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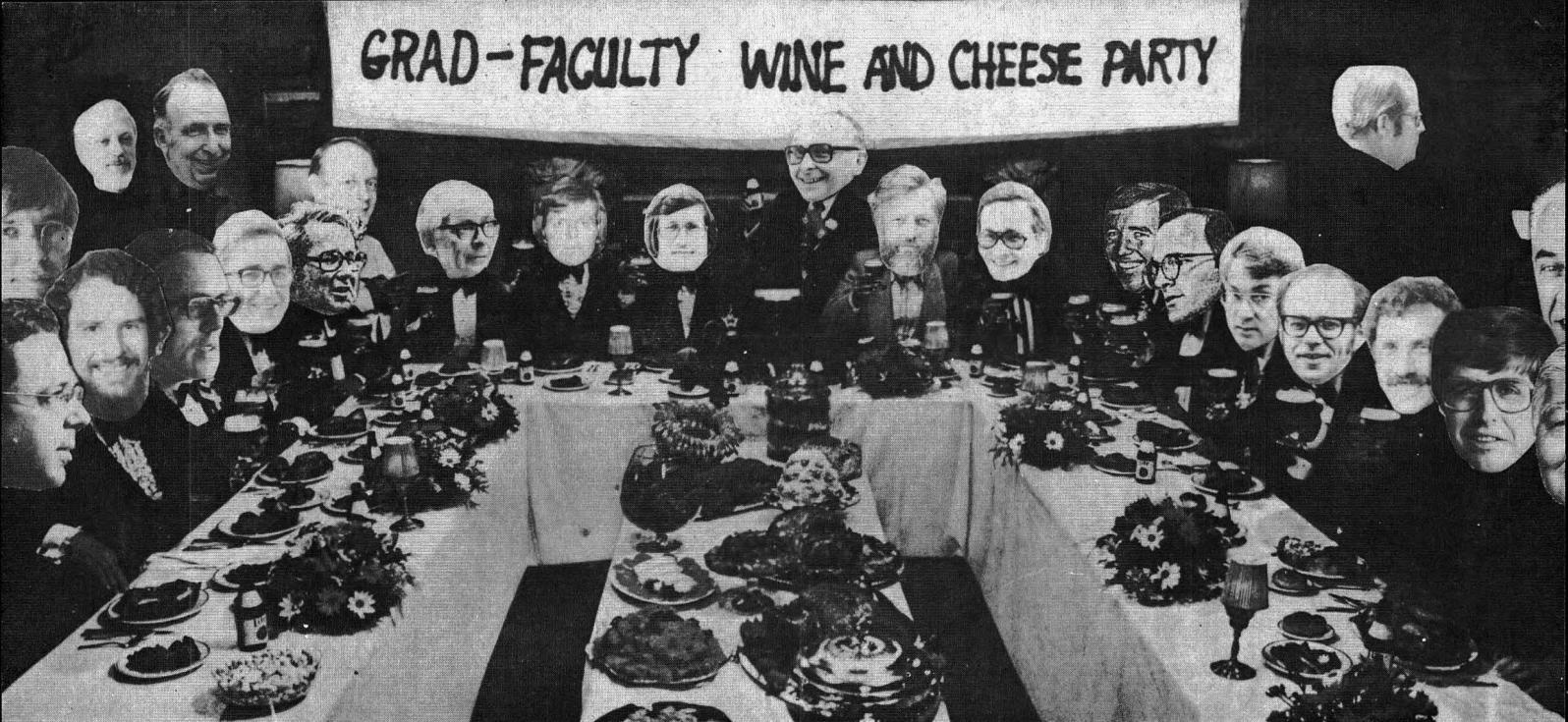
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The older students provided a clue-sheet for the new students at the Fall faculty-graduate student party.

ChE department

UNIVERSITY OF MINNESOTA

RUTHERFORD ARIS
U. Minnesota
Minneapolis, MN 55455

AS EARLY AS 1902, G. B. Frankforter of the Department of Chemistry wrote to Cyrus Northrop the President of the University of Minnesota to point out

"the importance of offering . . . a course of study in which both chemistry and engineering are represented. Such a source is now offered in all of the larger institutions of Germany and in nearly all of the larger Universities and technical institutions of this country.

"What I would respectfully recommend then is, that a course of study be offered which will meet the urgent demands of the present time. I will state that I have consulted the various members of the engineering faculty concerned and the plan meets with their most hearty approval. I will also say that in offering this new course, there need not be a single dollar of additional expense to the University.

