS MANAGER, OR OWNER Editor	

EDITORIAL AND BUSINESS ADDRESS

Department of Chemical Engineering
University of Florida
Gainesville, Florida 32611

Editor: *Ray Fahien* (904) 392-0857

Consulting Editor: *Mack Tyner*

Managing Editor:
Carole C. Yocum (904) 392-0861

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CHEMICAL ENGINEERING EDUCATION is published quarterly by Chemical Engineering Division, American Society for Engineering Education. The publication is edited at the Chemical Engineering Department, University of Florida. Second-class postage is paid at Gainesville, Florida, and at DeLeon Springs, Florida. Correspondence regarding editorial matter, circulation and changes of address should be addressed to the Editor at Gainesville, Florida 32611. Advertising rates and information are available from the advertising representatives. Plates and other advertising material may be sent directly to the printer: E. O. Painter Printing Co., P. O. Box 877, DeLeon Springs, Florida 32028. Subscription rate U.S., Canada, and Mexico is \$20 per year, \$15 per year mailed to members of AIChE and of the ChE Division of ASEE. Bulk subscription rates to ChE faculty on request. Write for prices on individual back copies. Copyright © 1985 Chemical Engineering Division of American Society for Engineering Education. The statements and opinions expressed in this periodical are those of the writers and not necessarily those of the ChE Division of the ASEE which body assumes no responsibility for them. Defective copies replaced if notified within 120 days.

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

Klaus D. Timmerhaus of the University of Colorado

MARTIN S. BARBER
University of Colorado
Boulder, CO 80309

THERE ARE SEVERAL Klaus Timmerhaus's. There is a patient, careful teacher much appreciated by his students. There is a researcher with varied, broadscale interests. There is a demanding, perfectionist administrator, somewhat abrasive toward his superiors but not towards his subordinates. There is an active officer and member of eleven professional and research societies known to a host of friends for both technical papers and analytic, what-is-ethically-required policy analyses. And there is a paradox: in most of these capacities Klaus appears to work full time!

In fact, Klaus's Spartan, efficient work schedule would be well worth study by anyone interested in maximum levels of human accomplishment. One item after another moves across his desk; written, edited, or marked for action with lead pencil in a minute script that can put more than 300 words on a page. Each item gets an allotted amount of time; drafting is so precise that revision is seldom necessary.

His day at the desk is unbroken except for three noon hours per week spent in equally efficient exercise: he does not jog; he runs. A brown-bag lunch at the desk later is not allowed to interrupt output. An additional pile of work goes home with him after a ten-hour day.

Klaus's research interests have concerned ultra-high pressures, cryogenics, or both. Since the energy crunch of 1973, they have also turned toward energy economics and conservation. His recent book, *Energy Conservation in Arid Lands*, has drawn praise not only from colleagues, but also from some American Indians who inhabit arid lands.

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Said CU's former dean of engineering Max S. Peters, himself a widely known and honored chemical engineer: "I have known Klaus since 1951 and have worked closely with him for more than the past twenty years, and I can honestly say that he is the most conscientious and dedicated person I have ever known. He truly is a great chemical engineer in every aspect of our field in addition to being a true friend and a wonderful person."

Klaus graduated from high school in Palatine, Ill., winning three letters in track and serving as a student editor and student body president. As a chemical engineering student at the University of Illinois he worked in a hospital and became an ambulance driver and one of the few chemical engineers who has ever delivered a baby.

During World War II he served as a radar instructor and coached championship track teams. Back at the university after the war, he played hockey and competed in four track events. A neck fracture sustained in an auto accident in January of his senior year slowed him only briefly; at the end of April he was back in competition with a cast on his neck and his arm in a sling, winning the first race he entered. Later that spring he won the National AAU Junior Championship in the 1500 meter event.

He still runs in senior events, recently taking up speed walking at the urging of Max Peters and taking first in his age category in his first 5-k race. He has served for many years as an official in high school and college track events.

Klaus earned his degrees at Illinois, participating with his graduate adviser, H. G. Drickamer, and others on several papers—on high pressure science, appropriately enough. He joined the University of Colorado faculty in 1953 after nearly two years of employment by Cal Research (Standard Oil of California) in Richmond, California, as a project design engineer. He became associate dean of engineering in 1963. The College of Engineering and Applied Science of the University of Colorado is a three-campus organization, and Klaus's responsibilities extend to all three campuses. Primarily, they concern graduate and research activities, but in practice they involve most aspects of engineering education, from undergraduate accreditation to faculty evaluation.

Klaus is also director of the three-campus Engineering Research Center, whose grants in force have increased from less than \$200,000 in 1953 to more than \$9 million in 1984, while graduate enrollment has grown from 90 to 550. These research gains have involved extensive work with faculty members to develop research ideas and locate suitable funding sources. Klaus scrutinizes each research proposal that leaves the college, working with faculty members to increase clarity and ensure that each request tallies with the needs of the funding agency to which it is addressed. Not all possible projects are solicited: with the rare exception of projects serving Colorado groups, no research project is accepted unless it has clear-cut educational value.

Klaus's research interests have generally concerned ultra-high pressures, cryogenics, or both. Since the energy crunch of 1973, they have also turned toward energy economics and conservation. His recent book, *Energy Conservation in Arid Lands*, has drawn praise not only from colleagues, but also from some American Indians who inhabit arid lands.

As a cryogenic consultant, Klaus has been involved with such projects as a major natural gas liquefaction plant in the Mideast and the nation's largest superconducting particle accelerator. Klaus sees good opportunities and a new future ahead for the chemical industries, even though he foresees that oil producing nations will see that it is not in their best interests to ship raw materials and

will build the chemical plants and oil refineries that will permit them to export more valuable finished products. "Chemical engineering needs to diversify into many different industries that can benefit from the specialized training given to its graduates," he said. "For example, biotechnology holds great promise. It can produce chemicals, pharmaceuticals, coatings, paints, and plastics from renewable natural resources. These industries build on principles of mass and energy balance of chemicals and materials which are the heart of chemical engineering."

He recommends that some chemical engineers look for careers in the solid state area. "Electrical

In fact, Klaus's Spartan, efficient work schedule would be well worth study by anyone interested in maximum levels of human accomplishment. One item after another moves across his desk . . .

engineers have a big problem in obtaining ultra-pure silicon wafers. This is a chemical engineering problem and not an electrical engineering problem and should be taught by chemical engineers." Similarly, he looks for chemical engineers to show the way in developing new separation techniques, augmenting dwindling energy reserves with unique renewable energy processes, perfecting new conservation approaches, developing greater reliability and safety in consumer products, and initiating entirely new manufacturing processes in outer space. He has been a proponent in AIChE of examining this situation and is active in the New Technology Committee that has been set up by AIChE to consider future directions and opportunities for chemical engineering. All in all, he sees myriad new areas for chemical engineers.

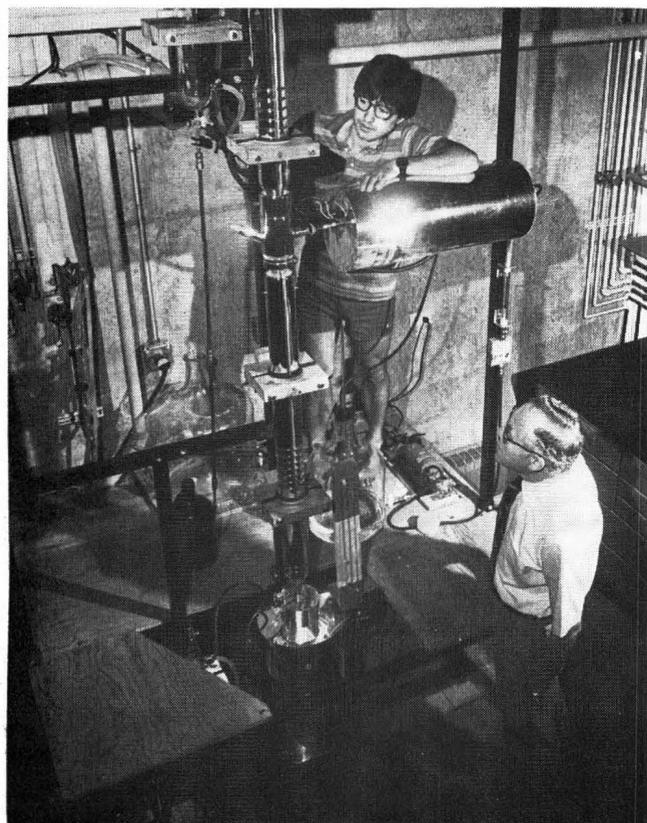
Among Klaus's current research interests is the thermal conductivity-convection relationship in porous insulation materials. Recent consulting experience has led him to believe that current values for convection in these materials are too conservative, and he is planning checks on the data. He is also studying the effect of a number of variables on the distillation efficiency of simple hydrocarbon mixtures.

As an educator, he also has some concerns about future trends in university research: "We should keep in mind that the university is not just a research facility: teaching is still our main function and teaching is getting short shrift in many

As an educator, he also has some concerns about future trends in university research: "We should keep in mind that the university is not just a research facility: teaching is still our main function and teaching is getting short shrift in many instances. We must keep a careful balance and not push the pendulum too far.

instances. We must keep a careful balance and not push the pendulum too far." He believes that all faculty should be involved in research to help them in their teaching activities. He stresses, however, that we need to be careful to maintain a balanced perspective.

"The better students will be successful in spite of this trend; however, students who are less



Dean Timmerhaus and graduate student Hasan Dindi check a fractional distillation column in which the separation of simple hydrocarbons is being studied.

academically inclined and/or who are not interested in advanced degrees will be the mainstay of industry. We must keep them capable or we will all lose out."

Some implications of the information revolution also concern him. "There exists among engineers the recognition that more and more our improving communications systems are transferring more and more data, so that we are getting clogged

with information. We need to devise ways of sifting and picking out what is pertinent.

"Computers can help with this problem, but we need to avoid excessive reliance upon computers. A computer search is no better than the key-wording that it is based upon. We need to remain aware that what comes out is no better than what is put in. Computer simulation also has pitfalls. Flawed models can lead to accidents and catastrophes. Simulations need to be checked against results.

"I believe that computers must be brought into education and integrated into it. We also need to integrate in other new concepts. We must take a new approach to teaching safety principles, and also economics, as an integral part of chemical engineering. Today, no part of a process or product can be allowed to remain unsafe. There will be serious and unpleasant consequences if we do not face up to the requirements of safety. If we are using a process that is unsafe because pressure is too high, or flow is too great, or the temperature is too high, we may need to change the process so that it is safe.

"We are likely to trip up on what we cut out for economy reasons. Safety relief valves should be placed in the right places and in the right numbers when the plant is designed—not after it is built.

"Therefore, in our design courses we must teach chemical engineering, safety, and economics all in the same problems. Safety and economics are subjects that we educators have wanted to leave to industry, while they wanted to leave them to us. Education is where they belong; if they are learned then they will be more likely to stick."

Klaus himself is a member of the Advisory Board for the National Institute of Occupational Safety and Health (NIOSH) and is incorporating what he recommends into a new book on cryogenic processes that he is preparing with Thomas M. Flynn.

Among Klaus's other achievements has been preparing a proposal for and securing an NSF matching grant worth \$1.325 million (in 1966 dollars) for construction of CU's Engineering Center. As chairman, cochairman, or the like he

has been involved with securing other grants with a value of about \$6 million. He has also managed from time to time to serve as college safety officer, acting chairman of the aerospace department, and on more than 70 campus committee assignments.

His output of professional publications is somewhat awesome: He has edited 25 volumes of *Advances in Cryogenic Engineering*; 17 in the *International Cryogenics Monograph* series; 4 of *Low Temperature Physics*, and 2 of *The Proceedings of the AIRAPT International High Pressure Conference*. He is coauthor with Max Peters of two editions of the very popular *Plant Design and Economics for Chemical Engineers*.

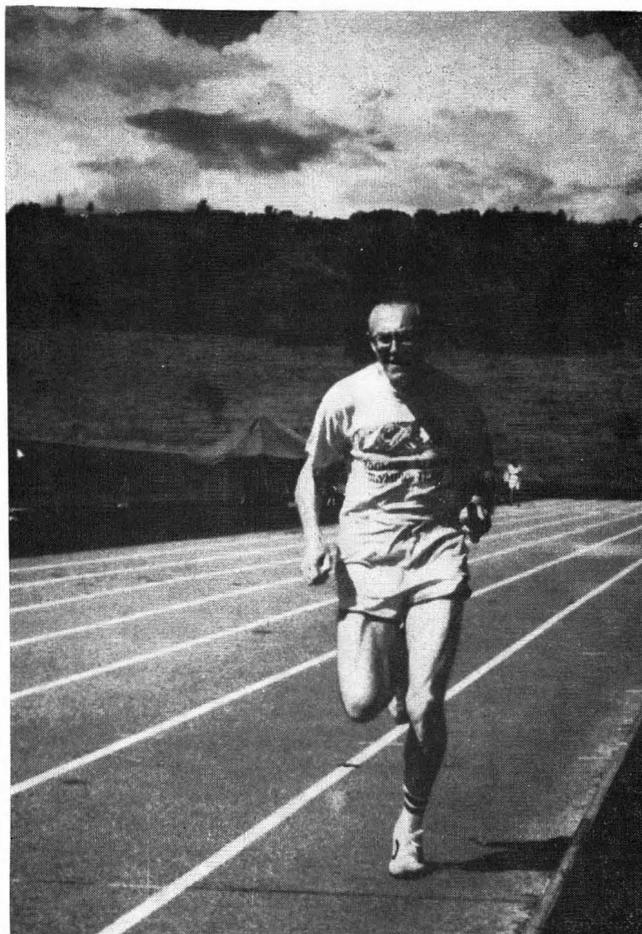
He has also published more than 70 technical publications in refereed journals, presented more than 70 technical presentations at national professional society meetings and has given more than 100 presentations to national, regional, and university audiences.

The variety of his service has nearly been matched by the varieties of honors it has brought him; if he doesn't hold the record for awards to a chemical engineering professor he must be a top contender.

He was one of three American academicians appointed as the first Foreign Corresponding Member of the Verein Deutscher Ingenieure, has been elected as a fellow of the American Society for the Advancement of Science and AIChE, and a diplomate of the American Academy of Environmental Engineering. He is an elected member of the National Academy of Engineering and the Austrian Academy of Science. The 1981 Cryogenic Engineering Conference was dedicated to him in recognition of his 25 years of service to cryogenics.

Among a few of his major awards are the second Samuel C. Collins Award of the Cryogenic conference, presented in 1967; the George Westinghouse award (for outstanding teaching) presented at the Diamond Jubilee meeting of the American Society for Engineering Education in 1968; the Alpha Chi Sigma Award of AIChE, which has also awarded him its Founders Award and named him in 1983 as an Eminent Chemical Engineer. His most recent award (at press time) was the Distinguished Public Service Award of the National Science Foundation.

His awards from the University of Colorado include the Distinguished Engineering Alumnus Award, even though he is not an alumnus of the



A familiar figure on the track.

University of Colorado, the Robert L. Stearns Award for distinguished faculty service, and numerous student-recognition awards for his teaching and service.

Among the numerous professional society offices he has filled have been the presidency of the AIChE, membership on the National Science Foundation Advisory Council, and a regional directorship of Sigma Xi. He has served for many years on the U. S. National Committee for the International Institute of Refrigeration, and is its 1982-85 chairman. He is a vice president of the Scientific Council of the International Institute of Refrigeration and a former president of the Southwestern and Rocky Mountain Division of the AAAS.

Klaus's wife Jean keeps their life organized while he works, and accompanies him upon some of his constant professional travels. Hobbies the couple share include hiking and fishing in Colorado's mountains. □

CHE AT THE**UNIVERSITY OF MARYLAND**

T. W. CADMAN AND R. B. BECKMANN

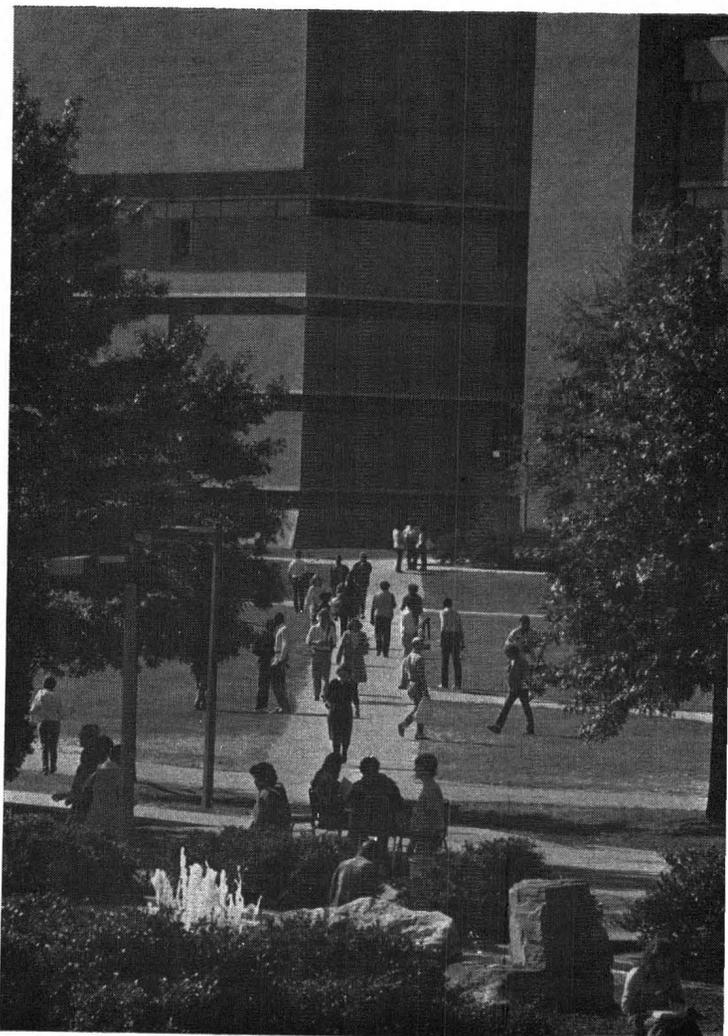
*University of Maryland
College Park, MD 20742*

ENGINEERING AT MARYLAND dates back to course instruction in surveying and construction given in 1859 within the Maryland Agricultural College. From this historical perspective, chemical engineering is a relative newcomer to Maryland. Formal degree programs in mechanical (1894), civil (1900), and electrical (1908) predate chemical engineering, as do a series of reorganizations which led to the University of Maryland system and the College of Engineering as we know them today.

Chemical engineering at the University of Maryland began in 1937 when, under founder and first chairman Wilbert J. Huff, the four year program leading to the baccalaureate degree (BS) was introduced. Graduate programs at the MS and the PhD levels were initiated in 1938 and 1939 respectively, marking the first of the graduate degree programs within the College of Engineering at the University of Maryland.

Today chemical engineering is one of eight programs within the College of Engineering and one of three programs administered through the Department of Chemical and Nuclear Engineering. Approximately 80 BS, 12 MS, and 3 PhD candidates graduate from the chemical engineering program per year at the present time.

The University of Maryland is a comprehensive public system of five campuses: The University of Maryland at Baltimore (UMAB), the University of Maryland Baltimore County (UMBC), the University of Maryland College Park (UMCP), the University of Maryland Eastern Shore (UMES) and the University of Maryland University College (UMUC). The College of Engineering is one of 16 colleges and professional schools



in the university.

Prior to 1984-'85, the degree granting activities of the college were only at the College Park campus. Effective this fall, undergraduate degree programs in chemical engineering and mechanical engineering are also offered at UMBC, and plans have been approved which permit the initiation of graduate engineering degree programs. The programs at both UMCP and UMBC are coordinated by the Dean of the College of Engineer-

The present is a time of rapid progressive change at the University of Maryland. . . . One of the newest additions to the College of Engineering is the Engineering Research Center, established to promote industry-university interactions.

ing, George Dieter, residing at UMCP and Associate Dean Albert Gomezplata, residing at UMBC. The college offers accredited four year BS degree programs in designated fields of engineering, including chemical engineering, as well as a co-op plan of study and a BS in engineering with interdisciplinary areas of specialization.

LOCATION OF CHE AND FACILITIES

As noted above, chemical engineering is offered as an undergraduate degree program at both UMCP and UMBC. Graduate degrees are offered only at UMCP. College Park is home for the majority of the program's current faculty and activities. The campus is located in an urban setting, triangulated by Annapolis (20 miles to the east), Baltimore City (25 miles to the northeast), and the White House in Washington, D.C. (10 miles to the southwest). The chemical engineering, nuclear engineering, and engineering materials programs form the Department of Chemical and Nuclear Engineering. Collectively they occupy the chemical engineering building on the northern side of the campus adjacent to chemistry, mathematics, physics and the other departments of engineering. UMBC is located in Catonsville, just southwest of the City of Baltimore. The campus features modern architecture in a rural setting.

Research facilities at College Park feature biochemical engineering laboratories, the laboratory for aerosol mechanics, the laboratory for process analysis and simulation, polymer characterization and process laboratories and multiphase flow laboratories. The nuclear engineering program provides access to a Co-60 source, a LINAC, a 250 kilowatt pool reactor and, most recently, a 300 psig, 1/3 scale thermal-hydraulic simulation loop of a nuclear reactor system. Facilities in X-ray analysis, crystal growth and materials testing are available in the engineering materials program.

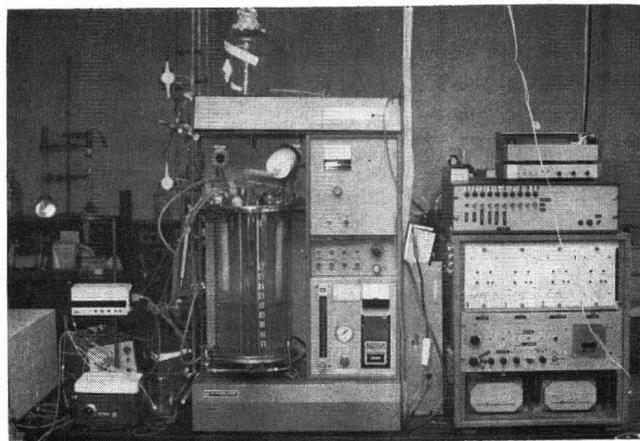
NEW ACTIVITIES AT MARYLAND

The present is a time of rapid progressive change at the University of Maryland. Under the

dynamic leadership of President John Toll and UMCP Chancellor John B. Slaughter, with Dean George Dieter at the helm for the College of Engineering, the change has been particularly significant for the college. Resources have been provided for a major enhancement of engineering at Maryland. An undergraduate enrollment limitation plan has been implemented on the College Park Campus and, as noted earlier, engineering programs have been initiated at UMBC.