I would also recommend that the School of Chemistry be separated from the College of Science, Literature and the Arts, in as much as the work is entirely foreign to that College. We graduate four men this year and there are some twenty members of the present Freshman class. With this new course which

is sure to be popular although it is an exceedingly difficult one, we shall be quite on a par with the School of Mines.

Very respectfully submitted,
 (Signed) G. B. Frankforter."

The School of Mines has since passed away but the "new course" continues to be both "popular" and "exceedingly difficult", and what president could fail to approve a program urged with such enthusiasm and costing "not a single dollar of additional expense."!

It was not until 1919 however that the curriculum was formalized as the "Chemical Engineering Course" and what was effectively a department arose as a division of the School of Chemistry. Charles A. Mann was promoted to the rank of professor with the title of acting head of the Division of Chemical Engineering. For the time being very inadequate quarters had to be used, and no satisfactory development of the experimental phases of chemical engineering could be put into operation until the completion of the fourth wing of the Chemistry Building. In the meantime, however, every effort was made to develop a satisfactory course in chemical engineering.

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TRANSITION

Twenty years later the department was still in the bowels of the chemistry building. Montillon and Montonna had joined Mann and were the three professors, with Rogers and Stoppel as assistant professors, Grove and Piret as instructors, and Armstrong, Chamberlain, Clegg, Eldredge among the teaching assistants. B. F. Ruth had been on the faculty; Amundson, Piercy and a host of others had graduated and the curriculum now contained Unit Operations, ChE Thermodynamics, Plant Design and Economics as well as courses on Explosives, Dyestuffs, Cellulose, Gas Manufacture and Sanitary Chemistry.

Thirty years later, just after Mann's death, Ceaglske and Piret were professors, Amundson and Stoppel associate professors and Stevenson, Preckshot and Madden assistant professors. The search outside the department for a new head was unsuccessful and Amundson, who had been made Acting Head in 1949, became the Head in 1951 and the big move from the basement of Chemistry to a new building was about to begin. It was a building of some 65,000 sq. ft. designed to handle 80 seniors and 100 graduate students. Apart from some dissatisfaction with certain of the materials (walls somewhat permeable to sound, for example) the building proved satisfactory but is once again stretched at its seams with the numbers of students. Many of the details of the transfer to the new building fell to some of the new faculty who had joined the department in the late 40's, notably to George Preckshot. There have been several episodes of remodeling, including the latest one to meet OSHA's requirements but in the fiscal climate of the moment there seems little prospect of the radical reorganization that is really necessary.

In the early 50's there were about eight members of the department, Ceaglske and Piret being the professors until joined by Amundson in '51 and Stoppel in '52. Isbin had come in 1950 and soon became an associate professor, being joined in that rank by Madden and Preckshot around the middle of the decade. Tsuchiya came in 1956 to bring the total number, including Hap Earle, to nine.

The pace of research increased in the 1950's also with such outstanding graduate students as Acrivos and Lapidus. Piret attracted a number of French students. Outstanding among them was Oleg Bilous who did his Ph.D. work with Piret

but also, on the side, wrote with Amundson some of the first papers on chemical reactors as dynamical systems.

During his sabbatical at Cambridge in 1954-5, Amundson not only wrote up much of this research but saw something of what could be done in a department when colleagues of diverse backgrounds are brought together and realized the potential of team teaching for developing really good cooperation. Toward the end of the decade he was able to put these ideas into effect as both numbers and research activity took off again. With Stoppel's death, but Isbin's promotion and Ranz's appointment, the tale of professors stood

... the department used to have a reputation for being dominantly theoretical. This was never really accurate, for there has always been a predominance of experimental programs.

at five, with three associate professors and an increasing number of assistants. Dahler, Fredrickson and Aris came in 1958 and were joined by Scriven in 1959. Edgar Piret left to be the Scientific Attaché in Paris. Davis came in 1963 and Keller in 1964 being followed in 1965, by Schmidt and Carr. These years also saw some of our outstanding graduates, such as Ramkrishna and Luss (and later Rhee and Varma), remaining for a short while as assistant professors. In 1969 there were nine professors (we avoid the neologism "full professors" as having too dyspeptic an image), three associates and three on the tenure track among a total of seven assistant professors. Of course it is not only the faculty that matter and graduates of the department probably remember best the outstanding figures of the staff: Ruth Nelson, who had everything at her finger tips or in a little 3x5 file box; Verne Nelsen, to whom the mysteries of stock and budget were as plain as day, and John Antolak without whom no experimental project got off the ground and but for whom the lab would have given up the ghost long before OSHA boxed it about with regulations.