One of the newest additions to the College of Engineering is the Engineering Research Center (ERC), established to promote industry-university interactions. Under Director Herb Rabin, an engineering extension service has been initiated to serve throughout the state, areas of technology have been identified for initial emphasis by the center, and plans are being drawn for an incubator program directed to the fostering of entrepreneurial activity.

The impact on chemical engineering has been quite significant. A particular emphasis has been placed on the enhancement of our biochemical engineering research program. An important as-



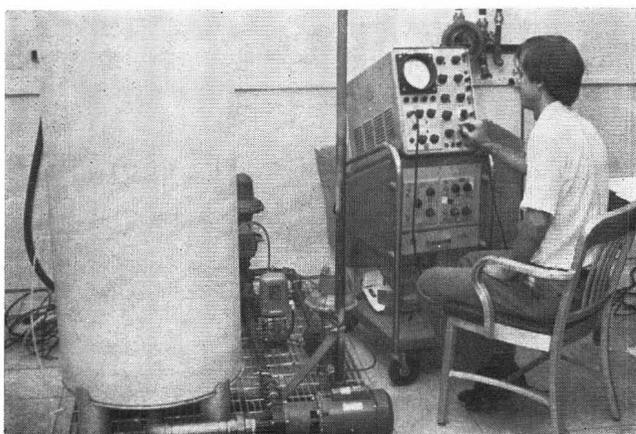
The 14 liter computer controlled fermentor in the Biochemical Engineering Laboratory.

pect of the enhancement is a co-operative undertaking with the ERC which has identified biochemical engineering as one of the areas for initial emphasis by the center. Under the auspices of the ERC, a 500 liter fermentor system together with auxiliary analysis and separations equipment has been ordered, with delivery expected in March 1985. In addition, the ERC staff position of Manager, Chemical Engineering Programs, has been established to coordinate collaborative research activities between the faculty and local

industry. As of this writing, candidates are being interviewed for this position. Initial emphasis is to be given to biochemical engineering and the closely related areas of process simulation and control research within chemical engineering.

The equipment acquisitions of the ERC in biochemical engineering are viewed as the first step in the development of a pilot plant facility for scale-up and developmental research on bioprocesses. The facility is to be located in the chemical engineering building, complementing the bench scale fermentors, analytical equipment, and PDP 11/34 data acquisition and control system presently in our biochemical engineering laboratories.

The emphasis on biochemical engineering within chemical engineering and the ERC reflects but one aspect of a university-wide emphasis on biotechnology. At the university level, Vice-Presi-



Undergraduate Steve Ahnert putting the final touches on a new liquid level module in the Undergraduate Process Control Laboratory.

dent of Academic Affairs Rita Colwell has initiated the formation of four centers emphasizing areas of biotechnology. The first is to be the Center for Advanced Research in Biotechnology (CARB), representing a collaborative effort between Montgomery County, the National Bureau of Standards and the University of Maryland. At the present time a full-time director for CARB is being recruited, and plans for a building for the activities of CARB at Shady Grove, Maryland, are being finalized.

The chemical engineering initiative at UMBC as well as the emphasis on biochemical engineering faculty additions at UMCP will increase the number of chemical engineering faculty in the Program to nearly twenty in the next several years and will provide unique opportunities for

interaction with faculty experts in the biosciences at UMBC, UMCP and UMAB. The enrollment limitation plan of the college is just beginning to alleviate a very heavy undergraduate load in chemical engineering, permitting the allocation of more faculty time and resources to the expansion of the PhD program and the research activities of the faculty. In addition to biochemical engineering, the program has particular research strengths in aerosol mechanics, process simulation and control, multiphase flow, and polymers. Within the department, polymers has been identified as a primary area for development in the Engineering Materials Program, directed by John D. Hoffman. Adding to an already strong metallurgy program under Richard J. Arsenault, the emphasis on polymers will provide opportunities for collaboration with the chemical engineering faculty working in the area. Overall, chemical engineering at the University of Maryland is very much alive and looking towards the future.

CURRENT PROGRAM FACULTY

Chemical engineering faculty at the University of Maryland currently number thirteen, with eleven having primary duties at UMCP and two at UMBC. Currently the program has two open faculty positions at College Park and plans to add three or four additional faculty at UMBC over the next two years.

An ever-present pipe and a collection of owl figurines are sufficient clues to identify **Robert B. Beckmann** (Wisconsin, 1944). On the off chance that one of the clues is missed, identity is insured if a bow string tie, immaculate doodling, a print-perfect style of written communication, or amusing tales of horror from the senior design course are detected. Bob served as chairman of the department in the early '60's, building the graduate program before moving on to a tour of duty as dean of the college. Well known for his work on behalf of accreditation across the country, Bob provides the capstone on the design requirement of the curriculum while annually adding to his repertoire of anecdotes.

Theodore W. Cadman (Carnegie-Mellon, 1966) serves as the department chairman and strives to maintain his sanity with an active research program involving process control innovations and applications to fermentation operations and modern process simulation techniques. He is also an avid microcomputer enthusiast with a particular zeal for incorporating their use throughout

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the chemical engineering curriculum. To relieve the stress and tensions of departmental administration, Ted is an intrepid gardener, within certain constraints (anything planted has to be hardy, perennial, and serve to minimize or lessen lawn mowing), an inveterate do-it-yourselfer home remodeler and, in case of severe frustrations, he lays concrete block at his Chesapeake Bay retreat.

Richard V. Calabrese (Massachusetts, 1976) has research interests in two primary areas: turbulent two phase flow and the transport and transformation of atmospheric pollutants. Turbulent circulation patterns and drop/bubble breakup correlations abound in his studies in the former area. In the latter, Rich has been wide-ranging. The prediction of polycyclic aromatic hydrocarbon (PAH's) concentrations as a result of residential wood burning is a current project. As is the consequence analysis of nuclear reactor accidents, a segment of an Information System Study being completed by the Nuclear Engineering Program and the University Research Foundation at Maryland.

With less than a year in the Program, **Kyu-Yong Choi** (Wisconsin-Madison, 1983) is still setting his feet at Maryland. A product of Wisconsin at Madison, studying under Dr. Harmon Ray, Kyu-Yong has selected polymerization reaction engineering, with an emphasis on control, as his primary research activity. Lately, he has been particularly busy initiating his experimental program.

Stowe Davison (Maryland, 1984) is the newest member of the faculty and the first to be hired for the degree program at UMBC. A graduate of Maryland, Stowe completed his doctorate under James Gentry. He is an expert in computer applications and has selected the theoretical and experimental study of aerosol charging to begin his academic research career. In addition to being a gifted teacher, Stowe is quite at home in the laboratory and lately has been putting his practical skills to the real test by virtually rebuilding his home in College Park.

Interested in a new process? See **Larry L. Gasner** (M.I.T., 1971). Larry has a practical engineering bent which stands him well in all of his activities. With primary interests in the development and scale-up of bioprocesses, Larry is

anxiously awaiting the arrival of the 500 liter fermentor system. Well, perhaps just a little less anxiously than implied, since Larry is looking forward to spending time in Germany with the vendor, finalizing the plans for the system and reviewing the construction progress.

James W. Gentry (Texas-Austin, 1969) brings his scientific and mathematical skills to bear on the study of aerosols. A prolific publisher of research findings on the behavior of non-spherical and ultrafine aerosols, Jim has an extensive collection of books and classical records including the collected works of 19th century mathematicians, bound sets of Texas Football, and the collected works of J. S. Bach.

Albert Gomezplata (Rensselaer, 1959) serves as Associate Dean of Engineering with responsibility for the activities at UMBC. As a member of the chemical engineering faculty since 1958 and a former chairman of the department, Al is well equipped to initiate the programs at Catonsville and to foster the development of chemical engineering at the Baltimore County campus. On a time available basis, Al crosses the street to his sailboat on the waters in Annapolis and is an avid do-it-yourselfer when it comes to keeping his automobile(s) running.

Juan Hong's (Purdue, 1979) forte is biochemical engineering with a particular focus on biomass and product formation and separation processes. An avid experimentalist, Juan is equally skilled in analysis and modeling techniques and, as many a graduate student will attest, presents a mean course in thermodynamics.

Although categorized under the nuclear engineering faculty in the listings of the Department, **Yih-Yun Hsu's** (Illinois, 1958) chemical engineering background and expertise in heat transfer and two-phase flow make him a valuable contributor to the program's activities. YY, as he is known, particularly enjoys teaching heat transfer to the Junior chemical engineers.

Mention interaction analysis and one is assured of attracting the attention of **Thomas J. McAvoy** (Princeton, 1964). Together with strategies for distillation column control and short-cut modeling techniques, Tom brings a practical, enthusiastic bent to process dynamics and control. In the ap-

appropriate season, bluefish on the Chesapeake Bay and ice hockey are known to be competitors. Tom is director for the Center for Process Analysis, Control and Simulation, promoting interaction with industry in practical applications of control. Among the center's activities are a biennial short course, "Applications of Advanced Control in the Chemical Process Industries," and a series of videotapes featuring international experts on dynamics and control. In addition to his research activities, Tom has modernized the undergraduate process control laboratory using modular experimental units featuring a liquid level system interfaced to an APPLE microcomputer data acquisition and control system.

Gregarious **Thomas M. Regan** (Tulane, 1967) serves as the undergraduate advisor for the chemical engineering program. In addition to being a mainstay in undergraduate course instruction, including unit operations laboratory, Tom has culinary skills which rate par excellence.

Wilburn C. Schroeder's (Michigan, 1933) part time professorial position in chemical engineering dates back to 1953. It has always been part time and Will is always in every weekday, breaking precisely at 11:30 AM for lunch with several of the faculty at a local restaurant. Lunch is well worth the while to hear of his trips to Indonesia to build ammonia plants, tales of his tour of Germany immediately after World War II while at the Bureau of Mines, or for a discussion of the latest coal conversion technology—including the Schroeder Process—or national politics and the state of the market on the hour. Will's personality and expertise in energy, coal technology, and economics are particularly appreciated by the seniors in his classes who are given a view of chemical engineering that is not reflected in any text.

One of the quietest members of the Program is **Theodore G. Smith** (Washington University, 1960). Ted's research interests are focused on the study of polymer blends and the properties of polymers, particularly mass transfer. This fall he has also undertaken the particularly challenging and interesting task of using microcomputers in the introductory sophomore class. With funds provided by the university and the college, 24 Zenith 150 microcomputers have been purchased for the undergraduate program. Microcomputers were also purchased for use in the introductory freshmen courses taught within mechanical engineering, so Ted should find his task somewhat easier the second time around.

ADDITIONAL FACULTY

Nuclear Engineering Program: Kazys K. Almenas (Warsaw, 1968); Dick Duffey (Maryland, 1956); Mohammed Modarres (M.I.T., 1979); Frank J. Munno (Florida, 1964); Gary A. Pertmer (Missouri-Columbia, 1978); Marvin L. Roush (Maryland, 1964); Joseph Silverman (Columbia, 1951).

Engineering Materials Program: Richard J. Arsenault (Northwestern, 1962); John D. Hoffman (Princeton, 1949); Marc L. Mansfield (Dartmouth, 1981).

ACKNOWLEDGMENTS

The review by Thomas M. Regan is greatly appreciated.

ChE book reviews

INTRODUCTION TO PROCESS ECONOMICS, 2nd Edition

*By F. A. Holland, F. A. Watson and J. K. Wilkinson
John Wiley & Sons, 1983, xv: + 346 pages. \$21.95.*

**Reviewed by V. W. Uhl
University of Virginia**

The scope of this book exceeds the title term "process economics" as generally understood. The latter half of the book treats topics which deal with management techniques and business considerations. Overall, the level and content put the work in the double category of an undergraduate text and an introduction for engineers in industry to economic evaluation and management topics. The book will first be generally characterized. After the contents are delineated, there is a detailed commentary and then a thumbnail appraisal.

The treatment, although orderly, is uneven with respect to writing quality, intensity of the text, and the mode of demonstrating concepts and techniques. Some handling is inadequate while other material appears extraneous. The wide disparity in the quality of the style—stodgy in the beginning, felicitous later—suggests that each author may have written different sections, and they did not collaborate on editing. Some concepts are artfully and thoroughly developed; then essentials such as assets and depreciation are improperly presented and clumsily explained. In the last half some listed topics, such as cost benefit

analysis, are barely more than mentioned. The figures lack distinction and clarity, the tables are typed and many lack titles. The references are up-to-date, but many expected attributions to sources are not given.

Part one, titled "Elements of Profitability Assessment," surveys within a logical structure: time value of money; items of cost, including their handling, e.g., depreciation, and breakeven analysis; use of profitability measures; estimation of capital investment; and the prediction of annual operating expenses. In scope it corresponds almost to the first (1974) edition. Chapter 3 thoroughly considers a range of methods for assessing probability (twelve in fact). Chapter 4, which deals with uncertainties in profitability estimates is out of place; it should have been coordinated with related material in the last half of the book.

"Elements of Decision Making" is the designation for the second half, doubled in length from the 1974 edition. The topics are properly classified by the two chapter headings as numerate methods and management considerations. The nine sections in the first of these chapters include: statistics and probability; curve fitting and trend analysis; utility functions; linear programming; forecasting; learning curves; and profit-volume analysis. The last three are new. The final chapter on management considerations looks at matters such as: types of accounting; price and cost trends; value engineering; cost-benefit analysis; marketing; risk and insurance; and inflation (an addition to the new edition).

The treatment of engineering cost analysis is comprehensive. Each chapter has several appropriate problems which serve to fulfill the book's role as a textbook. The concept of contribution, especially as the contribution to sales ratio (CSR), proves useful in the analysis of sales data. The subject of capital cost estimation is well done, and it is on an international basis. Noteworthy treatments in the second half of the book deal with utility functions and learning curves.

The book fails in its poor expression of some concepts, limited scope, and inadequate reflection of current practice. The manner in which the cardinal concept of "cash flow" (net profit after income taxes plus depreciation) is expressed is indirect and therefore confusing. Also, attempts to correlate technical economics (for prediction) with financial accounting (for historical record) are unorthodox and hence confusing. For instance,

EDITOR'S NOTE

CEE REDUCES BACKLOG

Due to a steady increase in the number of papers submitted in recent years, CEE was faced last year with a two-year backlog of papers. We accordingly took steps to 1) increase the number of pages of editorial matter in each issue, 2) reject papers of lesser quality, 3) request the shortening of papers of considerable length, and 4) solicit fewer papers. As a result, with the publication of this issue our backlog has nearly been cut in half.

We appreciate the patience of our prospective authors during this period and encourage our readers to continue to send us papers of high quality

Ray W. Fahien
Editor

assets are incorrectly perceived; gross profit is equated to net profit; the latter is taken as income before taxes which is contrary to the common accounting definition, at least in the U.S. The practices for handling depreciation are limited. For instance, the Accelerated Capital Recovery System (ACRS) enacted by U. S. federal legislation in 1980 is not mentioned. Only discrete interest is used for the computation of net present value (NPV) and internal rate of return at a time when the employment of continuous interest and the half-year convention is common and growing. The wider view of "engineering economy" is ignored, one which considers choice between alternatives which are of the nature of plant additions, process modifications, and equipment replacement. And the optimization of processes, either by mode of operation or sizing in design (often termed Economic Balance) are not considered.

Several topics in the second half, such as elementary statistics, have no place because of their elementary character. Others, such as cost-benefit analysis and marketing are treated in a summary fashion, so they constitute a mere mention of these subjects. And inflation is handled in too cursory and incomplete a way to be useful.

Unfortunately the awkward presentation of the first half of the material, further burdened by a clumsy and needlessly extensive nomenclature, renders this basically simple subject arcane. The work is also lacking in judgments. For instance no critique was offered for the dozen methods of profitability assessment described. Readers seek guidance and a rationale.

Overall the book is limited in scope, is misleading in places, and makes an essentially simple discipline difficult to master and tedious to consider. □

CHEATING-AN OUNCE OF PREVENTION ... or the Tragic Tale of the Dying Grandmother

RICHARD M. FELDER
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Raleigh, NC 27695

Note: The material in this paper was presented at an orientation program given by North Carolina State University to new faculty members and teaching assistants. The formal misconduct procedure discussed in response to Question 12 of course varies from one university to another, but the philosophy underlying the procedure is relatively standard.

IN THESE PAGES, I talk about cheating—how to minimize its occurrence (preventing it completely is generally too much to hope for), what to do when you suspect it, and what to do when you can prove it. I don't claim to be an expert on the topic—I'm not sure there is such an animal—but will simply offer a few ideas for consideration. Ultimately, all instructors must develop their own philosophies on cheating, based on their individual senses of justice, morality, and humor.

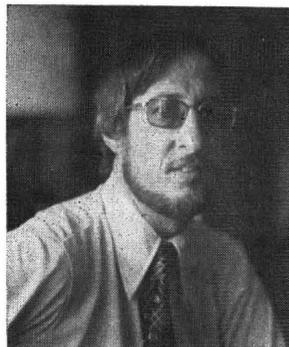
Here, then, are some questions a course instructor might ask about this uncomfortable subject, and some suggested answers.

1. *I'm going to be teaching a (small, large) (undergraduate, graduate) course. Is there likely to be cheating?*

Yes.

It may reflect the spirit of our times, or a decline in student morality, or the unchanging nature of the human species, or anything else you choose

The sad fact is, however, that as long as grades are important to students—as they probably will be—some students will do whatever they can to get the highest possible grades.



Richard M. Felder is a professor of ChE at N. C. State, where he has been since 1969. He received his BChE at City College of C.U.N.Y. and his PhD from Princeton. He has worked at the A.E.R.E., Harwell, Exxon Corporation, and Brookhaven National Laboratory, and has presented courses on chemical engineering principles, reactor design, process optimization, and radioisotope applications to various American and foreign industries and institutions. He is coauthor of the text, **Elementary Principles of Chemical Processes**.

to see in it. The sad fact is, however, that as long as grades are important to students—as they probably always will be—some students will do whatever they can to get the highest possible grades.

Clearly, the likelihood of cheating varies from one classroom situation to another. If you are teaching an advanced graduate course with eight excellent students, it is probably safe to leave the room during a test. On the other hand, if you teach a sophomore course with 200 students in a room that seats 200, and no one cheats or attempts to do so, you should nominate the class for the Guinness Book of World Records.

You may as well resign yourself to the fact that some students, impelled by desperation or a flexible moral code, will try to beat whatever system you impose, and guide yourself accordingly.

2. *Why should I be all that concerned about cheating?*

Most obviously, when students cheat and get away with it, it penalizes honest students, in some cases forcing them to cheat as well just to remain

competitive. More than this, however, it cheapens the value of the degree and adds to the probability that students will be officially declared qualified in fields in which they have no competence whatever. These incompetents could end up building our bridges, designing our nuclear reactors, removing our appendices, and possibly most serious of all, teaching our children.

3. *What forms does cheating take?*

There are two major categories: (a) cheating on homework and (b) cheating on tests. I'll take them up in turn.

4. *How do students cheat on homework?*

Cheating on homework involves getting solutions from somewhere other than one's own head, and turning them in as original. The sources include other students' solutions (either stolen or freely shared), back solutions in files (popular among fraternity members), and stolen textbook solution manuals. These are all traditional sources, known and loved for generations.

The current generation's contribution to the field is the stolen computer file. Instructors who store homework solutions on hard disks (as opposed to personal floppy disks) never know when some budding software wizard with an eye toward academic or financial gain might gain access to their files and copy and possibly reproduce and sell the solutions. Also, when the assignment involves writing a computer program, copying another student's solution file is often a trivial exercise for someone who knows his way around an operating system.

5. *How should I deal with homework cribbing?*

One way is to change the assignments each time the course is given, so that back files become useless. This imposes a tremendous additional work load on the instructor, however, and in the case of such things as laboratory courses may be impossible.

The instructor or grader can go through all the papers, looking for sets of identical solutions. However, it is difficult or impossible to prove anything in such cases. Students can always claim that they worked independently and coincidentally came up with identical answers, and you have no way of disproving them. If a student hands in a photocopy of a page from the solution manual, you would of course have a pretty good case

against him. However, the chances are that anyone that stupid will probably flunk out in the natural course of events, so that no extraordinary action may be called for.

My own solution for this problem is relatively simple, although it is strictly applicable only to technical courses. To the greatest extent possible, *eliminate the requirement that homework be done independently*. In fact, I always encourage students to work together, although I require them to hand in their own solutions. By working with others, students often learn how to solve problems that would have stumped them as individuals.

Of course, some students will get free rides this way, simply copying solutions without understanding them. However, these students will almost invariably be weeded out by the course tests. To be assured of this, include material of the type in question on the tests; ask questions about the

**On almost every test
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conduct of the experiments and the analysis of data in laboratory courses, and give brief programming exercises in courses that involve computer homework.

6. *How do students cheat on tests?*

Let me count the ways.

- **THE SNEAK PREVIEW:** Students get copies of the test before it is given, and come to class with the solutions already worked out.
- **THE EYES HAVE IT:** They copy from neighbors' papers—usually those adjacent or in the row ahead, sometimes in the row behind. (The latter requires more agility than the average engineering student possesses, and sometimes results in severe whiplash.)
- **THE NOTE OF PRECAUTION:** They copy from prewritten slips of paper, notebook covers, or easily accessed portions of their epidermis.
- **THE CALL OF (A WARPED) NATURE:** They go out of the examination room during the test, ostensibly to the bathroom, and either look up the answers or get by with a little help from their friends.
- **QUICK CHANGE ARTISTRY:** They pick up worked out solutions intended for distribution after the tests have been collected, and hastily correct their own solutions before handing their papers in. Since most students taking a test invariably wait until the last second to hand their papers in, and the

instructor is usually distracted by the mob around the front desk at this point, he can easily miss the student in the middle of the crowd pulling this particular stunt.

- **NOW YOU SEE IT, NOW YOU DON'T:** They don't hand in their test at all if they feel they have done poorly, then claim the grader lost it.
- **THREE-PAGE MONTE:** They substitute correct solutions for incorrect ones after the graded tests have been handed back, and claim that the grader made a mistake.
- **HISTORY REPEATING ITSELF:** They memorize solutions to previous examinations and simply write them down when the same questions reappear.

Any instructor lazy enough to use the same tests semester after semester invites the last of these activities. I do not consider it cheating, but a legitimate exercise for the enterprising student. The other methods cited above are a different story, however. As much as possible must be done to guard against them.

7. *How do I prevent cheating before the examination?*

The key word is security.

- Don't leave a copy of the test on your desk, or on your secretary's desk, or stored in your word processor where someone else can get access to it, or on the photocopy machine, or in a wastebasket in your office or the department office.
- When work is not being done on the test, keep all existing copies locked away in a safe place, like your personal file cabinet.
- Don't let work-study students photocopy a test—do it yourself, or have your secretary or teaching assistant do it, and immediately seal the copies in an envelope or folder and lock them away.
- Know how many copies were run off, and count them before the test is given. If the count is wrong, make up a new test, or see the following story.

A professor in our chemistry department once gave a test for which the answer page was the test paper. Before giving the test, he counted the copies, and found that he was short by two. He took the papers to the department office, used a paper cutter to remove about 1/8 inch from the bottom of each sheet, and then gave the test. Afterwards, he collected the solutions, stacked them vertically, pulled out the two that were longer than all the others, and invited the students they belonged to into his office for a little chat. I don't know what happened from there, but you get the point.

8. *How can I minimize cheating during the examination?*

- Most obviously, by keeping your eyes open. Be sure the examination is proctored at all times, and be on the lookout for suspicious behavior. (Keep the cold hard staring to a minimum, however—too much of a police-state atmosphere can intimidate students to a point that they become incapable of showing what they really know.)
- If there is room, request that students sit in alternate seats. If this is not possible, and if you have reason to believe that copying may be a problem in a particular class, you may find it convenient to make up and distribute alternate versions of the test to adjacent students. (Shuffle the order of the questions, or use different sets of numbers if calculations are involved.)
- If someone's eyes are obviously wandering during a test, silently call his attention to the fact that he is being observed. If you can't catch his eye, you might announce (humorously, if you can manage it) that group solutions will not be accepted, and look pointedly at him when he looks up. In extreme cases, you can quietly ask him to move to a more isolated location.
- Don't hand out worked-out solutions until you are absolutely certain you have collected all the test papers. One way to guarantee this is to hand them out in the period following the one in which the test was given.
- Before grading the papers, log them in, so you will know immediately who did not submit one.

9. *How can I minimize cheating after the examination?*

- If possible, use examination booklets, so that substitution of corrected pages for original ones is made more difficult.
- Make copies of all graded solution papers, or of some of them if there are too many to copy them all, before handing them back. Then, if a student comes to you and complains that the grader made a mistake, comparing his paper with the copy will tell you whether he was really misgraded, or whether he's trying to pull the old switcheroo on you.
- Note the names of all students who present questionable claims of misgrading. If you can't disprove their claims, give them the benefit of the doubt, and change their grades—but on subsequent tests, be sure to copy their graded solutions before handing them back, even if you copy no others.

10. *Does the type of test determine how likely students are to cheat on it?*

To a considerable extent, yes. The tests which are most likely to be cheated on are those with answers that are easy to copy (e.g. true-false and multiple choice tests), and those which seem unfair to the students. Generally speaking, if you want to construct an engineering course test that is both pedagogically sound and difficult to cheat on, I recommend the following:

- Require full problem solutions, not just simple answers, and be liberal with partial credit.
- Give only open-book tests.
- Give tests that are easy to read and possible to solve.

If the answer to a question is “true” or “(d)” or 675°C, it is a trivial matter to ascertain this fact from the adjacent student and get full credit, while on a problem that takes several pages to work out the cheater’s task is much more arduous. Requiring detailed solutions and giving partial credit makes life more complicated for the instructor and the graders, but it helps assure that students who understand the course material are not unduly penalized for careless mistakes, and it minimizes the chance of a student getting full credit for copying a correct answer without having the vaguest idea of how to do the problem.

I have strong feelings on the question of open-book versus closed-book tests. What I want to know is whether my students can take the material I have given them—course notes, worked out problems, and a course text—and use it to solve problems; I really do not care how much data they can cram into their short-term memories the night before the quiz. An open book test allows me to find out what I want to know; it tests the students’ understanding, not their memory, and it also provides a closer simulation of the tests that await them in their careers. As a fringe benefit, open-book tests eliminate the usefulness of inscribing or scotch-taping facts, formulas, and conversion factors on shirtsleeves and under socks.

There is no question but that a poorly constructed test invites cheating. I know a professor who seems to delight in making up test questions that even his faculty colleagues cannot decipher. In some cases the problems are trivial; the only trick is to figure out what is being asked. Students faced with this sort of thing tend to panic, envisioning zeros on the quiz since they do not even know how to get started, and they often take whatever measures they can to get out of their dilemma.

Another feature of some tests that drives students up the wall is the mistake-ridden problem that either has absurd solutions or cannot be solved at all. Such problems almost invariably appear when the instructor makes up the quiz at the last minute and does not bother to work out the solutions himself. If this is a chronic occurrence in a course, students tend to be much more inclined to share solutions than they might otherwise be.

Finally, we have the instructor who likes to make up tests for which the average is in the 20’s or 30’s. Rightly or wrongly, students regard such tests as basically unfair, and they often feel little remorse about cheating on them. I believe that tests like this are little more than ego trips for the professor—they do not serve any useful pedagogical purpose.

The closest I have ever come to cheating on a test was on my graduate school thermodynamics final. The whole course was a disaster—the text spoke about one body of material, the lectures about completely unrelated material, there were no quizzes—and the final examination had no apparent relation to either the book or the lectures. Fortunately, I was not led into temptation because there was no one to copy from—we were all in the same boat. I got a 9 on the exam (out of a possible 100). It was good enough for a B in the course; two hot-shots who got 12 and 11 got A’s. However, I truly believe that if I had cheated on this travesty, God would have forgiven me.

11. What about students who miss tests?

On almost every test some students will not show up and will later appear in your office with stories that will astound you with their inventiveness, pathos, and sheer chutzpah. “My alarm didn’t go off,” is probably the most popular story, followed by, “My car wouldn’t start,” and complaints of every malady known to medical science and some that medical science has yet to catch up with.

All instructors hate make-up tests. It’s hard enough to construct a fair test that covers everything you want to cover, that discriminates between students who are excellent, good, fair, and poor, and that can be finished within the allotted time slot. Having to do it twice is one of the great pains of higher education. To avoid it, some instructors allow no excuses except certified doctors’ notes, and in the absence of such documentation a test grade of zero is assigned. (This approach is particularly appropriate if the instructor makes a practice of dropping the lowest test grade.) Others give students the benefit of the doubt and routinely give make-up tests, often taking them from previous years.

I tend to fall into the latter category, but I have my limits. Two students who missed a quiz last year came into my office and indicated that they had to go back home to stay by their dying grandmother’s bedside. Since I had already given

one of these students a make-up test earlier in the semester (it seems his alarm clock had failed to go off, and then his car wouldn't start), I was a trifle skeptical, so after they left my office I called his home and inquired. There was no dying grandmother. The two students got zeros on the quiz, and they can expect to be watched with hawk's eyes for the remainder of their academic careers.

12 What should I do when I suspect a student of cheating?

It depends strongly on the grounds for your suspicion. Unless you have fairly clear evidence, the best procedure is to do nothing. It is better to miss an occasional violation than to subject an honest student to implications of dishonesty and possibly to public embarrassment.

If a student's paper shows evidence of foul play—it duplicates another paper too closely, for example, or it indicates ability completely inconsistent with previous performance, or it seems to have been tampered with after being graded and returned—calling the student into your office and asking him to discuss it with you is a first step. You might say you are not clear about how he arrived at his answers, and ask him to go over what he did. Or you can point out the things that make you suspicious and ask for explanations.

If the student denies all wrongdoing (as he usually will) and you have no way of proving conclusively that he cheated, give him the benefit of the doubt and drop the matter. If in fact he cheated, the fact that he was called in may be enough to keep him honest thereafter.

13. What should I do when I have clear proof that a student cheated?

All universities have administrative policies and procedures for dealing with this situation. Briefly, the N.C. State academic misconduct procedure involves confronting the student with the charges against him; filing a report on the case with the Department of Student Development if the student admits guilt; or referring the case to the Student Attorney General for a formal hearing if no admission is forthcoming.

Unless the instructor filing charges recommends a stronger sanction, a student who admits guilt or is found guilty by the hearing panel is given a zero on the assignment or test he cheated on and is placed on academic misconduct probation for the remainder of his career at the university.

A record of the incident is placed in his permanent file, but does not appear on his transcript. A second violation results in suspension.

In most cases, instructors choose to avoid this procedure, either to keep students from getting black marks on their records or to avoid time-consuming red tape. They may take individual action ranging from assigning a grade of zero on a particular test to failing the student in the course, and in some instances recommending or demanding that he drop out of the curriculum.

Quite obviously, individual discipline is risky: a student may claim that his rights have been violated, and the instructor may find himself involved in much more red tape than he ever would have had to deal with by proceeding through official channels. The safest procedure is to adhere to the university policy—and it is mandatory to do so when penalties more severe than low test grades are involved.

The first step of the academic misconduct procedure is confronting the student with the charges against him, and requesting an admission of guilt. Before doing this, however, you should reread the university policy and inform the student of the consequences of admitting guilt and of denying it. Make a written transcript of the proceedings and have the student sign it attesting to its accuracy. A copy of the transcript can serve as the report to the Department of Student Development. Finally, make sure that you retain copies of any incriminating evidence, so that if a formal hearing is necessary you will be able to substantiate the charges that led to the procedure being initiated.

Finally, if a student in one of your courses has been proven guilty of cheating, I believe you should make your departmental colleagues aware of it. I once caught a student who tampered with a graded test and failed him on the test. Attempting to be fair to him, I said nothing about the incident to anyone. He managed to pass the course, made his way through the rest of the curriculum, and graduated. Subsequent to his graduation, it came out that almost every instructor who had him in their courses experienced difficulties of a similar nature, and all of them did what I did. He literally cheated his way through college and is now certified to practice chemical engineering, which is a frightening thought to me.

If my colleagues and I had just talked to each other, we would have been on the lookout for this type of behavior from him, and when it occurred, we would have known enough to proceed through

the university judicial system. He would have been placed on misconduct probation, and there is a good chance that his academic career would have been appropriately terminated. As it is, we can only hope that he is not now in a position to do too much damage.

CONCLUSION

These are distasteful things to have to write. I like and admire most students—if I didn't, I would find another profession. I detest the thought that I have to undertake the precautions outlined in this paper, which in a sense tar all students with the same brush.

I started my teaching career filled with an idealistic humanitarianism which held that if you assume the best in people they will reward you by living up to your expectations. Unfortunately, I quickly found out that it does not always work that way. My idealism was interpreted by the dishonest students as a license to cheat with impunity

and by the honest ones as a sign that I didn't care about the cheating that they all knew was going on. I eventually concluded that taking precautions against cheating, regardless of the implications of these precautions, and dealing firmly with proven cheaters, were the fairest things I could do for my students.

Most students are basically honest. Most cheating incidents do not reflect chronic behavior patterns, but slips resulting from momentary panic. As an instructor, you should keep this in mind: always give students the benefit of the doubt when a reasonable doubt exists, and do all you can to avoid blackening their records and jeopardizing their futures by overreacting to minor ethical slips. At the same time, make it quite clear to your students that cheating is unacceptable, and back your words up when it becomes necessary to do so. By so doing, you will be serving the interests of the students, yourself, your faculty colleagues, and the university as a whole. □

ChE book reviews

THE PRACTICAL USE OF THEORY IN FLUID FLOW. Book I: Inertial Flows

*By S. W. Churchill; Etnaner Press,
Thornton, PA 19373 (1980)*

Reviewed by

David G. Thomas

Oak Ridge National Laboratory

The selection of words and their order in the title of this text describe the emphasis and objectives of the author. To accomplish this, simple derivations from first principles are used to explain practical problems that occur in single phase compressible and incompressible flows. The basic physics of the flow phenomena is retained even when developing approximate models which often are of sufficient accuracy for engineering applications. More to the point, because empirical models are avoided whenever possible, increased confidence in the generality of the result is developed.

This is an unusual book in several respects. It is not listed in the 1983-84 edition of Books in Print. Under the umbrella of the general title are included 7 books, of which the one under review

is the first. Other titles in the series are:

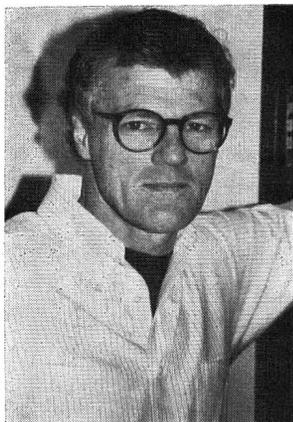
- II One-dimensional Laminar Flows
- III The General Equations of Motion
- IV Unconfined Multidimensional Flows
- V Confined Multidimensional Laminar Flows
- VI Confined Turbulent Flows
- VII Flows Through Dispersed Media

The division of subject matter indicated above results in an unusual grouping of topics on both compressible and incompressible flow in Book I. For instance, successive chapter titles are: Ch. 1, Reversible Expansions and Compressions; Ch. 2, Expansions at Low Velocity; Ch. 3, Maximum Reversible Rates of Flow for a Gas; Ch. 4, Jet Propulsion Engines; Ch. 5, Maximum Rate of Flow of Gas Through a Pipe; Ch. 6, Sudden Expansions and Contractions; Ch. 7, Shock Waves; Ch. 8, Detonation Waves in Gases; Ch. 9, Surface Waves, and Ch. 10, Cavitation, Incipient Vaporization and Aerodynamic Heating. There are an average of 20 problems for each chapter and it would be essential to solve the majority of them to gain full benefit from the approach selected by the author. Not only do the problems require an understanding of the basic principles but some developments of importance are deferred to the problem sets. Numerical methods are avoided. This book is suitable for a senior or first year graduate course. □

A SIMPLE GEOMETRICAL DERIVATION OF THE SPATIAL AVERAGING THEOREM

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THE CHEMICAL ENGINEERING approach to transport phenomena usually begins with the study of fluid mechanics, moves on to heat transfer, and completes the introductory sequence with a study of diffusion and mass transfer. This sequence is normally restricted to single phase transport phenomena, or situations in which the influence of the second phase is represented only in terms of a boundary condition. The beginning sequence is often treated with great care as the Navier-Stokes equations slowly evolve [17, Chap. 5], the thermal energy equation rises from the morass of Cartesian tensor analysis [10, Sec. 10-1], and the complexities of multicomponent transport phenomena [3, Sec. 18.3] complete the initial foray into the world of partial differential equations. What follows is



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The key mathematical theorem used in these three studies is known as the spatial averaging theorem, and it was presented independently by the above workers in 1967. In each study a different route to the averaging theorem was used . . .

crucial to chemical engineering: *multiphase transport phenomena*. However, the disparity between the precise analysis encountered in *single phase* transport phenomena and the qualitative treatment of *multiphase* transport phenomena often causes our students to question the efficacy of engineering science and encourages faculty members to adopt the position that it simply is not worth the trouble. Clearly, the transition from axioms and well-posed problems to applications and ill-posed problems deserves our attention.

The connection between single phase transport phenomena and multiphase transport phenomena is easily accomplished by means of the spatial averaging theorem. This approach was originally developed by Anderson and Jackson [1] who derived the equations of motion for a fluidized bed, by Slattery [15] who studied the problem of viscoelastic flow in porous media, and by the author [18] who used the method to derive a dispersion equation for mass transport in porous media and, more importantly, to outline a method of closure. The key mathematical theorem used in these three studies is known as the *spatial averaging theorem*, and it was presented independently by the above workers in 1967. In each study a different route to the averaging theorem was used, and since 1967 there have been numerous other treatments of this mathematical problem [2, 8, 11, 19]. The process is not yet terminated, for in recent papers Cushman [6, 7] has raised the issue of the need for time and space-dependent averaging volumes, and Veverka [16] has commented on possible limitations of the averaging theorem. Howes and

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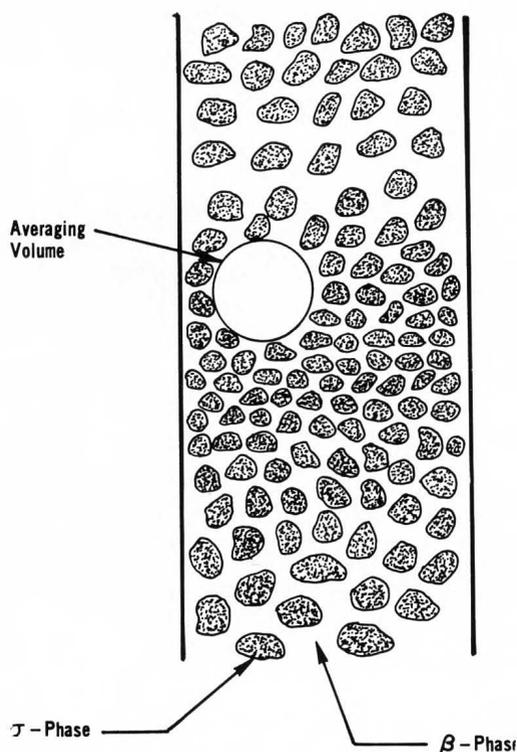


FIGURE 1. A two-phase system

Whitaker [13] have examined the questions raised by Veverka and find them to be unimportant for cases of practical interest. The objective of this paper is not to produce a new result, but merely to provide a route to the averaging theorem that can be used in our undergraduate classes.

PHYSICAL PROBLEM

In Fig. 1 a two-phase system is illustrated with the continuous phase identified as the β -phase and the discontinuous phase identified as the σ -phase. One could think of this system as a bubble column or as a fixed bed reactor. We direct our attention to the β -phase and note that the species continuity equation can be expressed as

$$\frac{\partial c_A}{\partial t} + \nabla \cdot \mathbf{N}_A = R_A \quad (1)$$

Here c_A represents the molar concentration of species A, the molar flux is given explicitly by

$$\mathbf{N}_A = c_A \mathbf{V}_A \quad (2)$$

and the molar rate of production per unit volume of species A owing to homogeneous chemical reaction is represented by R_A . It should be clear that we are thinking of the β -phase as a fluid and the

σ -phase can be either a non-porous solid, a porous solid, a liquid, or a gas. It will be sufficient for our purposes to consider only the mass transfer process in the β -phase.

Obviously we are unable to determine the details of the concentration field in the β -phase and some type of averaging procedure is in order. The method of volume averaging is based on the assumption that a *local* average concentration and a *local* average rate of reaction will suffice for design purposes. To this end, we associate with every point in space an averaging volume such as the sphere illustrated in Fig. 1. We designate the averaging volume by v and average values computed on the basis of this volume are assigned to the centroid of the volume. Since there is an averaging volume associated with every point in space, i.e. in both the β and the σ -phases, we can generate a field of average values of the concentration, temperature, etc.

In the method of volume averaging there are numerous types of averages. This is perhaps best illustrated in a recent paper dealing with diffusion and reaction in a micropore-macropore model of a porous medium [22, 23]. In that work one finds four different volume averages and eleven different concentrations for a single species. In general, there are two averages that one needs and the first of these is referred to as the *phase average* which is defined by

$$\langle c_A \rangle = \frac{1}{V} \int_{V_\beta(t)} c_A \, dV \quad (3)$$

Here $V_\beta(t)$ represents the volume of the β -phase contained within the averaging volume which can be expressed as

$$v = V_\beta(t) + V_\sigma(t) \quad (4)$$

Note that while the individual volumes, $V_\beta(t)$ and $V_\sigma(t)$, may be functions of time and space, the averaging volume is not.

When the point concentration of species A is constant, we see from Eq. 3 that the phase average

concentration is not equal to that constant value. Because of this, we usually prefer to work with the *intrinsic phase average* concentration which is defined by

$$\langle c_A \rangle^\beta = \frac{1}{V_\beta(t)} \int_{V_\beta(t)} c_A \, dV \quad (5)$$

These two average concentrations are related by

$$\langle c_A \rangle = \epsilon_\beta \langle c_A \rangle^\beta \quad (6)$$

in which ϵ_β is the volume fraction of the β -phase given by

$$\epsilon_\beta = V_\beta(t)/V \quad (7)$$

The averaging procedure is best initiated in terms of the phase average, and thus we integrate

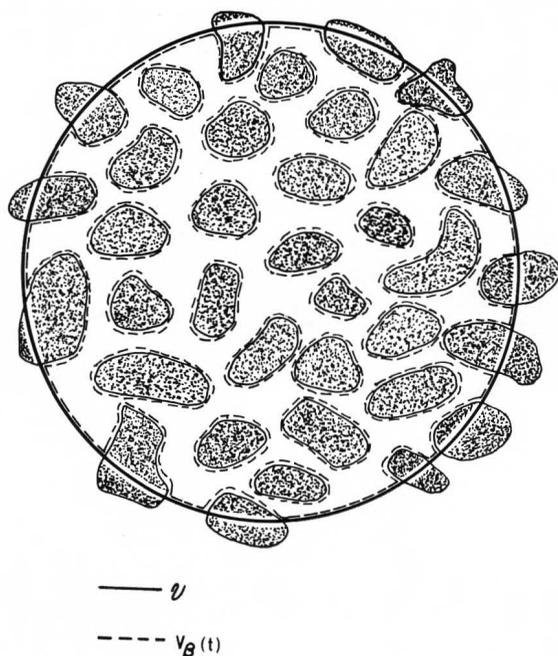


FIGURE 2. Averaging volume for a two-phase system

Eq. 1 over the volume $V_\beta(t)$ and divide by v to obtain

$$\frac{1}{V} \int_{V_\beta(t)} \frac{\partial c_A}{\partial t} \, dV + \frac{1}{V} \int_{V_\beta(t)} \nabla \cdot \mathbf{N}_A \, dV = \frac{1}{V} \int_{V_\beta(t)} R_A \, dV \quad (8)$$

Use of the traditional nomenclature illustrated by Eq. 3 leads to the form

$$\left\langle \frac{\partial c_A}{\partial t} \right\rangle + \langle \nabla \cdot \mathbf{N}_A \rangle = \langle R_A \rangle \quad (9)$$

Here it is clear that we must be able to interchange differentiation with respect to both time and space with time-dependent spatial integration if we are to obtain a governing differential equation for the average concentration. The general transport theorem [17, Sec. 3.4] will allow us to treat the first term in Eq. 9 in a precise manner, and what is needed here is a rule for interchanging spatial integration with spatial differentiation. Clearly we seek a three-dimensional form of the Leibnitz rule using the same simple approach currently available in the derivation of the general transport theorem.

MATHEMATICAL PROBLEM

In general we require an averaging volume to contain many "pores" or "particles" of both phases in order to obtain smooth and representative values [5, 19]. Such an averaging volume is illustrated in Fig. 2 in which we have clearly identified v and $V_\beta(t)$. The volume of the β -phase is bounded by two surfaces that we identify as

$A_{\beta\sigma}(t)$	interfacial area
$A_{\beta e}(t)$	area of entrances and exits

and for the purposes of our derivation it is sufficient to consider the simple system shown in Fig. 3. There we have illustrated two averaging volumes with the centroids separated by a distance Δs along a straight line, the orientation of which is designed by the unit vector λ .

The objective here is to derive the three-dimensional Leibnitz rule which can be expressed as

$$\frac{\partial}{\partial t} \int_{V_\beta(t)} c_A \, dV = \int_{V_\beta(t)} \nabla \cdot c_A \, dV - \int_{A_{\beta\sigma}(t)} n_{\beta\sigma} c_A \, dA \quad (10)$$

Rather than deal directly with the gradient, it is more convenient to begin with the directional derivative [17, Sec. 7.4] and use the definition of the derivative to write

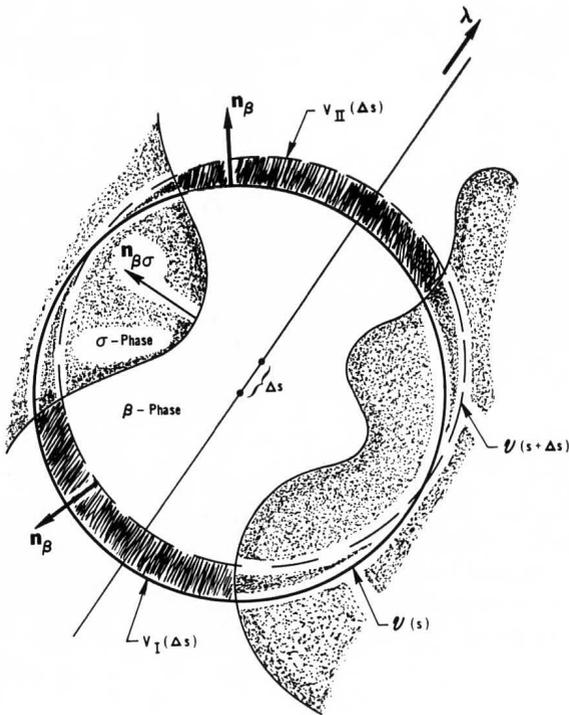


FIGURE 3. A uniform translation

of the general transport theorem [17, Sec. 3.4] in order to evaluate the integrals on the right hand side of Eq. 12. Each point on the surface of the averaging volume $\nu(s)$ is translated a distance Δs in the λ -direction in order to construct the volumes $V_I(\Delta s, t)$ and $V_{II}(\Delta s, t)$, and the details of the geometry are illustrated in Fig. 4. Our next step in this analysis requires that we represent the volume integrals over $V_I(\Delta s, t)$ and $V_{II}(\Delta s, t)$ in terms of the surface areas A_I and A_{II} . These two areas are identified by the unit outwardly directed normal vector \mathbf{n}_β shown in Fig. 3, and as $\Delta s \rightarrow 0$ these two areas will be coincident with the area of entrances and exits, $A_{\beta e}(t)$. When the averaging volume undergoes a displacement Δs , an element of the surface will generate a cylinder as illustrated in Fig. 4. The differential volume elements illustrated in Fig. 4 can be expressed as

$$dV_{II} = \Delta s \, dA_{CS} \quad (13)$$

where dA_{CS} represents the cross-sectional area of the cylinder under consideration. The *cross-sectional area* is related to the *surface area* element by

$$\lambda \cdot \nabla \int_{V_B(s,t)} c_A \, dV = \frac{d}{ds} \int_{V_B(s,t)} c_A \, dV$$

$$= \lim_{\Delta s \rightarrow 0} \frac{\int_{V_B(s+\Delta s,t)} c_A \, dV - \int_{V_B(s,t)} c_A \, dV}{\Delta s} \quad (11)$$

$$dA_{CS} = \lambda \cdot \mathbf{n}_\beta \, dA_{II} \quad \text{over } A_{II} \quad (14a)$$

$$dA_{CS} = -\lambda \cdot \mathbf{n}_\beta \, dA_I \quad \text{over } A_I \quad (14b)$$

These relations allow us to express the volume
Continued on page 50.

Clearly the intersection of the two integrals will cancel in Eq. 11 so that we obtain

$$\frac{d}{ds} \int_{V_B(s,t)} c_A \, dV = \lim_{\Delta s \rightarrow 0} \frac{\int_{V_{II}(\Delta s,t)} c_A \, dV - \int_{V_I(\Delta s,t)} c_A \, dV}{\Delta s} \quad (12)$$

Since the two volumes, $V_I(\Delta s, t)$ and $V_{II}(\Delta s, t)$, tend to zero as $\Delta s \rightarrow 0$, we can use the simple geometrical arguments presented in the derivation

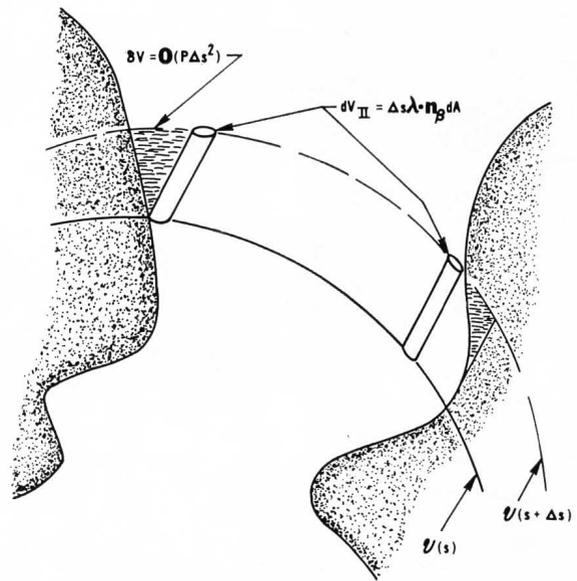


FIGURE 4

TOWARD ENCOURAGING CREATIVITY IN STUDENTS

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THE WORD "CREATIVITY" has been much abused because it is difficult to define precisely. In common speech, it is often used for a negative purpose: educators, politicians and administrators are criticized for "not being creative" but, upon further investigation, that criticism often means only that the critic doesn't approve of what the educator, or politician or administrator, is doing. In American society, where we tend to worship whatever is new and where we tend to condemn whatever is old, the word "creative" is a positive adjective, a word of praise, while the more-commonly-used phrase "lack of creativity" is a sign of condemnation.

The dictionary doesn't help much. *Webster's Unabridged Dictionary* refers, on the one hand, to creativity as "making something out of nothing" as in the Bible where God created the earth, and



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on the other hand, to social or legal acts, as in government where Congress creates a new law, or to artistic acts where a painter or sculptor creates a work of art.

None of these definitions are satisfactory when we consider creativity in science or in the education of scientists and engineers. Within that context, I much prefer a definition which I once heard from a psychologist: A creative act is one where two ideas or concepts, previously believed to be totally separate, are for the first time, shown to be closely related. A creative act, in other words, is to show that two apparently distinct ideas or concepts are, in truth, not distinct but are merely two aspects of some more general unifying idea or concept. This definition helps us to find ways for encouraging creativity in chemical engineering students, especially graduate students.

Let me now illustrate this definition of creativity by some examples from the history of science and then indicate how that definition suggests some possibly useful procedures for educating creative scientists and engineers.

A striking example is provided by the history of thermodynamics. Until about 1870, thermodynamics (as the name implies) was the science of heat engines, a science concerned with the principles which govern the conversion of heat to mechanical work and vice versa. The research of Mayer, Joule, and Carnot showed that this conversion can be quantitatively described through simple mathematical relations which, however, are characterized by a lack of symmetry; the rules for converting work to heat are not the same as those for converting heat to work. It was this lack of symmetry which led Clausius to the concept of entropy and toward quantitative formulation of the first and second laws of thermodynamics.

While this theoretical development of thermodynamics was proceeding, there was at the same time significant experimental development in chemistry where the early pioneers of what we now call physical chemistry were measuring

Through his invention of a unifying concept—the chemical potential—Gibbs constructed a theoretical framework which has tremendously influenced and advanced many fields of science, with particularly beneficial effects in chemical engineering. Gibb's unifying action, showing the relationship between apparently separate fields of inquiry, is a striking example of what we mean by creativity.

yields of chemical reactions and distributions of components in mixtures among two or more phases. Until about 1870, no one recognized that there was a fundamental connection between what we now call chemical equilibria and phase equilibria. More important, no one had seen any connection between these chemical phenomena and the scientific principles of heat engines. Now, more than 100 years later, we recognize a connection because of our notions of asymmetry and irreversibility: it's easy to convert work to heat but it's not easy to go back again; it's easy to make water and carbon dioxide from methane and oxygen but it's not easy to do the reverse; it's easy to mix water and alcohol but, having mixed them, it's not easy to separate them to their former condition.

We all know that it was Gibbs who first recognized the connection between physical chemistry and thermodynamics, two sciences which, prior to Gibbs, had been believed to be unrelated. Through his invention of a unifying concept—the chemical potential—Gibbs constructed a theoretical framework which has tremendously influenced and advanced many fields of science, with particularly beneficial effects in chemical engineering. Gibb's unifying action, showing the relationship between apparently separate fields of inquiry, is a striking example of what we mean by creativity.

Gibbs' creative work related one science to another; he used the scientific principles of heat engines to obtain a theoretical treatment of equilibrium in chemical systems. However, the essence of creativity—tying together two separate ideas—need not be limited to those cases where both ideas come from the world of science. Creative acts interconnect intellectual ideas regardless of origin or classification. For example, Sigmund Freud's autobiographical writings indicate that psychoanalysis was born from the interaction of two major factors. First, as a young man, Freud worked in a psychiatric hospital in Paris where he treated women afflicted by hysteria; second, Freud had read the philosophical works of Friedrich Nietzsche and had been impressed by Nietzsche's observation that human behavior was only superficially conditioned by the rational rules

of society, while in its essential acts, human behavior was governed by deep-seated, irrational motives. Freud saw a connection by establishing the now well-known concepts of id and super ego which allowed him to interpret hysteria as a consequence of emotional suppression, usually dating back to early childhood; once the patient recognized the source of her problem, she could, with counseling, find an accommodation which often led to a cure. Freud's creative act was to apply to medicine what at that time was far-out, radical philosophy.

A third and final example is provided by the physicist Niels Bohr whose complementarity theory is now accepted by most scientists as one of the basic cornerstones of physics. This theory, also known as the Copenhagen interpretation of quantum mechanics, is a concept of nature which believes that duality is not an apparent, but a fundamental feature of natural phenomena: light is not uniquely corpuscular nor is it uniquely a wave; it is both, such that, depending on what observation we want to interpret, one is more evident and sometimes the other. If duality is fundamental, then classical causality and determinism are not possible, as shown by Heisenberg's uncertainty principle. According to the Copenhagen view, probability and statistics are not just approximations which follow from our inadequate knowledge; they are the fundamental laws which govern natural phenomena.

Bohr tells us that his theory of complementarity has two roots: spectroscopy and the philosophy of Søren Kierkegaard, a Dane like Bohr, who bitterly opposed the deterministic philosophy of Hegel that dominated Europe during the nineteenth century. Hegel's famous sequence (thesis, antithesis, synthesis) expressed the notion that with time, like a pendulum, a particular idea (or thesis) generates its opposite (antithesis) and that with more time, the two opposed ideas merge to form a new idea (synthesis). Kierkegaard was a deeply religious Christian who doubted that man could ever attain absolute knowledge; such knowledge was reserved for God. Kierkegaard denied that with time one idea is followed by its opposite; he stressed instead his belief that two

opposed ideas exist simultaneously. Opposites co-exist and if we examine any one deep truth, we find its opposite to be true as well. Kierkegaard's view is succinctly expressed by the title of one of his books, *Either/Or*.

Bohr studied Kierkegaard in his youth, shortly before he became interested in interpreting transitions of electronic energy states, as measured by spectroscopists. Before Bohr, most physicists had never heard of Kierkegaard and, even if they had, it would not have occurred to any one of them that Kierkegaard's highly abstract criticism of Hegel had any connection with electronic transitions. But Bohr saw the connection. His creative

If we accept the definition of creativity that I have indicated, then we must see to it that our students are exposed to a variety of subjects, including some that are remote from chemical engineering.

act was to establish an interpretation of physical phenomena using concepts from what was (and still is) obscure philosophy.

What do these examples suggest toward fostering creativity in education? If we accept the definition of creativity that I have indicated, then we must see to it that our students are exposed to a variety of subjects, including some that are remote from chemical engineering. If the essence of creativity is to do something new or to do something in a new way, then we should give our students the intellectual tools that are needed for novelty; to do that, our students should become familiar with modes of thinking and with procedures of inquiry which are different from those we use in common chemical engineering. Simply put, creativity is likely to be stimulated by intellectual breadth.

The most common argument for breadth is, that for professional success, a chemical engineer must not only be technically competent but must also be familiar with economics and with all those humane skills that allow him to interact positively with a variety of co-workers and that, in general, lead to good citizenship. A further argument is that our alumni are not only chemical engineers but also intelligent human beings who seek to fill their leisure hours with satisfying enjoyment, and therefore it is proper to include music, art and literature in a chemical engineering curriculum. Without in any way subtracting from the weight

of these arguments, I would add that breadth is necessary for creativity, not necessarily to produce a Gibbs or Freud or Bohr—because that is unlikely—but to provide our alumni with a broad attitude toward problems they are likely to encounter, to give them the capability to think beyond common chemical engineering when they face those new challenges—as they surely will—which cannot be solved by the conventional wisdom that is contained in standard chemical engineering.

In any one field of human endeavor, progress is inevitably attained by borrowing from another. The great advances recently made in medicine and in biology have come about primarily because of progress in experimental physics and analytical chemistry. Today, doctors can diagnose previously hard-to-detect pathology because of the CAT scanner which utilizes sophisticated x-ray technology combined with computers. Further, while recent discoveries in molecular biology promise to produce cures for serious diseases, they are only possible because of powerful electron microscopes, refined chromatographs and sensitive detectors of isotope radiation. Similarly, regardless of what opinions we may have of modern art and modern music, we recognize that the new art forms that are appearing in the United States and Europe are increasingly influenced by the encounters that our artists and musicians have with non-Western cultures, notably African, and with electronic tools and gadgets, including the computer. I mention all this only to emphasize once more that progress results from cross-fertilization and to stress that in any area of human activity, significant novelty is only achieved by going beyond the frontiers of that area through adoption of achievements from other areas.

Let me close by reflecting briefly on how these general ideas of breadth and creativity can be put into practice, given the inevitable boundary conditions under which we must operate. In undergraduate programs, our primary educational obligation is to impart professional competence such that our alumni, within a year or less, can make productive contributions to their employers. To achieve that end in a reasonable number of semesters, we tend to believe that we must fill the curriculum with numerous required courses, leaving little room for breadth. I suspect that we have gone too far in specific course requirements and that at least a few required courses are in our curriculum not because they are truly necessary but because of tradition (because the professors re-

sponsible for the curriculum took these courses when they were students) and because every professor in the department insists that *his* particular specialty must be taught to everyone, essentially because he likes to teach it.

If we are serious about encouraging creativity for undergraduates, we must open up the curriculum and encourage at least our better students to become familiar with intellectual concepts and tools that are not now common in chemical engineering. Clearly, not all students will benefit from such exposure, and therefore we should have flexibility such that our average students will do more or less what they do now but where the student with unusual potential is permitted and encouraged to deviate from the norm and to direct at least a part of his imagination toward other intellectual disciplines.

For graduate education, where the curriculum is less rigid, we should insist that our students take some high-level courses in other departments. By high-level, I mean courses with significant intellectual content; that is, courses taken by majors in other fields, and not survey courses designed for general education. Further, we should encourage independence and develop self-confidence by insisting that in their second year of graduate study, our

PhD students pass an oral proposition examination where the candidate proposes an original research project on a subject remote from his PhD thesis. The student must defend his proposal to a committee of professors that should include one or two colleagues from departments other than chemical engineering. Except for remoteness from his thesis, there should be no restriction concerning the subject of the proposed research. The important point is that the student must choose the proposed research topic himself, that he receive minimum guidance in preparing his defense and that in judging the proposal, the examining committee insist on high intellectual standards, regardless of utility.

Given the job-oriented goals of the chemical engineering curriculum, it is not likely, nor is it desirable, that there be a major shift in the intellectual menu for most chemical engineering students. But for those students who have creative potential, I hope that we can relax our sectarian interests and expose them to intellectual vistas that at present have nothing to do with contemporary chemical engineering but that some day, through the inventive genius of our younger colleagues, may broaden and enrich the domain of our profession. □

ChE book reviews

ENGINEERING WITH POLYMERS

by Peter C. Powell

Chapman & Hall, 733 Third Ave., New York;
\$49.95 HB, \$25 PB (1983)

Reviewed by

James M. McKelvey

Washington University

Engineering with Polymers by Peter C. Powell, Mechanical Engineering Department, Imperial College, London, is a text designed for final year undergraduate students in mechanical engineering. It assumes no prior knowledge of polymer science or chemistry on the part of the student. It is the author's stated intent to present the "minimum useful knowledge of engineering with polymers within a mechanical engineering degree course."

There are four main sections to the book: (1) The first four chapters provide an introduction to the language, terminology, and technology of polymers. This includes an introduction to polymer

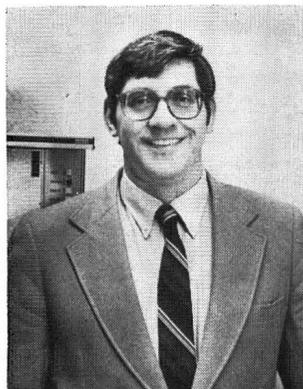
physics, polymer materials science, and polymer processing. (2) Two chapters provide an introduction to the mechanical behavior of polymeric materials, one on stiffness and the other on strength. (3) One chapter outlines the mechanics of fiber reinforced composites, and (4) Two chapters provide an introduction to polymer fluid flow, heat transfer and the effect of processing on properties.

Given the mechanical engineering orientation and purpose of the book it is not surprising that the book's most comprehensive treatment is given to the mechanical behavior of polymers and the mechanics of composites. The treatment of polymer processing is largely descriptive and somewhat superficial. A valuable part of the book are the problems associated with each chapter and an outline of the solutions, which makes the book well suited for self-study. The sections on polymer and composite mechanics would be a useful adjunct to a first course in polymers for chemical engineers, which would probably provide a more comprehensive introduction to property-structure relationships and processing. □

COMPUTER-ASSISTED LABORATORY STATIONS

WILLIAM J. SNYDER, MICHAEL E. HANYAK
Bucknell University
Lewisburg, PA 17837

RAPID INCREASES IN technology, computer literacy requirements, and the current trend to achieve the BS degree in four years or less, create heavy academic pressures on engineering students. With laboratories occupying approximately one third of the student's scheduled time, it is essential that this time be used efficiently by both students and faculty. Current students are demanding more participation in the practical aspects of chemical engineering [1]. However, universities are unable to provide the type of equipment used in industry because of budget constraints, and thus most academic engineering equipment dates from the 1950's. An article in *Chemical Engineering News* [2] describes the deteriorating quality of chemical engineering education as a result of faculty shortages and equipment obsolescence.



William J. Snyder received his BS, MS and PhD degrees at Penn State. He worked for R. W. Coughlin as a postdoc at Lehigh University before moving to Bucknell University. His chemical interests are in thermodynamics, kinetics, polymer science and computer-aided design. He is currently performing research on polymer degradation and chemical sensors. (L)



Michael E. Hanyak received his BS at Penn State, MS at Carnegie-Mellon and PhD at the University of Pennsylvania. After working at Air Products for three years on developing a steady-state process simulator for cryogenic systems, Dr. Hanyak moved to Bucknell in 1974. His chemical engineering interests are in computer-aided design and thermodynamics. (R)

... universities are unable to provide the type of equipment used in industry because of budget constraints, and thus most academic engineering equipment dates from the 1950's.

Also, in the university environment, increased demand on scholarly development by the faculty, larger enrollments, and the low priority of laboratory development have exacerbated the problem.

One way of alleviating some aspects of this problem while increasing the effectiveness of laboratory time is to implement the concept of computer-aided laboratory stations (CALs).

By augmenting the laboratory with computer stations for data acquisition and control, many advantages are obtained, such as

- Increasing the efficiency of student laboratory time
- Providing necessary training for skills needed in industry
- Increasing the student's capability of performing complex and complete data analysis
- Providing students with the opportunity to analyze real problems, exercise engineering judgment, and

TABLE 1
Contents of a Laboratory Station

- Apple II Plus System—48K
- Disk II Floppy Disk & Interface
- Language System with PASCAL
- Second Disk II Drive
- Thermal Printer
- 80-column Video Board
- FORTRAN Compiler Software
- IMI ADALAB Add-On Package
- IMI ADA-AMP Instrumentation Amplifier
- IMI TEMPSense Software
- IMI VIDICHART, Scientific Plotter, and Curve Filter Software
- Secure Equipment Cart
- Electronic Hardware
 - Two Prototyping/Hobby Cards
 - Three Transformers
 - Filters & Circuit Breakers
 - Rack panels & Mounting chassis
 - Nine Relays
 - Thermocouple Jacks & Plugs

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FIGURE 1. Computer Assisted Laboratory Station

- express creativity
- Increasing faculty efficiency, but not at the cost of student interaction.

REQUIREMENTS OF CALS

A laboratory station must be able to receive analog or digital data from sensors, to condition signals, and to either create a display or store the data. Students need to interact with the station by programming in higher level languages such as BASIC, FORTRAN, and PASCAL instead of assembly language. The station should be linked to a mainframe computer by a high speed modem for long term data storage, statistical analysis, and text or graphic output. For the control of laboratory processes, the station must be able to send digital or analog signals to stepping motors and voltage controlled instrumentation. The station should provide a visual status report upon request, contain alarms, and produce good hard copy. Finally, because of space limitations the station is restricted to the size of a small desk or carrel and should be of modular construction.

CALS DESCRIPTION

The critical state of laboratory instruction clearly dictates the focused use of the computer for data acquisition and control. Realizing the advantages of CALS, the Chemical Engineering Department at Bucknell designed and constructed

two portable stations at a cost of approximately \$6000 per station (1981 prices). Each station contains an Apple II Plus computer, a television monitor, two disk drives, a language card, a thermal printer, an 80-column video board, a micromodem, and the ADALAB system from Interactive Microwave, Inc. (IMI). Table 1 describes this equipment in more detail. In addition, software in BASIC from IMI is provided for data acquisition, control and data analysis.

All the equipment, including manuals and disk storage racks, is contained in a mobile 3' x 5' x 2' security cabinet. The portable CAL (Fig. 1) allows students to roll the station to their experiment, plug in wires that monitor temperature, pressure, or composition and to run software to acquire data. Also, the students can write programs to control the experiment. For powerful data analysis, students can transfer the data from Apple diskettes to Bucknell's time-sharing computer using the micromodem. In addition, the student has access to a small graphics tablet (Fig. 2) connected to the Apple for digitizing data that



FIGURE 2. Digitizing Station

is not convenient for data logging but is needed in a computer file.

A TYPICAL EXPERIMENT

The characteristic response is an important consideration when selecting or specifying sensors. For example, accurate control of humidity is often required in chemical processes and in heating-ventillation-air conditioning systems (HVACs). A knowledge of sensor response time over a range of operating conditions is necessary for the determination of a transfer function with humidity

... the work load on the faculty is reduced without sacrificing quality. The use of the CAL concept for a portable station provides flexibility and ease of operation without expensive duplication of equipment. Educational laboratories now can simulate industrial environments at a minimum cost.

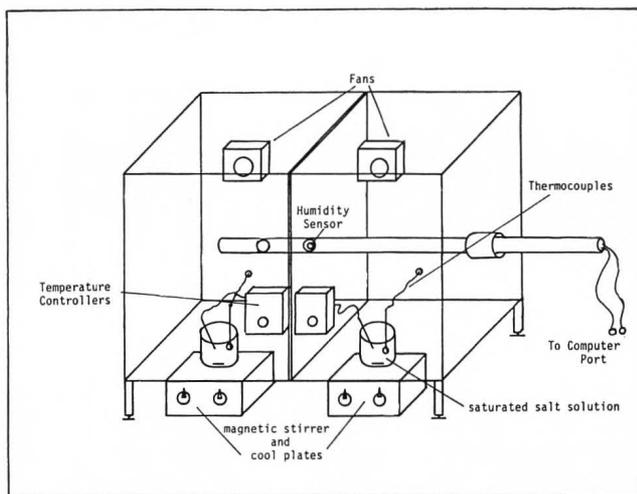


FIGURE 3. Diagram of Humidity Chamber

as the measured variable. The objective of this experiment is to determine the response times of a solid state humidity sensor at various humidity conditions and to develop an empirical model for the sensor.

The sensor used in this experiment is a small (0.5 cm) fast response solid state device. Figs. 3 and 4 show an environmental chamber for subjecting the sensor to step changes in humidity. The humidity in each well-mixed chamber is controlled by varying the temperatures of saturated salt solutions. The sensor is mounted on a sliding rod and can be rapidly transferred from one chamber to the other. The voltage output from the sensor (0-3 volts dc) is sent to an ADALAB

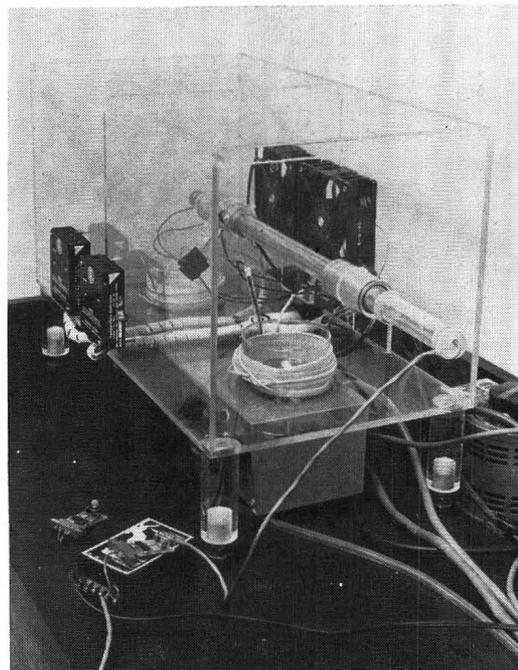


FIGURE 4. Humidity Chamber

system which is controlled by the Apple computer. Use of the VIDICHART software enables data acquisition of sensor voltage. Typical sensor response data expressed in terms of a first order time constant are shown in Table 2 and Fig. 5.

SUMMARY

Personal computers, when configured for laboratory use, not only increase the efficiency of students but provide an exciting experience for

TABLE 2
Calculated Sensor Response Data

Salt	Soln. Temp °C	Air Temp. °C	RH, %	Trial 1 t, secs.	Trial 2 t, secs.
Run #1					
Potassium Fluoride	31.5	30.4	26.5	75.0	75.2
Sodium chloride	24.0	28.4	75.5	82.8	82.5
Run #2					
Lithium chloride	11.7	25.4	11.0	12.2	12.5
Potassium sulfate	10.8	25.8	98.1	15.8	15.8
Run #3					
Lithium chloride	24.1	25.3	11.5	1.4	1.3
Potassium sulfate	23.8	25.2	97.3	9.0	9.1

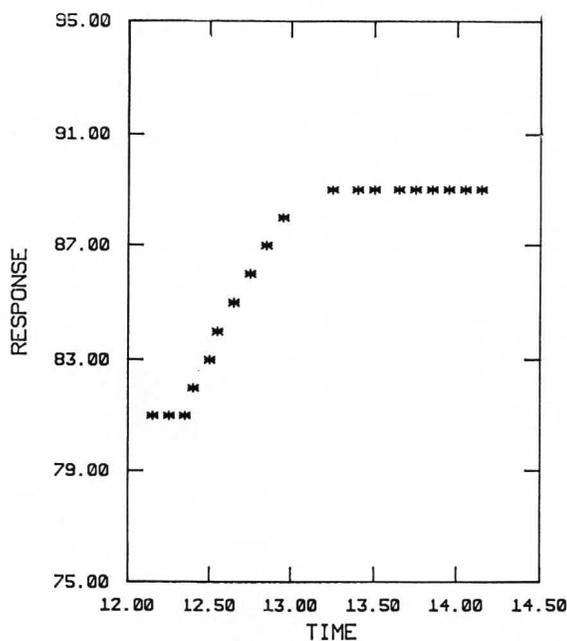


FIGURE 5. Sensor Output

ChE book reviews

DIFFUSION IN LIQUIDS

by H. V. Tyrrell, and K. R. Harris.

Butterworths (1984). 448 pages, \$75.00.

Reviewed by E. N. Lightfoot
University of Wisconsin

This book, originally conceived as a revision of Tyrrell's "Diffusion and Heat Flow in Liquids," is intended to give the non-specialist a balanced summary of the literature on both theoretical and practical aspects of diffusion in liquids, of sufficient depth to provide effective access. Both translational and rotational diffusion under the influence of arbitrary driving forces, in binary as well as multi-component systems, are discussed. It was deemed that heat flow could no longer be included in a book of reasonable length without undue sacrifice of depth.

The first four chapters are used to establish the foundations of transport theory, starting with the classical phenomenological description. The phenomenological introduction is followed by a summary of non-equilibrium statistical mechanics which permits, at least in principle, the calculation of transport properties from molecular parameters. The primary purpose of these chapters is to pro-

vide a unified treatment adequate for understanding modern methods of interpreting experimental data.

Chapter 5 provides rather detailed descriptions of the most widely useful techniques for gathering data, and Chapters 6 to 8 are devoted to interpreting experimental results in terms of kinetic theory and physical models.

Translational diffusion coefficients have been measured for well over a century, and many classic techniques have been highly refined and are still widely used. Among those described by the authors are optical techniques based on Gouy and Rayleigh interference phenomena (much improved in the last decades by the availability of lasers), diaphragm cells, use of Taylor dispersion (which has become important because of its speed), and light scattering.

Photon correlation techniques have made light scattering methods particularly important for macromolecules such as proteins, but effective use of these methods requires understanding of the underlying physics, as does the use of nuclear magnetic resonance for description of rotational diffusion. Largely because of this need Chapter 5 is rather long and detailed.

Chapter 6 is devoted to the interpretation or

ACKNOWLEDGEMENT

We would like to thank Robert J. Murcek for his ideas and time in implementing the CALS.

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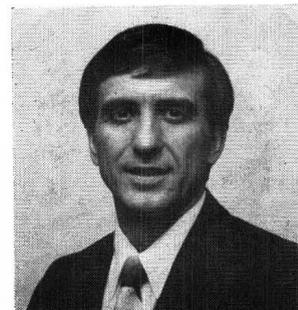
A SEQUENTIAL DESIGN LABORATORY EXPERIMENT FOR SEPARATING PARTICLES BY FLUIDIZATION PRINCIPLES

DONALD D. JOYE
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Villanova, PA 19085

ONE OF THE MOST frequent activities of practicing chemical engineers is design—in one form or another. Yet the laboratory rarely, if ever, provides experience in this area. Many good reasons exist for this, but these will not be discussed here. Rather, one experiment will be discussed in the hopes of stimulating similar experiences for chemical engineering students in laboratory.

The laboratory experiment in sequential design was organized around a central problem—to separate a mixture of essentially two kinds of particles by fluidization principles. Fluidization had only been touched upon briefly in a previous course, so the subject matter was new but not completely unfamiliar. The problem was defined as follows: in certain processes solid particles are treated to expand their structure or create large internal pore volume. Not every particle is successfully treated, and the need exists for separating the untreated or poorly-treated particles from those that meet the product requirements. The particles differ in density and size, so that some fluidization or elutriation technique can be used for the separation. The overall objective of this semester-long exercise was to design, build, and operate an apparatus to solve the problem. Fluidization laboratory exercises have been described previously [1] but not in the sense of a design problem with the goal of building a functioning unit.

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Donald D. Joye is currently Assistant Professor of chemical engineering at Villanova University. He joined the staff at Villanova in 1981 after previous teaching and industrial experience. He received his BSE degree in chemical engineering from Princeton University in 1967 and his MS and PhD from Lehigh University in 1969 and 1972, respectively. Dr. Joye's research interests are in fluid mechanics and related fields, heat transfer, and the unit operations. He is a registered patent agent and has particular interests in teaching problem solving skills and the innovation process.

Each lab group worked on a separate step of the design in a sequence selected by the instructor in a manner similar to the way a design team might function. All lab groups were required to read and understand basic fluidization principles as described in standard textbooks such as Foust, et al. [2], McCabe and Smith [3], etc. Each group, when its time came for the lab, was given an assignment and shown why that particular job needed to be done.

Students working in the early stages needed to characterize the particles with respect to size (equivalent diameter) and true density, in order to calculate terminal speeds and fluidization velocities. The particles were highly irregular, which made the job somewhat challenging. Particles of a given kind were not all the same size, so some statistics [4] were used to quantify expected variations. Other lab groups tested these results by finding terminal speeds experimentally. Fluidization theory was then used by subsequent groups to select an appropriate fluid velocity that would carry the light particles out with the fluid and

leave the others behind. Design of the column and selection of the prime mover from materials available in the lab (a design constraint) were then carried out. Several groups then participated in constructing and testing the unit. Finally, operation of the equipment to achieve the desired objective was undertaken—with all groups watching the final test runs.

THEORY

Fluidization theory and drag force phenomena on particles are well-known and well-documented [5]. Irregularity of the particle shape, however, creates some interesting problems for the students. What is the diameter of an irregularly shaped particle? Would a shape factor be appropriate? Necessary? How does one measure true density when the geometry cannot be characterized clearly? Most of these questions were answered by application of fluidization principles and problem solving skills.

Calculation of terminal speed also involves unknowns. Air was selected as the fluid due to the nature of the particles. The terminal speeds of the particles in air could be calculated after the regime of fall was known. The trial-and-error method of Foust et al [2] or the K-factor approach of McCabe and Smith [3] could be used here. Then the appropriate terminal speed equation could be selected. For example, if the fall of the particle through air were in the Newton's Law region where the Reynolds numbers are relatively high, e.g. greater than about 500 but less than about 200,000, the terminal speed can be calculated by

$$v_t = 1.75 \sqrt{g D_p (\rho_p - \rho) / \rho} \quad (1)$$

where v_t = terminal speed
 g = acceleration of gravity
 D_p = (equivalent) diameter of particle
 ρ_p = density of particle
 ρ = density of fluid.

The minimum fluidization velocity is the gas velocity at which fluidization begins. Prior to this condition air would pass through a bed of particles without disturbing them (packed bed). Once the minimum fluidization velocity is exceeded, the bed expands and is said to be fluidized, up until the terminal speed is reached. At this point the particles are carried along with the fluid, and a stable bed of particles no longer exists. The Ergun equation [2, 3, 5] can be used with a substitution for the pressure drop term to give an equation from

The overall design concept was that of a vertical column of a certain height and diameter connected to an air blower with the appropriate pressure drop—throughput characteristics.

which the minimum fluidization velocity can be calculated [3]

$$\frac{1.75 D_p^2 \rho^2 v_o^2}{\phi \epsilon_M^3 \mu^2} + \frac{150 D_p \rho (1 - \epsilon_M) v_o}{\phi^2 \epsilon_M^3 \mu} - \frac{D_p^3 g \rho (\rho_p - \rho)}{\mu^2} = 0 \quad (2)$$

where ϕ = shape factor
 ϵ_M = packed bed porosity
 v_o = superficial (average) velocity.

In this case the shape factor was set equal to 1.0, because the geometry of the particles could not be quantified by well-known methods. The bed porosity was measured experimentally.

Once the terminal speed and minimum fluidization velocity have been determined, a porosity diagram (shown in the next section) can be constructed for both kinds of particles. From this diagram an appropriate air velocity can be selected. In addition, this diagram shows what will be happening to the other kinds of particles at the selected operational air velocity.

Design of the column reduces to selecting an appropriate column diameter considering the particle diameters and the fact of fluidization. Blower sizing can then be done on the basis of volume throughput and pressure drop. The pressure drop through the fluidized bed can be estimated by equating the force exerted on the solids to the force of gravity minus the buoyant force of the displaced fluid [3]

$$\Delta P = g h_M (1 - \epsilon_M) (\rho_p - \rho) \quad (3)$$

where ΔP = pressure drop
 h_M = height of packed bed of solids

This pressure drop is essentially constant for batch fluidization (prior to entrainment). When a mixture of particle types is present, and one type is being entrained while the other is not, it becomes difficult to calculate the bed pressure drop accurately and some estimate must be used.

SEQUENTIAL ASSIGNMENTS AND RESULTS

Twelve lab groups participated in this experiment. The first six groups worked on preliminary design calculations, and the last six worked on the design, construction, operation, and checking of

calculations.

The first lab group determined an average diameter and density for the relatively dense and non-porous particles. This was accomplished by weighing sets of particles and dropping them into a graduated cylinder partly filled with oil, so that the volume change could be observed. The fluid used in the cylinder was oil, which would slow down or prevent absorption of the liquid by the particles. The average density was found to be 1.23 g/cc. The total volume of a known number of particles was then used to calculate a volume-average diameter based on spherical geometry. This diameter was 0.574 cm. The methods of achieving the assigned objectives were left to the

more porous particles. These particles were very porous and much more irregular than the others. Volume displacement techniques were much more difficult to perform. These particles were also more fragile than the dense ones. One group decided to take ruler measurements of the longest and shortest diameter they could measure and average the results. This gave an arithmetic average diameter of 1.47 cm with a standard deviation of 0.34 for a sample size of 50. The second group decided to measure diameter by terminal speed experiments. This gave 1.19 cm for the diameter with a standard deviation of 0.21 for a sample size of about 20. One group calculated a density based on weight of the particle, the arithmetic

The separation was successfully effected by the last group, and a good time was had by all at the demonstration. What material was used for the particles? Popped and unpopped popcorn kernels. Needless to say, the students consumed the data with enthusiasm.

group members with little input from the instructor.

The second lab group also worked on the dense, nonporous particles. They used a similar technique for density measurement but with water as the working fluid. Their density was 1.31 g/cc, slightly higher than the previous group's value. This could be explained in part by water absorption reducing the displaced volume, and in part by variation in samples taken from the broad particle population. An overall average density of 1.27 was used. To find the equivalent diameter this group decided to try a terminal speed experiment. They first dropped spheres of known diameter and weight into a heavy mineral oil to determine its viscosity (Reynolds numbers were in the Stokes' Law region [2, 3]), then dropped particles into the same oil, measured the terminal speed, and used the Stokes' Law terminal speed equation to calculate a diameter (Reynolds numbers for this case were just less than 1.0 and Stokes' Law could be used). This projected diameter was found to be 0.476 cm, which is less than the previous estimate. The particles were not spherical and apparently slightly elongated, so that the smaller cross-section would be perpendicular to the flow direction in free-fall experiments. This group also calculated the packed bed porosity by volume displacement (of oil this time) and the minimum fluidization velocity from Eq. 3. Packed bed porosity, ϵ_M , was 0.36, and the minimum fluidization velocity in air at 23°C was 1.13 m/s.

The next two groups worked on the less dense,

average diameter and spherical geometry. The average density was 0.042 g/cc with a standard deviation of .022, quite a large spread. The average terminal speed of these particles in air was measured to be about 3.5 m/s with a standard deviation of 0.31. Distance of fall was about 4 m, so true terminal speeds were probably a bit higher.

The following two groups completed the preliminary calculations by determining the terminal speed in air of both dense and light particles, finding minimum fluidization velocity and packed bed porosity of the light particles and evaluating the distance vs. speed relationship in free fall to establish the reliability of terminal speed experiments. One of these groups calculated density and porosity by pouring oil into a beaker filled with particles. A screen was used to keep the particles submerged. Weights and volumes were recorded. They reported a density of 0.08 g/cc and a porosity, ϵ_M , of 0.68. This density was considered to be too high because of absorption of oil and compaction and breakage of the particles, so an average of the two density estimates was used. The calculated minimum fluidization velocity for the light particles was 1.04 m/s in air at 23°C.

The terminal speed of the more dense particles falling through air was also measured experimentally. In the early measurements, however, the particles fell so rapidly through 4 meter distance that accurate timing could not be done. Thus, another group needed to establish what distance was needed to reach terminal speed, and what distance

was required to get an accurate measure for terminal speed. This can be carried out by a graphical integration of the force-balance equation as discussed by McCabe and Smith [3] when distance is set equal to the integral of $v dt$. The results showed that the light particles needed about 2.75 m to reach 95% of terminal speed, while the more dense particles needed about 22 m to reach 95% of their terminal speeds. Terminal speed experiments for the light particles were then repeated, subtracting out the distance required to reach terminal speed and timing the fall from this point on. The results were not significantly different than before. For the more dense particles a place greater than 22 m tall and still safe for students to be running an experiment could not be found on campus, so the students decided to settle for the stairwell of a building five stories high and time the fall for the last two stories. The average terminal speed was calculated from 45 runs to be 16.2 m/s with a standard deviation of 3.1.

The results for preliminary calculations are summarized in Table 1. This information can be used to construct a bed porosity chart as shown in Fig. 1. The data points on the figure are from experimental tests discussed subsequently.

FINAL APPARATUS AND PERFORMANCE

During the remainder of the semester six other groups worked on the design of the separator using the information provided by the first six groups. The overall design concept was that of a vertical column of a certain height and diameter connected to an air blower with the appropriate pressure drop—throughput characteristics. Two groups rummaged about the lab looking for suitable equipment. Eventually a plastic column .203 m (8-inches) nominal diameter and about 1.2 m long was found and deemed suitable. Squirrel cage blow-

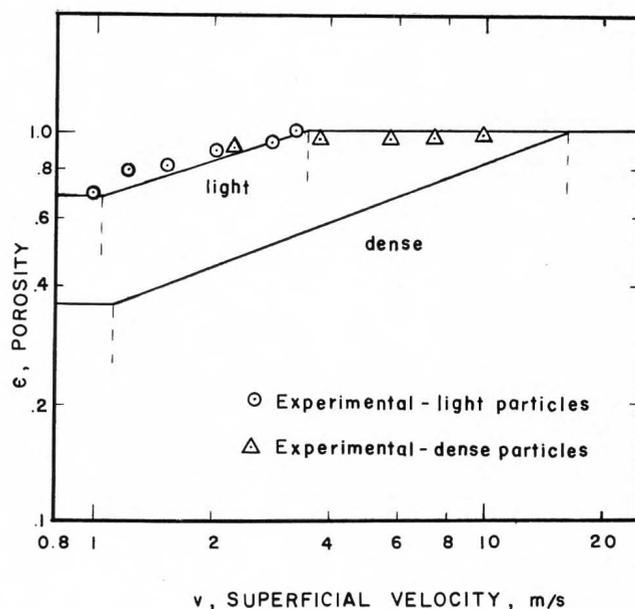


FIGURE 1. Porosity diagram for light and dense particles with experimental results.

ers were considered and discarded on the basis of insufficient throughput and probably not enough pressure drop. Finally a 0.75 kW (1 hp) centrifugal blower was decided upon. Estimations were made rather roughly in this stage. A safe design velocity was chosen to be about 4.5 m/s, at which point over 90% of the light particles would be entrained, and the dense particles would be in a fluidized state. The bed height could only be guessed at, since the amount of dense particles in the feed was not precisely known. The percentage of dense particles (by number) in the feed was estimated to be $10\% \pm 5$.

The third group constructed the apparatus. Some modifications were, of course, necessary. A screen was placed at the bottom of the column to prevent material from entering the blower. It was decided to operate batchwise given the constraints, and an adaptor had to be fabricated to connect the .203 m (8-inch) diameter column to the .127 m (5-inch) diameter blower outlet pipe. Of course no specifications were available for the blower, so the students had to determine the throughput experimentally. The inlet side of the blower contained a throttle plate and an orifice-manometer setup to do just that. A schematic of the apparatus is shown in Fig. 2. It soon became obvious that a means for collecting the entrained particles was required. A fourth group designed a collector, but after considering the effort required to build it, decided to

TABLE 1
Summary of Results of Preliminary
Design Calculations

QUANTITY	DENSE PARTICLES	LIGHT PARTICLES
Estimated diameter, cm	0.574	1.47
Terminal speed diameter, cm	0.476	1.19
Average density, g/cc	1.27	0.06
Packed bed porosity, ϵ_M	0.36	0.68
Min. fluidization velocity, m/s	1.13	1.04
Terminal speed in air, m/s	16.2	3.5

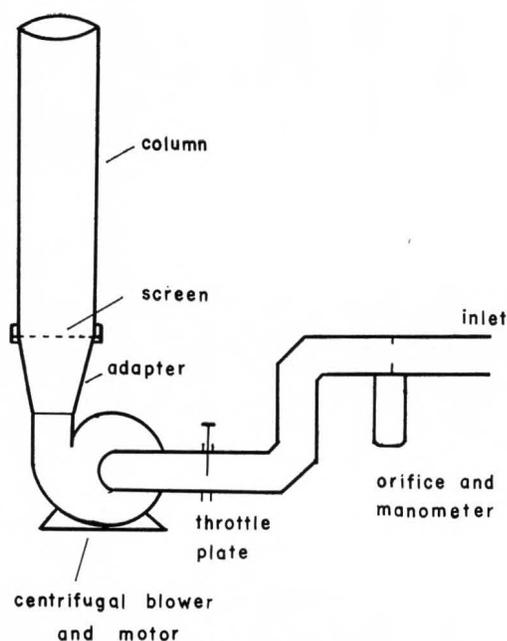


FIGURE 2. Apparatus

make do with a large plastic trash bag with holes punched in it.

The estimated pressure drop was about 5 cm (2 inches) of water; the required throughput was $0.13 \text{ m}^3/\text{s}$ (280 cfm) of air at 23°C , and the input power required was about 0.1 kW (.125 hp). With a blower of .75 kW (1 hp) rating, the (installed) maximum throughput was found to be $0.2 \text{ m}^3/\text{s}$ (425 cfm), which was plenty adequate, if not a bit oversized.

The last two groups operated the column. One group checked the predicted porosity diagram, and the other group operated the column for separation. From the data points shown in Fig. 1, the predicted porosity curve was closely approximated in the case of the light particles. In the case of the dense particles, the experimental results were nowhere near the predicted curve. One could easily see the reason for this during the operation of the unit when the dense particles alone were present. Air from the blower was not uniformly distributed across the column cross-section. In fact it appeared that circulation currents were present, such that half the bed was not even fluidized, while the other half was shooting about inside the column. Only a crude estimate of the bed height could be made. This situation was clearly different from textbook expectations and gave the students a real insight into the difficulties of maintaining fluidized beds. The light particles

were larger, less dense and required a lower velocity for fluidization, such that the above phenomena, though still present, was much reduced in intensity. Designing an air distributor could have been undertaken at this point to overcome the problem—but wasn't because of lack of time. This would have brought the experimental data for the dense particles more in line with expectations from theory.

The separation was successfully effected by the last group, and a good time was had by all at the demonstration. What material was used for the particles? Popped and unpopped popcorn kernels. Needless to say, the students consumed the data with enthusiasm.

CONCLUSIONS

The foregoing has presented the details of an unconventional laboratory exercise which brings design experience to the students in a laboratory setting. In addition the exercise has proved powerfully supportive of the following teaching values:

- How to deal with the unexpected.
- How to deal with constraints.
- How to make engineering decisions where precise measurement is impossible or when good information is not available.
- How to size and modify equipment.
- How to accomplish an overall objective by breaking down the larger job into smaller parts and working to solve one part at a time.
- The value of checking back and evaluating past work.
- Gives students satisfaction at seeing the job done successfully and understanding where their part fit into the whole effort.
- Challenges the students with a real-world problem that has an achievable solution reasonably within their grasp.
- It was fun, something students could relate to easily.
- Stimulated students to think beyond the immediate solution, for example several students recognized that the apparatus would not do for home application! □

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ChE book reviews

FINITE ELEMENTS: MATHEMATICAL ASPECTS, Vol. IV

By J. T. Oden and G. F. Carey;
Prentice-Hall, Englewood Cliffs, NJ 07632
(1983) \$29.00 Cloth

Reviewed by
Bruce A. Finlayson
University of Washington

The finite element method is becoming increasingly popular as a method for solving differential equations in chemical engineering. Consequently, students are demanding information about it even if their professors obtained their training before finite element methods were well-known. For this reason, short concise books on the finite element method are especially welcome. This book is Volume IV in a series of six books by the authors. Each book is a succinct book on this subject. Since chemical engineers may be more interested in the other volumes in the series the topics are listed here: Volume I—An Introduction; Volume II—A Second Course; Volume III—Computational Aspects; Volume V—Special Problems in Solid Mechanics; Volume VI—Fluid Mechanics.

Volume IV begins with the chapter on nomenclature, defining Sobelov spaces for example. This beginning chapter emphasizes to the reader that it is the mathematical aspects of the theory that are to be presented. The next chapter on interpolation theory shows the best error estimates that can be achieved since a finite element approximation to solutions of differential equations can never be better than the interpolation of the exact solution. Then 3 remaining chapters deal with elliptic boundary value problems: the regular approach, a mixed method, and a hybrid method. In the mixed method one solves for the function and derivative (like temperature and heat flux) while in the hybrid method one relaxes interelement continuity and adds a Lagrange multiplier constraint.

In all three chapters, the variational theory is first presented, thereby changing the differential equation to a variational statement. Then error estimates are provided for the finite element approximations of these problems and theorems are proved under which they apply. Finally example applications are given usually to the Poisson equa-

tion or the heat conduction equation with a known generation term.

A book such as this is heavy going unless the reader has some exposure to functional analysis, although the theorems are clearly identified and can be used without studying the proof. Some of the conditions of the theory (Babuska-Brezzi condition) could not be used, though, without a functional analysis background. Thus this book will appeal to a small segment of the chemical engineering audience, but is a welcome companion to the other volumes in the series. □

ChE letters

FIRST ChE DOCTORAL DEGREES GRANTED

Dear Sir:

Since I think it is important that you know this, I take great pleasure in informing you that on July 4, 1984, the "Universidad Nacional del Litoral," in the city of Santa Fe, Argentina, granted the first doctoral degree in Chemical Engineering in this country, the thesis work having been carried out at the Institute of Technological Development for the Chemical Industry (INTEC). The second doctoral degree, this time conferred to a woman, was also granted by UNL and INTEC.

Sincerely yours,

Dr. Alberto E. Cassano
INTEC

ChE books received

Machine Design Fundamentals: A Practical Approach, U. Hindhede, J. R. Zimmerman, R. B. Hopkins, R. J. Erisman, W. C. Hull, and J. D. Lang; John Wiley and Sons, New York, 10158; 642 pages, \$43.95 (1984)

Handbook of Industrial Water Conditioning, Eighth Edition; Betz, Trevose, PA 19047; 437 pages (1983)

Coal Liquefaction Products, Vol. 1. Edited by H. D. Schultz; Wiley-Interscience, NY 10158; 415 pages, \$65.00 (1983)

Plastics Products Design Handbook, Part B: Processes and Design for Processes, Edited by Edward Miller; Marcel Dekker, Inc., NY 10016; 392 pages, \$55.00 (1983)

Pascal Applications for the Sciences: A Self-Teaching Guide, Richard E. Crandall; John Wiley & Sons, New York; 246 pages, \$14.55 (1984)

A RESOURCE-BASED APPROACH TO ChE EDUCATION

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THERE IS A GRAVE need to modernize chemical engineering education within universities. This contribution presents the current problems and describes the proposed plan of the Queensland department to implement a scheme for resource-based education in chemical engineering. The financial cost over the period 1984-1989 is estimated to be as high as half a million dollars. Additional efforts of dedication and self-sacrifice by staff are necessary but cannot be quantified.

THE PROBLEM

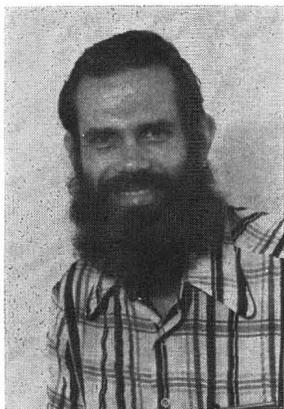
The traditional mode of instruction in chemical engineering over the past forty years has mainly been lectures supplemented by some prob-

lem and laboratory classes, and yet outside the university a major information revolution has taken place. In the light of these changes the time is prudent to evaluate whether better use of new resources can alleviate the problems that are perceived by this department. These problems are touched on in the following paragraphs.

Content. The content of the degree course is expanding in response to rapid growth in both the breadth and depth of engineering knowledge. The rapidly expanding base of engineering knowledge tends to submerge and confuse students' understanding of fundamental principles.

Structural Changes. The graduate in industry has at his command a vast resource of information in databases and computer software packages. He is no longer expected to carry out routine engineering calculations but, rather, has to select the correct computer package and critically evaluate the results. To perform these tasks a student

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waste-water treatment, grinding circuits, and mineral flotation. (C)

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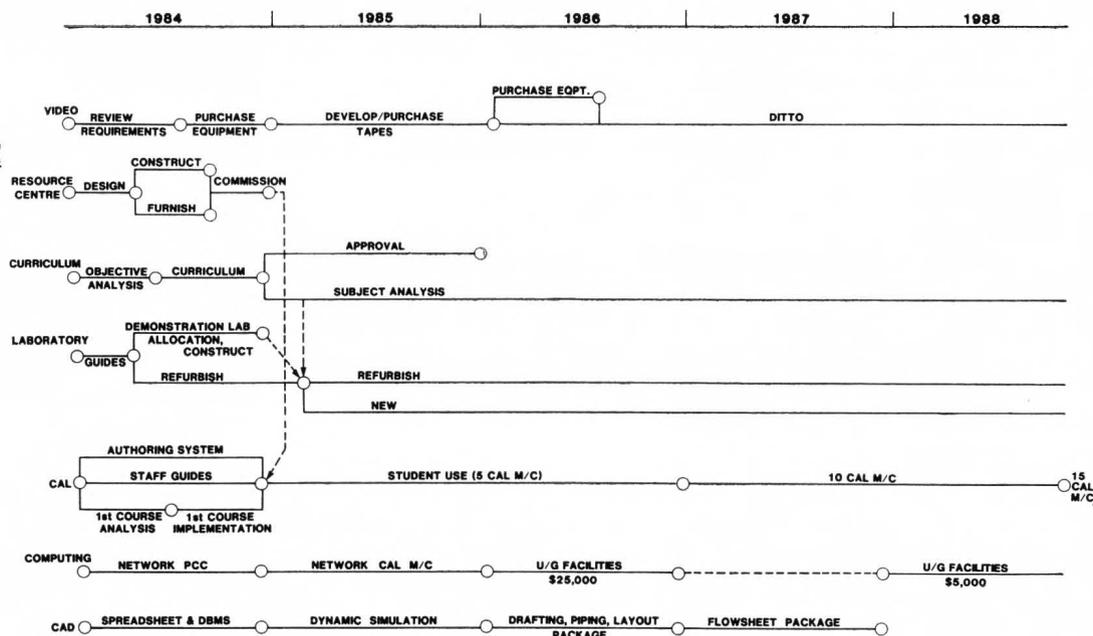


FIGURE 1.

should be thoroughly grounded in fundamentals and exposed to various software packages.

Laboratory. Much of the laboratory equipment and many experiments in the Queensland Department of Chemical Engineering are becoming obsolete. As a result, some of the skills students are being taught are increasingly irrelevant in a modern industrial environment. Indeed, in many areas industrial practice is far in advance of our laboratory experiments.

Student/Staff Ratio. The increasing student/staff ratio means less feedback to students in terms of comments on tutorial problems and practical reports. We need to promote more interactive teaching practices and more efficient use of student-staff contact time, i.e. more opportunity for individual contact and discussion and fewer formal "one-way" lectures.

Literacy. In the age of electronic media, incoming students are less inclined and less able to extract information efficiently from books. While we may decry this trend, we must nevertheless adapt to it. Course notes, directed reading, and information databases are some possible aids in this area.

Motivation. The changing social environment and the secondary school environment are no longer producing students who are "automatically" motivated. We need to introduce instructional techniques to instill motivation as well as concepts

and knowledge. Course and subject objectives and the increased use of interactive media and personal contact will assist.

A SOLUTION: RESOURCE-BASED EDUCATION

To meet the challenge of educating chemical engineers for the 1990s, a fundamental evaluation of the curriculum and the mode of instruction is being carried out in the department. It is recognized that the traditional mode of instruction needs to be reviewed, together with curriculum re-evaluation.

After much discussion in the department during 1983, a plan has evolved to change the mode of instruction towards a resource-based and partly self-paced learning environment.

The plan is to implement the new mode progressively from 1985, after a detailed curriculum re-evaluation and writing of aims and objectives for the course and individual subjects has been carried out. Fig. 1 shows the current planning diagram for the project. The main features of the new scheme are described in the following paragraphs.

1. Reducing the total number of lectures given in the course and reserving the remaining lectures to concentrate on fundamental principles. Currently there are a large number of lectures and students are often unable to discriminate be-

The traditional mode of instruction in chemical engineering over the past forty years has mainly been lectures supplemented by some problem and laboratory classes, and yet outside the university a major information revolution has taken place.

tween fundamental principles and the vast amount of factual material presented.

2. Setting up self-paced laboratories, with long opening hours attended by academic staff. The laboratories will be refurbished to modern engineering standards and experiments will be designed to meet specific objectives. Written or video tape aids will be available to assist students in carrying out experiments. The objectives of these experiments may be (i) teaching of experimental design, (ii) demonstration of difficult to understand concepts, and (iii) simulation of experiments carried out in industry. Currently, students are required to carry out specific experiments at scheduled classes. In a class-like atmosphere with many students working at one time, staff-student contact often takes the form of staff advising students what to do rather than discussion of the results and underlying precepts. By providing better guidance on how experiments should be conducted, more time will be available for discussion of results. The quality of staff-student contact will improve.

3. Setting up a laboratory of demonstration experiments. They will be very simple and easy to operate experiments for illustrating basic principles and a variety of observed phenomena. Many will be transportable to lecture or tutorial and all will be accessible to students whenever they wish. The ability to observe phenomena in the laboratory without the usual long preparation, procedures, and reporting and being able to choose their own time and pace should provide students with motivation and a valuable complement to other resources.

4. Setting up a self-paced computer-aided learning (CAL) laboratory with long opening hours attended by academic staff. Only material specifically suited for CAL will be taught in this mode. Some CAL courseware will be prepared by our own staff and where possible some will be purchased. To significantly reduce the time required for preparation of CAL lessons, the lesson will be prepared with the understanding that a tutor will be available nearby to provide assistance to students. The staff member will be in attendance during opening hours to discuss problems with students providing effective personal contact. Cur-

rently a student is taught through lectures, often at a pace not appropriate to him and at a time when he may not be receptive, and with little or no opportunity for review.

5. Making available a comprehensive range of chemical engineering software packages, physical and chemical properties data package, computer-aided design packages, etc. We are in the process of building up such a library of packages. Students will be exposed to resources comparable to those available in industry. They will be trained in the use of computer databases for access to reference knowledge and in critical evaluation of computer results in a manner required of them as practicing engineers in industry.

6. Making available audio-visual reference material. Much industrial training is presented today with the aid of professional audio-visual aids. Some of these quality aids are also ideal university teaching aids and an attempt will be made to obtain such materials wherever possible. Audio-visual materials, particularly video-tapes, offer the opportunity of bringing the industrial environment to the student when the student requires this information. Presently the student receives this information only from field trips or printed media, the timing of which may not coincide with the need for such knowledge.

CURRICULUM REVISION

In redesigning a course, as opposed to starting from nothing, there are certain pragmatic constraints. In the present case, the department controls only the second to fourth years of the course. This period has been divided into:

- **Background science subjects whose content is generally determined by many votes.**
- **Core chemical engineering subjects which define the basic graduate requirements.**
- **Elective subjects which will be used to enable the student to gain some breadth and also some depth in a particular specialist area.**

The elective specialist areas are mainly determined by the expertise of the staff. The other elective subjects are a "smorgasbord" of subjects offered within and outside the department. The current review is of the core chemical engineering curriculum.

Course Aims. The development of aims for the core course is following the traditional systems approach by starting with a small number of general aims for the graduate:

- Given the task of making a product from given raw materials with the maximum economic return, the graduate should be able to synthesize a suitable integrated set of unit operations (ability to synthesize an integrated process).
- Given the task of designing or analyzing a unit operation or process, the graduate should be able to formulate a model in terms of the basic mechanisms involved (fluid mechanics, thermodynamics, heat transfer, mass transfer, reaction kinetics) and to solve the resulting equations to determine conditions for optimum performance or performance for given conditions (ability to design or analyze parts of a process).
- Given a process plant and a set of environmental constraints, the graduate should be able to determine the optimum conditions for operating the process and to design a measurement and control system and/or operating strategies to maintain the process at the optimum conditions despite disturbances (ability to operate a process).
- Given a task to perform and sufficient resources, the graduate should be able to plan and organize the resources to complete the task in minimum time (ability to perform).
- Given a message to communicate, the graduate should have the written and oral skills to effectively communicate with those above, at, or below his/her level of responsibility and/or expertise.

These global aims have been hierarchically decomposed into about 80 more specific aims.

The next stage was to assign some weighting or importance to each aim. The professional engineering institutions have certain requirements in this regard. Therefore the aims were grouped according to their guidelines which defined some group weightings. Individual aims were then weighted within these groups by staff consensus.

The aims were then reordered into six groups (two semesters each of three years) taking into account the fact that many are prerequisite for others, the available contact hours (which varies somewhat by semester), and the natural grouping by content. This defined subjects each with 2 to 5 aims and a weighting which could be converted into a credit point figure.

Subject Objectives. There is a large literature on objectives and on their preparation, typified by texts such as Rowntree [4] and Briggs [1]. They are generally prepared by hierarchical decomposition and then ordered and represented as flowcharts,

network diagrams, logic diagrams, etc. Himmelblau [2] has done this very nicely and this text is used as the basis of an introductory second year subject.

In the present project, academic staff will be given half-years off their normal duties to prepare objectives and then instructional material for subjects in their area of expertise or knowledge. Eventually each of the core chemical engineering subjects will be defined by a set of objectives relating back to the course aims.

It is hoped that such detailed subject specifications will avoid the overlap and gap problems which usually develop in courses over the years. It is also more likely to succeed in core subjects where knowledge is not at the forefront of research and is reasonably static.

Teaching Strategies. The core section of the course will be resource-based and will combine the strategies of guided discovery and of conver-

After much discussion in the department during 1983, a plan has evolved to change the mode of instruction towards a resource-based and partly self-paced learning environment

sational learning as defined by Pask and Lewis [3].

Both these strategies consider the student to be a problem solver and consider knowledge to be an elaborate structure or network of concepts. The extent of the structure or network will be defined by the subject objectives.

The guided-discovery strategy has the teacher defining the knowledge structure and dividing it to set the students a series of sub-goals which they explore using resources and problems supplied by the teacher. For example, the teacher may define a sub-goal by a lecture and supply a study guide, laboratory experiment, and problem sheets as resources and then assess progress individually in tutorials and by a test. Using this strategy, a typical subject might be divided into six two-week modules, each started with a lecture and followed by two tutorials and a test.

The conversational-learning strategy has the teacher defining the knowledge structure, but allowing the student much more freedom. The student decides upon the order in which material is covered and is free to use supplied resources and

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EXTENDED FORM OF THE GIBBS PHASE RULE

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THE FOLLOWING EXTENDED form of the Gibbs Phase rule can be used to determine the degrees of freedom possessed by a system consisting of several species which partake in one or more chemical reactions.

$$f = (N - r - s) - p + 2 - t + u \quad (1)$$

where f = degrees of freedom

N = species

r = independent reaction equilibria

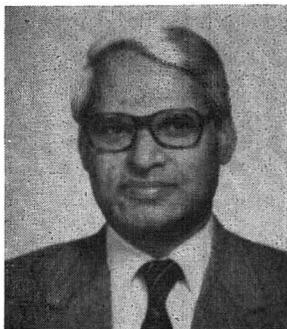
s = stoichiometric constraints

p = phases

t = special or additional constraints

u = special or additional variables

A species is defined as a chemically distinct entity. For instance, in a system comprised of $H_2O(g)$ and $H_2O(l)$ the number of species is but one. On the other hand, in the $H_2(g) - O_2(g) - H_2O(g)$ system, there are three species. In any system, once the species that occur have been



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identified then the corresponding atom matrix can be constructed. For this purpose, each species is represented by a line vector of atom coefficients. For the said $H_2(g) - O_2(g) - H_2O(g)$ system we obtain

	H	O
$H_2O(g)$	2	1
$H_2(g)$	2	0
$O_2(g)$	0	2

The resulting atom matrix is reduced to an echelon form utilizing standard procedures [1]. This gives

$$\begin{bmatrix} 2 & 1 \\ 2 & 0 \\ 0 & 2 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & \frac{1}{2} \\ 0 & 1 \\ 0 & 0 \end{bmatrix} = E$$

The rank of the echelon matrix E , defined as the number of non-zero rows, is seen to be 2. This also happens to be the rank of the parent matrix. Thus

$$c^* = \text{rank of the atom matrix} = 2.$$

It is well to note that underlying this system, there are but two kinds of atoms—namely H and O. Thus, the above findings with regard to the rank of the atom matrix may appear to be entirely predictable; and it may be supposed that c^* is equal to k where k is defined as the kinds of atoms that comprise the species present in the system. However, careful examination uncovers the fallacy of such a supposition. The following example illustrates the point. In the $CaCO_3(s) - CaO(s) - CO_2(g)$ system, it is clear that there are three kinds (Ca, C, and O) of atoms. The corresponding atom matrix is constructed as follows:

	Ca	C	O
$CaCO_3(s)$	1	1	3
$CaO(s)$	1	0	1
$CO_2(g)$	0	1	2

This is reduced to the echelon form in the usual

The stoichiometric constraint is a unique constricting relationship between the mole fractions of two or more species occurring in a given phase. It is well to note that the scope of the stoichiometric constraint does not extend beyond the particular phase that is under consideration.

manner.

$$\begin{bmatrix} 1 & 1 & 3 \\ 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 1 & 3 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{bmatrix} = E$$

Thus, the rank c^* of the atom matrix is only 2 despite the fact that there are three kinds of atoms underlying the species. In general,

$$c^* \leq k \quad (2)$$

The number of independent reactions that occur in a system comprised of N species is linked to the rank of the atom matrix in accordance with the Gibbs stoichiometric rule [2].

$$0 < r \leq (N - c^*) \quad (3)$$

The equality sign gives r^* the maximum number of linearly independent reactions that are required to describe the system. Therefore, f^* , the minimum number of degrees of freedom the system possesses becomes equal to

$$f^* = (* - s) - p + 2 - t + u \quad (4)$$

where $c^* = (N - r^*)$, and r^* is the maximum number of linearly independent reactions occurring in the system.

NUMBER OF COMPONENTS AND STOICHIOMETRIC CONSTRAINTS

The number of components (c) of a system is the smallest number of chemical species (or constituents) that must be specified in order to completely define the composition of the phases involved in the equilibrium. For a phase composed of α constituents, in the absence of stoichiometric constraints, one must specify $(\alpha - 1)$ mole fractions in order to fully define its composition. The last remaining mole fraction can be obtained, by difference, from the equation

$$x_1 + x_2 + \dots + x_{\alpha-2} + x_{\alpha-1} + x_\alpha = 1.0 \quad (5)$$

The number of components is not necessarily the same as the number of elements, or chemical species, or compounds present in the system.

The number of components can be greater than, equal to, or less than the number of initial substances from which the equilibrium system is synthesized in the laboratory. The number of com-

ponents, c , is not necessarily equal to the rank of the atom matrix constructed with the species occurring in the system under consideration. In general

$$c \leq c^* \leq k \quad (6)$$

where c^* and k have the same meaning as before. It will be noted that in the absence of any stoichiometric constraints, $c = c^* = (N - r^*)$.

It is important that we have a clear understanding of the concept of stoichiometric constraint. The *stoichiometric constraint* is a unique constricting relationship between the mole fractions of two or more species occurring in a given phase. It is well to note that the scope of the stoichiometric constraint does not extend beyond the particular phase that is under consideration. The constraint can be formulated in terms of mole fractions, as mentioned earlier, or in terms of partial pressures; and sometimes it is also expressed in terms of numbers of moles of species. Despite the fact that the numbers of moles of species are extensive variables (whereas the phase rule is a relationship between intensive variables), there is no internal inconsistency in this approach because the moles of species occurring in a given phase can be readily converted into mole fractions by division with total moles in that phase.

There is a distinction to be made between the stoichiometric constraint (in the present sense of the word) and the material balance equation; this distinction is most apparent in heterogeneous systems. A relationship that links numbers of moles of species from two or more phases ceases to be a stoichiometric constraint and simply becomes a material balance equation. This does not, however, preclude the reduction of two or more material balance equations into one or more stoichiometric constraints by appropriate algebraic operations. Also, one cannot write a stoichiometric constraint for a given phase that is in violation of the material balance equation for the larger system.

The number of components (c) in the system is given by

$$c = c^* - s = (N - r^* - s) \quad (7)$$

where s is the number of stoichiometric con-

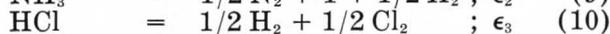
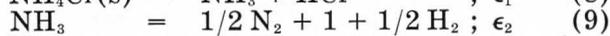
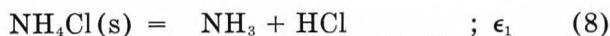
straints totaled over all the phases present in the system.

The existence of the stoichiometric constraint can be demonstrated quite rigorously by the use of the concept of "extent of reaction." A stoichiometric constraint is said to exist (i) if the atom ratio in a particular phase is equal to a ratio of two small integers, or (ii) when a simple relationship can be written linking two or more atom ratios in a particular phase. The following examples are instructive.

Suppose a system is prepared by placing an arbitrary amount of $\text{NH}_4\text{Cl}(\text{s})$ in an evacuated vessel. The temperature is raised, causing a portion of the salt to decompose into gaseous

While the method of extent of reaction is satisfactory for the purposes of formulating the stoichiometric constraints in a system, a simpler procedure may be advantageous in some instances.

products. The species present in the system include $\text{NH}_4\text{Cl}(\text{s})$, NH_3 , HCl , N_2 , H_2 , and Cl_2 . Since the rank of the atom matrix is 3, it follows that there are three linearly independent reactions. These reactions and the corresponding extents of reaction are



The number of moles of each species can be written in terms of the initial values and the extents of reaction.

$$n(\text{NH}_4\text{Cl}) = n^\circ(\text{NH}_4\text{Cl}) - \epsilon_1$$

$$n(\text{NH}_3) = \epsilon_1 - \epsilon_2$$

$$n(\text{HCl}) = \epsilon_1 - \epsilon_3$$

$$n(\text{N}_2) = 0.5 \epsilon_2$$

$$n(\text{H}_2) = 1.5 \epsilon_2 + 0.5 \epsilon_3$$

$$n(\text{Cl}_2) = 0.5 \epsilon_3$$

There are five "new" species, all occurring in the gas-phase. The numbers of moles (or mole fractions) of these five new species are seen to be expressed in terms of three extents of reaction. This means that only three of these quantities are independent. This can be demonstrated quite readily by the matrix methods.

$$\begin{array}{c} \text{NH}_3 \\ \text{HCl} \\ \text{N}_2 \\ \text{H}_2 \\ \text{Cl}_2 \end{array} \begin{array}{ccc} \epsilon_1 & \epsilon_2 & \epsilon_3 \\ 1 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 0.5 & 0 \\ 0 & 1.5 & 0.5 \\ 0 & 0 & 0.5 \end{array} \rightarrow \begin{array}{ccc} \boxed{1} & \boxed{-1} & \boxed{0} \\ \boxed{0} & \boxed{1} & \boxed{-1} \\ \boxed{0} & \boxed{0} & \boxed{1} \\ \boxed{0} & \boxed{0} & \boxed{0} \\ \boxed{0} & \boxed{0} & \boxed{0} \end{array} = \mathbf{E}$$

The echelon matrix (\mathbf{E}) shown on the right has a rank of 3 indicating that only three independent vectors exist. Thus, intuitively, we anticipate the existence of two stoichiometric constraints. For the g.atoms of each element in the gas-phase, we have

$$\begin{array}{l} \text{N} = n(\text{NH}_3) + 2n(\text{N}_2) = \epsilon_1 \\ \text{H} = 3n(\text{NH}_3) + n(\text{HCl}) + 2n(\text{H}_2) = 4\epsilon_1 \\ \text{Cl} = n(\text{HCl}) + 2n(\text{Cl}_2) = \epsilon_1 \end{array}$$

Two independent atom ratios can be written between these three elements. Thus

$$\frac{\text{H}}{\text{N}} = \frac{4\epsilon_1}{\epsilon_1} = \frac{4}{1} \quad ; \quad \frac{\text{H}}{\text{Cl}} = \frac{4\epsilon_1}{\epsilon_1} = \frac{4}{1}$$

Substitutions provide

$$n(\text{HCl}) + 2n(\text{H}_2) = n(\text{NH}_3) + 8n(\text{N}_2)$$

$$3n(\text{NH}_3) + 2n(\text{H}_2) = 3n(\text{HCl}) + 8n(\text{Cl}_2)$$

Division by the total number of moles of gaseous species yields

$$x(\text{HCl}) + 2x(\text{H}_2) = x(\text{NH}_3) + 8x(\text{N}_2) \quad (11)$$

$$3x(\text{NH}_3) + 2x(\text{H}_2) = 3x(\text{HCl}) + 8x(\text{Cl}_2) \quad (12)$$

where $x(i)$ is the mole fraction of the i th species in the gas-phase. Thus, we have uncovered two stoichiometric constraints (applicable in the gas-phase) for this system. That the atom ratios H/N and H/Cl in the product-gas mixture will be equal to 4/1 can be readily surmised by an inspection of the stoichiometry of the original $\text{NH}_4\text{Cl}(\text{s})$ species from which the gas-phase has evolved.

We can determine the number of components in this system by the application of Eq. (7). It will be noted that

$$\begin{array}{l} \text{N} = 6 \text{ (one solid + five gases)} \quad ; \quad r^* = 3 \quad ; \quad c^* = 3 \\ s = \text{Number of stoichiometric constraints} = 2 \end{array}$$

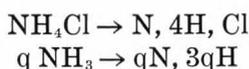
Substitutions yield

$$c = (6 - 3 - 2) = 1$$

We may now consider a variation of the foregoing illustration. Suppose that the system is prepared by placing a mixture of arbitrary amounts of $\text{NH}_4\text{Cl}(\text{s})/\text{NH}_3(\text{g})$ in an evacuated vessel and at equilibrium there are present HCl , N_2 , H_2 , and Cl_2 in addition to the two initial substances. It is readily seen that in this particular example, the atom ratios H/N and H/Cl of the gas-phase are not equal to 4/1. However, there does exist a simple

There is one kind of special constraint that resembles a stoichiometric constraint. This emanates from the condition of electroneutrality in ionic systems . . .

relationship between the atom ratios. Since the initial mixture is composed of arbitrary amounts of the two constituents, let us suppose that it consisted of q moles of NH_3 per mole of $\text{NH}_4\text{Cl}(\text{s})$. Since the four new species are generated from these two compounds, we can write



Furthermore

$$\frac{\text{N}}{\text{Cl}} = \text{RNL} = 1 + q \quad ; \quad \frac{\text{H}}{\text{Cl}} = \text{RHL} = 4 + 3q$$

where RNL and RHL are atom ratios in the gas-phase. By eliminating q , we obtain the following relation that links the two atom ratios:

$$\text{RHL} = 3 \text{RNL} + 1 \quad (13)$$

In light of this, we can conclude that there indeed exists a stoichiometric constraint in this system. The same conclusion can also be reached in a slightly different way. In terms of extents of reaction

$$\begin{aligned} n(\text{NH}_4\text{Cl}) &= n^\circ(\text{NH}_4\text{Cl}) - \epsilon_1 \\ n(\text{NH}_3) &= n^\circ(\text{NH}_3) + \epsilon_1 - \epsilon_2 \\ n(\text{HCl}) &= \epsilon_1 - \epsilon_3 \\ n(\text{N}_2) &= 0.5 \epsilon_2 \\ n(\text{H}_2) &= 1.5 \epsilon_2 + 0.5 \epsilon_3 \\ n(\text{Cl}_2) &= 0.5 \epsilon_3 \end{aligned}$$

Since the last four equations involve only three independent parameters, viz., ϵ_1 , ϵ_2 , and ϵ_3 , it is clear that only three of these equations are truly independent. The remaining can be obtained by a linear combination of the others. It is a relatively simple exercise to show that

$$3 n(\text{N}_2) = 1.5 \epsilon_2 = n(\text{H}_2) - n(\text{Cl}_2)$$

or

$$3 x(\text{N}_2) + x(\text{Cl}_2) = x(\text{H}_2) \quad (14)$$

which is the stoichiometric constraint for the system. The very same relationship can also be deduced by starting with Eq. (13).

In this system also we have $N = 6$, $c^* = 3$, and $r^* = 3$. Furthermore, $s = 1$. This provides

$$c = \text{Number of components} = c^* - s = 2$$

The systems $\text{NH}_4\text{Cl}(\text{s})/\text{HCl}(\text{g})$, $\text{NH}_4\text{Cl}(\text{s})/\text{N}_2(\text{g})$, $\text{NH}_4\text{Cl}(\text{s})/\text{H}_2(\text{g})$, and $\text{NH}_4\text{Cl}(\text{s})/\text{Cl}_2(\text{g})$

can be treated in a similar manner. In each of these, one can write a simple relationship with the atom ratios from which the stoichiometric constraint can be derived.

Let us consider a system that is prepared by placing $\text{MgSO}_4(\text{s})$ in an evacuated vessel and is allowed to equilibrate. The species present include $\text{MgO}(\text{s})$, SO_3 , SO_2 , SO , O_2 , S , S_2 , S_3 , S_4 , S_5 , S_6 , S_7 , and S_8 in addition to the original $\text{MgSO}_4(\text{s})$. The atom matrix has a rank of 3 and the maximum number of independent reaction equilibria is 11. The concentrations of the 12 new gaseous species generated in the system can be expressed in terms of 11 independent extents of reaction. Thus, there exists one stoichiometric constraint in the gas-phase. It can be easily shown that

$$\frac{\text{O}}{\text{S}} = \frac{3}{1} = \frac{3n(\text{SO}_3) + 2n(\text{SO}_2) + n(\text{SO}) + 2n(\text{O}_2)}{n(\text{SO}_3) + n(\text{SO}_2) + n(\text{SO}) + \sum_j n(\text{S}_j)} \quad (15)$$

This translates into the following stoichiometric constraint

$$x(\text{SO}_2) + 2 x(\text{SO}) + 3 \sum_j j x(\text{S}_j) = 2x(\text{O}_2) \quad (16)$$

Additionally $N = 14$, $c^* = 3$, $r^* = 11$ and $s = 1$. Substitutions yield

$$c = c^* - s = 2$$

This result is correct despite the fact that the system was prepared from a single substance.

While the method of extent of reaction is satisfactory for the purposes of formulating the stoichiometric constraints in a system, a simpler procedure may be advantageous in some instances. Suppose that a homogeneous system is prepared from I number of constituents. At equilibrium, this single-phase system contains N species of which I are the initial constituents. The rank of the atom matrix of N species is c^* and a maximum of r^* reactions are required to describe the system. We have

$$J = N - I \quad (17)$$

where J is the number of "new" species generated by the r^* reactions. The number of stoichiometric constraints s present in the system is given by

$$s = J - r^* = N - I - r^* = c^* - I \quad (18)$$

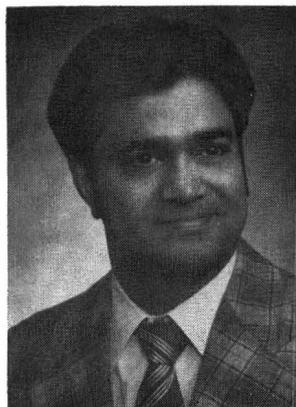
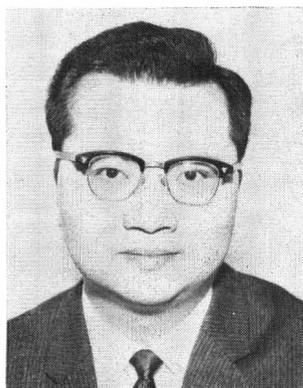
This relationship is directly applicable to single-

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SIMULATION OF SIMPLE CONTROLLED PROCESSES WITH DEAD-TIME

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THE STUDY OF SYSTEMS with dead-time in under-graduate process control is important due to the fact that a large number of chemical process systems exhibit apparent dead-time characteristics and that the dead-time is detrimental to control. The topic dealing with the determination of closed-loop response of processes containing dead-time is typically not covered in under-graduate process control, possibly because the solution by Laplace transforms requires the use of Pade ap-



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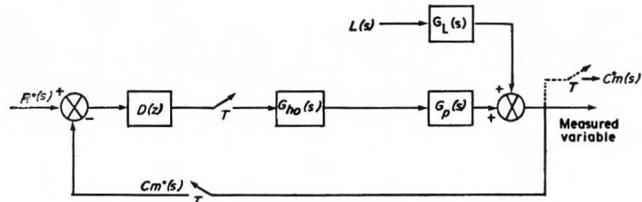


FIGURE 1. Typical sampled-data control system.

proximation for dead-time which makes the procedure lengthy and tedious. In this paper a computer-aided method is described which simplifies the procedure.

The method is based on the premise that the closed loop response of a sampled-data control system shown in Fig. 1, approaches that of the equivalent analog system (i.e., one without samplers and zero-order hold) as the sampling period is reduced. Thus, by suitable selection of the sampling period, the conventional (analog) control system can be analyzed by the z-transform method.

SYSTEM EQUATIONS

The scope of the program described in this paper is limited to the analysis of simple processes containing one or two time constants, a gain, and a dead-time element.

The closed-loop pulse transfer function of the sampled-data control system shown in Fig. 1 is

$$C(Z) = \frac{D(Z) G_{ho} G_p(Z)}{1 + D(Z) G_{ho} G_p(Z)} R(Z) + \frac{G_L L(Z)}{1 + D(Z) G_{ho} G_p(Z)} \quad (1)$$

The terms in Eq. (1) are indicated in Fig. 1.

The sampled-data system can be analyzed either for set point changes or for load changes. For set point changes, the expression for $R(Z)$ is of the form

$$R(Z) = \frac{a + bZ^{-1} + cZ^{-2}}{d + eZ^{-1} + fZ^{-2}} \quad (2)$$

The method is based on the premise that the closed loop response of a sample-data control system . . . approaches that of the equivalent analog system . . . as the sampling period is reduced.

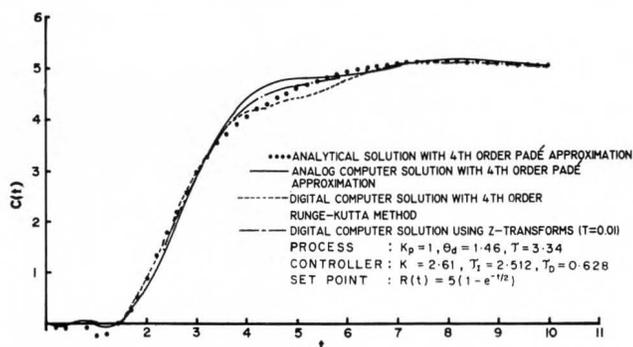


FIGURE 2. Set point response of the equivalent analog control and sampled-data control systems.

where a,b,c,d,e,f are user selected constants.

The appropriate expressions for D and G_p are inserted in Eq. (1) and the resultant equation is simplified to give

$$C(Z) = \frac{C_1 + C_2 Z^{-1} + C_3 Z^{-2} + \dots}{D_1 + D_2 Z^{-1} + D_3 Z^{-2} + \dots} \quad (3)$$

The constants in Eq. (3) are functions of the process parameters (K_p , θ_d , τ or K_p , θ_d , τ_1 , τ_2), controller parameters (K_c , τ_1 , τ_d) and the sampling period, T. Eq. (3) upon inversion by long division gives the closed-loop response at the various sampling instants. The load response of the process can be similarly evaluated [1].

PROGRAM DEVELOPMENT AND TESTING

A digital computer program written in double precision Fortran to solve Eq. (3) has been developed and tested. A listing of the program is available from the authors upon request. The user must specify as inputs the parameters of the process and controller, whether set point response or load response is desired and the sampling period.

The closed-loop response of an illustrative process is shown in Fig. 2. Also shown is the digital computer solution based on fourth-order Runge-Kutta integration and the analog computer solution based on the fourth-order Pade approximation. The sampling period for the z-transform-based solution is 0.01 time units. It may be observed that the sampled-data system approximates the conventional system well.

The z-transform based computer program should be useful in undergraduate process control. The undergraduate student, of course, will probably not be able to handle z-transforms. However, all that the student needs to know for the purpose of executing the program is the nature of the input data needed and the format of the results to be expected. □

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ChE book reviews

ELEMENTARY CHEMICAL ENGINEERING, Second Edition

By Max S. Peters, McGraw-Hill Book Company, NY (1983) \$32

Reviewed by E. V. Collins
Iowa State University

The text covers the traditional topics of stoichiometry, unit-operations, chemical technology, and plant design. A complete nomenclature table is found at the beginning of each chapter where appropriate. Since this text is intended for students with no calculus background, there is no coverage of unsteady-state conditions.

This text is very well suited to a freshman level over-view course of the field of chemical engineering. We have used the first edition of this text in a survey course for other engineering disciplines. Worked out example problems are well chosen and used liberally throughout the text. Homework problems are available where appropriate, covering rather a wide spectrum of difficulty. Five homework problems are indicated as appropriate for computer solution. These cover a variety of applications, e.g. look-up table preparation, an iterative solution for a fluid flow system, and a matrix solution for a material balance problem.

The author used parallel solutions to example problems in first the American engineering system and then the SI system of units. It is unfortunate that the physical properties tables in the appendix are all given in American engineering system of units. This perpetuates the use of the American engineering units, since all data must be converted to the SI system of units. □

GIBBS PHASE RULE

Continued from page 43.

phase systems only. For the more complex systems involving several phases, the more detailed 'extent of reaction method' should be employed.

The number of stoichiometric constraints in any particular phase is equal to the number of new chemical species (as distinguished from the 'old' or 'initial' species from which the system is prepared) occurring in that phase less the maximum number of linearly independent reactions required to describe the system. The number of components is equal to the rank of the atom matrix less the total number of stoichiometric constraints summed over all phases.

SPECIAL CONSTRAINTS

In contrast to the stoichiometric constraints which are preordained by the particular stoichiometry of the reaction system, the special constraint 't' has something of an arbitrary quality. One particular form this constraint often takes is that of specifying the pressure. For example, the total pressure of the system may be specifically fixed as in the case of equilibrium phase diagrams for alloy systems which are determined at a constant pressure of 1 atm. Alternatively, the partial pressure of a gaseous species (or the activity of a component in a condensed phase) may be specifically set at a particular value. Each such specific choice constitutes a special (or additional) constraint and results in a parallel loss in the degrees of freedom enjoyed by the system under consideration.

There is one kind of special constraint that resembles a stoichiometric constraint. This emanates from the condition of electroneutrality in ionic systems: the total charges on cationic species must exactly match those on the anionic species. In some systems, the electroneutrality constraint can be redundant because it may simply be a linear combination of independent stoichiometric constraints. So a check must always be made on the linear independence of the constraints before they are imposed on the system.

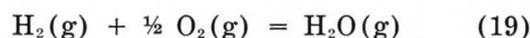
The effect of the special constraint on the number of components in a system is of some interest. When the imposed special constraint relates to phase-composition (i.e., mole fraction, partial pressure, or activity) it reduces the number of components in the same manner as does a stoichiometric constraint.

The discussion of the extended form of the Gibbs phase rule will not be complete without a consideration of its application. Each of the following examples is designed to illustrate a specific feature of the extended rule.

APPLICATIONS

H₂(g)-O₂(g)-H₂O(g) system

This is prepared by filling the vessel with a mixture of hydrogen, oxygen and water vapor. The system is allowed to equilibrate. It is seen that $N = 3$ and $c^* = 2$; hence $r^* = 1$. The lone independent reaction equilibrium is



There are no stoichiometric or special constraints; and no special variables are involved. Furthermore this is a single-phase system. Substitutions give

$$f = (3 - 1 - 0) - 1 + 2 - 0 - 0 = 3 \\ c = 2 - 0 = 2$$

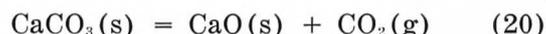
We can specify (1) temperature (2) total pressure and (3) a composition parameter such as the H/O atom ratio of the gas-phase.

$$\frac{\text{H}}{\text{O}} = \frac{2n(\text{H}_2) + 2n(\text{H}_2\text{O})}{n(\text{H}_2\text{O}) + 2n(\text{O}_2)} \\ = \frac{2P(\text{H}_2) + 2P(\text{H}_2\text{O})}{P(\text{H}_2\text{O}) + 2P(\text{O}_2)}$$

where $n(i)$ and $P(i)$ respectively denote the number of moles and partial pressure of the i th species.

CaCO₃(s)-CaO(s)-CO₂(g) system

Suppose that solid calcium carbonate is placed in an evacuated vessel and is allowed to dissociate and reach equilibrium. The species present in the equilibrated system are CaCO₃(s), CaO(s) and CO₂(g). As noted earlier, the atom matrix constructed of these three species has a rank of 2. The only reaction equilibrium to be considered is



No stoichiometric constraint exists because the products CaO(s) and CO₂(g) occur in different phases (unlike SO₂ and O₂ in the dissociation of solid MgSO₄ mentioned earlier). Thus $N = 3$, $c^* =$

2, $r^* = 1$, $p = 3$ and $s = t = u = 0$. Substitutions give

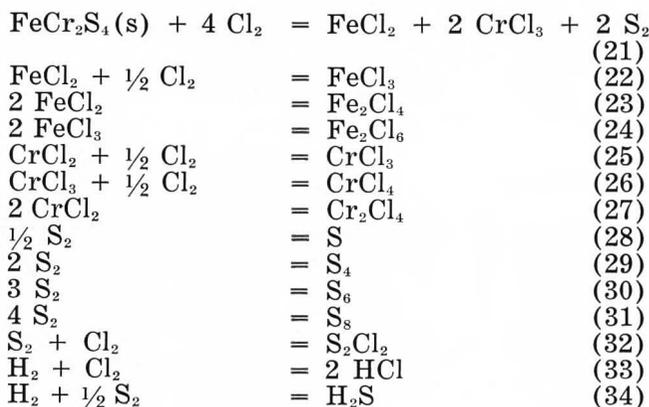
$$f = (3 - 1 - 0) - 3 + 2 - 0 = 1$$

$$c = 2 - 0 = 2$$

This is a univariant system which is completely described if temperature or pressure is specified.

FeCr₂S₄(s)-HCl(g)-Cl₂(g) system

This chemical transport system is prepared by placing a mixture of these three species in an evacuated vessel held at an appropriate temperature. At equilibrium the gas-phase is observed to contain 18 species: FeCl₂, Fe₂Cl₄, FeCl₃, Fe₂Cl₆, CrCl₂, CrCl₃, CrCl₄, Cr₂Cl₄, S, S₂, S₄, S₆, S₈, S₂Cl₂, H₂, Cl₂, HCl, and H₂S respectively, and no condensed phases other than FeCr₂S₄(s) occur. The atom matrix constructed of these nineteen species has a rank of 5. Thus $N = 19$ and $c^* = 5$; therefore $r^* = 14$. The maximum number of linearly independent reactions that are required to describe the system fully, thus, is seen to be 14. These are as follows



It is of particular interest to note that there are two stoichiometric constraints inherent in this manner of preparation of the vapor transport system. All of the Fe, Cr and S atoms in the gas-phase (albeit present in the form of various molecular species) originate with the solid FeCr₂S₄; also since no other condensed phase appears, the following obtains

$$\frac{\text{Cr}}{\text{Fe}} = \frac{2}{1} = \frac{P(\text{CrCl}_2) + P(\text{CrCl}_3) + P(\text{CrCl}_4) + 2P(\text{Cr}_2\text{Cl}_4)}{P(\text{FeCl}_2) + P(\text{FeCl}_3) + 2P(\text{Fe}_2\text{Cl}_4) + 2P(\text{Fe}_2\text{Cl}_6)}$$

$$\frac{\text{Cr}}{\text{S}} = \frac{2}{4} = \frac{P(\text{CrCl}_2) + P(\text{CrCl}_3) + P(\text{CrCl}_4) + 2P(\text{Cr}_2\text{Cl}_4)}{P(\text{S}) + 2P(\text{S}_2) + 4P(\text{S}_4) + 6P(\text{S}_6) + 8P(\text{S}_8) + 2P(\text{S}_2\text{Cl}_2) + P(\text{H}_2\text{S})}$$

Each of these relationships constitutes a stoichiometric constraint. There are no special constraints or variables that have to be reckoned with. Thus, we have

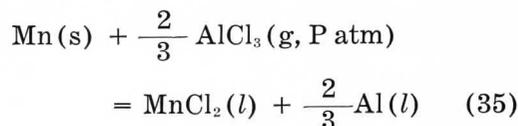
$$f = (19 - 14 - 2) - 2 + 2 - 0 = 3$$

$$c = 5 - 2 = 3$$

Three system properties have to be specified. These may be selected as (i) temperature (ii) initial chlorine pressure in the system, $P^\circ(\text{Cl}_2)$ and (iii) Cl/H atom ratio of the gas-phase. The specification of temperature yields 14 equilibrium constant expressions, one for each of the reactions identified above. These 14 relations together with the two stoichiometric constraint equations coupled with the values of $P^\circ(\text{Cl}_2)$ and Cl/H should enable the determination of the equilibrium partial pressures of the 18 gaseous species that occur in the system. An iterative method of calculation suitable for complex systems is presented in a recent publication [3].

Mn(s)-AlCl₃(g)-MnCl₂(l)-Al(l) system

For this four-phase, four species system, the atom matrix has a rank of three. The only independent reaction equilibrium is



Suppose that the pressure of AlCl₃(g) is arbitrarily set at 1 atm. This would constitute a special constraint. There are no stoichiometric constraints or special variables. Therefore $N = 4$; $r^* = 1$; $s = 0$; $p = 4$; $t = 1$ and $u = 0$. Substitutions yield

$$f = 0$$

$$c = c^* - s = 3$$

The system, when subject to the single special constraint stipulated above, becomes invariant. This simply means that there is but one unique temperature (T_e) at which the four-phase system is in a state of equilibrium for a $P(\text{AlCl}_3)$ of 1

atm. The value of T_e can be found as follows. For the reaction equilibrium

$$\Delta G = 0 = \Delta G_r^\circ(\text{MnCl}_2) - \left(\frac{2}{3}\right) \Delta G_r^\circ(\text{AlCl}_3)$$

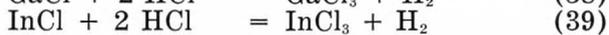
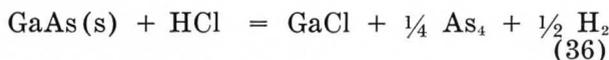
Using the tabulated data [4] on the standard free energies of formation (ΔG_r°), we find

$$\begin{aligned} 0 &= -39,162 + 41.601 T_e \\ T_e &= 941.4 \text{ K} \end{aligned}$$

The equilibrium $\text{Mn}(s) - \text{AlCl}_3(g) - \text{MnCl}_2(l) - \text{Al}(l)$ is unique in that it occurs only at this temperature when all the species are in their respective natural standard states. Had $P(\text{AlCl}_3)$ been specified as, say, 0.95 atm instead of 1.0 atm, then we would find that the corresponding value of T_e becomes 935 K. Only one special constraint may be imposed when $T_e = 935\text{K}$: for example, we cannot arbitrarily set $P(\text{AlCl}_3)$ at, say, 0.95 atm and at the same time fix the activity of aluminum (presumably present as a liquid alloy) at, say, 0.8. This would result in negative degrees of freedom which has no physical significance.

Ga-In-As-H-Cl system

The mixed crystal (solid solution) $\text{Ga}_x\text{In}_{1-x}\text{As}$ is grown from vapor phase. The system is prepared by introducing a gas mixture consisting of $\text{GaCl}(g)$, $\text{InCl}(g)$, $\text{As}_4(g)$, $\text{HCl}(g)$ and $\text{H}_2(g)$ into the crystal growth system. At equilibrium, there are present eight gaseous species (GaCl_3 , InCl_3 and As_2 in addition to the initial five) and two condensed phase species $\text{GaAs}(s)$ and $\text{InAs}(s)$. Since $c^* = 5$, it follows that $r^* = 5$. These five independent equilibria are:



There are no stoichiometric or special constraints. In order to facilitate the equilibrium calculation, however, sometimes two hypothetical species, $\text{GaAs}(g)$ and $\text{InAs}(g)$, are introduced. The number of moles of $\text{GaAs}(g)$ and $\text{InAs}(g)$ (hypothetically) present in the equilibrated system is simply equal to the number of moles of deposited GaAs and InAs respectively. The hypothetical

species constitute special variables. Thus $N = 10$; $r^* = 5$; $p = 2$; $s = t = 0$; and $u = 2$. Substitution gives

$$\begin{aligned} f &= (10 - 5 - 0) - 2 + 2 - 0 + 2 = 7 \\ c &= 5 - 0 = 5 \end{aligned}$$

These seven degrees of freedom are satisfied by specifying (1) temperature, (2) total pressure, (3) Cl/H atom ratio, (4) $n^\circ(\text{Ga})$, (5) $n^\circ(\text{In})$, (6) $n^\circ(\text{As})$, and (7) interaction parameter Ω for the GaAs-InAs regular solution. In here $n^\circ(\text{Ga})$, etc., denotes the number of g atoms of Ga, etc. in the initial gas-phase albeit present in the form of GaCl , etc. The atom balance equation for Ga is

$$n^\circ(\text{Ga}) = n^\circ(\text{GaCl}) = n(\text{GaCl}) + n(\text{GaCl}_3) + n^*(\text{GaAs})$$

where $n^*(\text{GaAs})$ represents the contribution due to the hypothetical species. Other atom balance equations can be written similarly.

FINAL COMMENTS

In attempting to make an equilibrium calculation in complex systems, a necessary and useful prerequisite is to conduct phase rule analysis of the system. Such an analysis helps clarify the essential elements of the calculation procedure. The extended form of the Gibbs phase rule presented here is especially useful in analyzing multicomponent heterogeneous systems. \square

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NOMENCLATURE

c	number of components
c^*	rank of atom matrix
f	degrees of freedom
f^*	minimum number of degrees of freedom
$\Delta G_r^\circ(\text{AlCl}_3)$	standard free energy of formation of $\text{AlCl}_3(g)$
$\Delta G_r^\circ(\text{MnCl}_2)$	standard free energy of formation of $\text{MnCl}_2(l)$
I	initial constituents
J	new species

k	kinds of atoms or elements
n(i)	number of moles of the ith species
n°(i)	initial number of moles of the ith species
N	species
p	number of phases
r	independent reaction equilibria
r*	maximum number of independent reaction equilibria
RHL	H/Cl atom ratio
RNL	N/Cl atom ratio
s	stoichiometric constraints
t	special or additional constraints
u	special or additional variables
x(i)	mole fraction of the ith species
Greek letters	
ϵ_i	extent of reaction for the ith reaction

REVIEW: Diffusion in Liquids

Continued from page 29.

correlation of experimental data, via kinetic theory and, more extensively, such approximations as hydrodynamic and free volume theories. A separate section is provided for electrolytes. The utility of these theories is discussed for binary and ternary nonelectrolytes in Chapter 7 and for binary electrolytes and fused salts in Chapter 8.

This is a densely written book of high technical quality, and it is difficult to write a definitive review without extensive study, a procedure not feasible for this reviewer. However, I think it fair to say that this is a useful and reliable treatise, but that it will not attract large numbers of chemical engineers as readers. Much of the material presented is available elsewhere in equivalent form, and little attention has been paid to the problems of those wishing to use the subject matter in typical engineering applications. However, this book should prove valuable to those engaged in serious experimental or theoretical investigations and who wish to be sure that the basis of their work is sound. A few examples are given below to back up these comments.

The phenomenological discussion of Chapters 2 and 3 is representative of both the strengths and weaknesses of this book. The discussion of the Onsager reciprocal relation clears up a number of widely held misconceptions in a clear definitive manner, but little is done to provide the reader with convenient sets of diffusion equations, or of means to test and interrelate the wide variety of apparently different expressions found in the diffusion literature. The authors confine them-

selves largely to the flux expressions used by a relatively narrow group of physical chemists cited in the acknowledgement. These have not for the most part found widespread acceptance by chemical engineers, and it is not a simple matter to relate them to those which are more common. The means for making these inter-relations is provided in Chapter 3, but this reviewer did not find the treatment a convenient one to use. However, the definitions of mutual, self- and intra-diffusion coefficients in Chapter 1 are quite clear, and very useful as there has been much confusion about these terms.

Chapter 5 is, in this reviewer's opinion, highly useful, and a real strength of the book. The discussion of experimental techniques is detailed and practical, and also generally sound in terms of underlying theory. I do have a minor criticism in the discussion of Taylor dispersion in that the extensive literature on departures from Taylor's asymptotic theory is not referenced. Such departures can be important and may result from end effects or a variety of flow disturbances. This objection is, however, more than balanced by the strength of the discussion of errors in the use of light scattering. The authors have done much here to clear up longstanding controversies as to the significance of measurements made in concentrated solutions.

I found the organization of Chapters 6 through 8 awkward, but it may be that I did not take enough time to accommodate to it. It is clear that the authors have a prejudice which results in more attention to even doubtful theory than to useful empiricism. Thus they ignore many useful empirical and semi-empirical correlations totally. However, they do present a substantial amount of data and discuss it critically in the light of available theory, and these discussions should prove highly useful to many readers. They do seem more concerned with the experimental proof of the Onsager reciprocal relation than with the practical description of multicomponent diffusion problems, but in this they are constrained by the limited amount of practically useful information available.

On balance I expect to find this monograph a most welcome addition to my library, and a challenge to those like myself, with more applied tastes than the authors, to meet the above objections. I think this is the most authoritative source available in the area of diffusion, which is accessible to an engineering audience. □

RESOURCE-BASED EDUCATION

Continued from page 39.

to find others. The teacher acts as a resource and an adviser while retaining some assessing and monitoring roles. This strategy is generally used for design projects, and can be used to extend the more gifted students.

CONCLUSIONS

Successfully carrying out this major program of modernization will require

- A commitment by the departmental staff to the new concept
- The willingness of departmental staff to make short-term sacrifices
- The diversion of financial resources to fund the scheme.

Discussion within the department during 1983 has resulted in enthusiastic support from the staff and a commitment by the staff to the concept. As part of the plan each staff member will be relieved in turn of normal duties to be retrained in CAL and video techniques and to prepare new resources. The total financial resources required, including cost for staff retraining, is estimated to be in excess of half a million dollars.

While each element in the proposed mode of operation is not novel, the implementation of the integrated package on a departmental basis in chemical engineering is both new and challenging. This is the beginning. □

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SPATIAL AVERAGING THEOREM

Continued from page 21.

integrals in Eq. 14 in terms of area integrals according to

$$dV_I = - \Delta s \lambda \cdot n_{\beta} dA_I \quad (15a)$$

$$dV_{II} = + \Delta s \lambda \cdot n_{\beta} dA_{II} \quad (15b)$$

There is a minor problem in the use of these relations at the contact point between the surface of the averaging volume and the β - σ interface. As indicated in Fig. 4 the error is on the order of $P\Delta s^2$ where P is the length of the contact line between the surface of the averaging volume and the β - σ interface. Use of Eq. 15 in Eq. 12 along with the estimate of the error

$$\delta V = Q(P\Delta s^2) \quad (16)$$

leads to

$$\frac{d}{ds} \int_{V_{\beta}(s,t)} c_A dV = \lim_{\Delta s \rightarrow 0} \left[\frac{\int_{A_{II}(s,t)} c_A \Delta s \lambda \cdot n_{\beta} dA_{II} + \int_{A_I(s,t)} c_A \Delta s \lambda \cdot n_{\beta} dA_I + Q(c_A P \Delta s^2)}{\Delta s} \right] \quad (17)$$

Since Δs and λ are independent of position, they can be removed from the integrals and in the limit as $\Delta s \rightarrow 0$ we obtain

$$\frac{d}{ds} \int_{V_{\beta}(s,t)} c_A dV = \lambda \cdot \int_{A_{\beta e}(s,t)} n_{\beta} c_A dA \quad (18)$$

Here we have used

$$A_{\beta e}(s,t) = \lim_{\Delta s \rightarrow 0} \left(A_I(s,t) + A_{II}(s,t) \right) \quad (19)$$

and expressing the derivative with respect to s in the form

$$\frac{d}{ds} = \lambda \cdot \nabla \quad (20)$$

quite obviously leads to

$$\nabla \int_{V_{\beta}(t)} c_A dV = \int_{A_{\beta e}(t)} n_{\beta} c_A dA \quad (21)$$

since λ is arbitrary. This is Eq. 7 of Slattery's derivation [15] and in terms of the nomenclature indicated in Eq. 3 we obtain

$$\nabla \cdot \langle c_A \rangle = \frac{1}{V} \int_{A_{\beta e}(t)} n_{\beta} c_A dA \quad (22)$$

while the vector form of this result is obviously given by

$$\nabla \cdot \langle N_A \rangle = \frac{1}{V} \int_{A_{\beta e}(t)} n_{\beta} \cdot N_A dA \quad (23)$$

The spatial averaging theorem can be obtained by use of the divergence theorem

$$\frac{1}{V} \int_{V_{\beta}(t)} \nabla c_A dV = \frac{1}{V} \int_{A_{\beta e}(t)} n_{\beta} c_A dA + \frac{1}{V} \int_{A_{\beta \sigma}(t)} n_{\beta \sigma} c_A dA \quad (24)$$

along with Eq. 22 to arrive at the result

$$\langle \nabla c_A \rangle = \nabla \cdot \langle c_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} n_{\beta \sigma} c_A dA \quad (25)$$

The analogous form for a vector is given by

$$\langle \nabla \cdot N_A \rangle = \nabla \cdot \langle N_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} n_{\beta \sigma} \cdot N_A dA \quad (26)$$

We are now in a position to continue our analysis of Eq. 9 using the general transport theorem and the spatial averaging theorem to interchange differentiation and integration.

CLOSURE

The general transport equation provides the relation

$$\frac{d}{dt} \int_{V_{\beta}(t)} c_A dV = \int_{V_{\beta}(t)} \frac{\partial c_A}{\partial t} dV + \int_{A_{\beta \sigma}(t)} c_A w \cdot n_{\beta \sigma} dA \quad (27)$$

in which we have used $w \cdot n_{\beta \sigma}$ to represent the normal component of the velocity of the β - σ interface, and we have made use of the fact that the normal component of velocity of the surface $A_{\beta e}(t)$ is zero. Use of this result allows us to express Eq. 9 in the form

$$\frac{d}{dt} \left(\frac{1}{V} \int_{V_{\beta}(t)} c_A dV \right) - \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A w \cdot n_{\beta \sigma} dA + \langle \nabla \cdot N_A \rangle = \langle R_A \rangle \quad (28)$$

and the spatial averaging theorem given by Eq. 26 can be used to obtain

$$\frac{\partial \langle c_A \rangle}{\partial t} + \nabla \cdot \langle c_A v_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A (v_A - w) \cdot n_{\beta \sigma} dA = \langle R_A \rangle \quad (29)$$

Since the phase average concentration is associated with a fixed point in space we have used the partial time derivative in writing Eq. 29, and we have used Eq. 2 to express N_A in terms of the concentration and the species velocity. From Eq. 23 we see that $\nabla \cdot \langle c_A v_A \rangle$ represents the flux at entrances and exits and under most circumstances [21, Sec. 7.4] diffusion is negligible compared to convection at entrances and exits and Eq. 29 can be written as

$$\frac{\partial \langle c_A \rangle}{\partial t} + \nabla \cdot \langle c_A v_A \rangle + \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A (v_A - w) \cdot n_{\beta \sigma} dA = \langle R_A \rangle \quad (30)$$

Because the intrinsic phase average concentration is preferred, we can use the representation given by Eq. 6 to write

$$\begin{aligned} \frac{\partial}{\partial t} \left[\epsilon_{\beta} \langle c_A \rangle^{\beta} \right] + \nabla \cdot \left[\epsilon_{\beta} \langle c_A v_A \rangle^{\beta} \right] \\ + \frac{1}{V} \int_{A_{\beta \sigma}(t)} c_A (v_A - w) \cdot n_{\beta \sigma} dA = \epsilon_{\beta} \langle R_A \rangle^{\beta} \quad (31) \end{aligned}$$

At this point we follow the procedure used in the time averaging of turbulent transport processes and make use of Gray's [12] spatial decomposition to write

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