In 1970 the Dean, disbanding the School of Mines and Metallurgy, allowed some of the more scientific types to come to chemical engineering and it became a department of Chemical Engineering and Materials Science, almost half as large again as before. The development of the department in the 1970's was governed by two considerations; namely, the need to integrate into it

the newly acquired aspect of materials science and to maintain and strengthen the standing that, by this time, the department had acquired. The area of polymers was a natural bridge between the chemical and the material ends of the operation and Macosko came in 1970, starting a very active program in polymer processing and rheology. Thomas was with us from '73 to '77 when he returned to Massachusetts, changing places with Tirrell, whose powerful progress has been recognized both internally and externally, by a Dreyfus Award and a Sloan Fellowship. Then Wellinghoff, a polymer morphologist, came to strengthen the bridge from the materials science side in 1978. Meanwhile, Gerberich had come in as a metallurgical materials scientist and Hutchinson, an electron microscopist (who had been part of the transfer of 1970) had left for the University of Washington. George Stephanopoulos came from the University of Florida to bring a great strength in the theory of design and control and was with us from 1974 to 1980, when, to our regret, he returned to Greece.

When, in 1974 (after 25 years of headship) Amundson asked to be relieved, his colleagues, much as they deplored the suggestion, could scarcely refuse. Aris was Head for four years and was succeeded by Keller in 1978. The department's magnanimity was further tested in 1980 when Keller was appointed the Academic Vice-President of the University of Minnesota and, bowing to the greater good of the greater number, we forged ahead under Davis' dynamic leadership. This brought in, in 1980, four new faculty members; two, Cussler and Evans, at a senior level and two, Jensen and Griffin, at the junior.

THE PRESENT

The continuing strength and harmony of the faculty is the final tribute to Amundson's years of building, for it survived his departure in 1976. On May 17, 1979, a date not inappropriate to one of Norwegian descent, we were able to incorporate Amundson's achievement into the permanent fabric of the University by renaming the chemical engineering building after him. As was commented at the time, there is no one in the engineering profession who should be in any doubt as to the subject taught in an Amundson Hall.

The strength of the department lies not merely in the achievement of its individual members, which has attracted the usual round of awards, but in the easy spirit of cooperation which marks it. At

This building has been named

AMUNDSON HALL

in honor of

NEAL RUSSELL AMUNDSON

for twenty-five years Head of the Department of Chemical Engineering and Materials Science and Regents' Professor of Chemical Engineering who, by his example and insistence on the highest academic standards, has built, not merely a building, but a department and has left his mark both on the University of Minnesota and on the whole profession of chemical engineering.

No one in the engineering profession would have any doubt as to the discipline taught in an Amundson Hall.

the graduate level this is manifested in the cooperative supervision of students, not in any regimented or organized fashion, but as the opportunity evolves naturally. We have been fortunate over the years in attracting some excellent students and this, of course, makes such cooperation easy. This team spirit is fostered at the undergraduate level by the system of team teaching. Graduate students spend the first quarter getting acquainted with the work of the different members of the department and organizing their preferences. This results in the assignment to an advisor at the beginning of the second quarter of their graduate experience and allows them to get moving on their research during the first summer. Though course work continues into the second year, the student presents a dossier showing the beginning of his or her research by the seventh quarter and faces, at this time, an oral preliminary examination on graduate course work. Beyond this the student is free to spend full time on research. The different groups of graduate students jointly or severally supervised by the faculty have different modes of operation; some meet regularly for group seminars but others work rather more individually. The general attitude is that it is the subject matter that counts and the way in which it can be developed in the intellectual context of the university.

Over the years the department has been

fortunate in its visitors and has entertained for sabbatical or other visits such persons as K. G. Denbigh, H. Kramer, E. Wicke, L. Waldmann, W. Schowalter, H. Brenner, W. Resnick, E. Rotstein, R. W. Fahien, J. Sinfelt and R. Rosensweig to name but a few. We also benefit from the adjunct professorships of not a few engineers in the Twin Cities area who come in and teach a course or take a lab with great enthusiasm and devotion, and who immensely enrich the student's experience by their industrial experience. K. J. Valentas, now the Vice-President for Engineering at Pillsbury, has taught a food engineering course for years: H. Kramer of General Mills, before his sudden death last year, had made a major contribution to the design course. Among the others, W. C. Johnson of 3M and B. Koepke of Honeywell have taught regularly as have J. Johnson, R. Minday, L. White and many more.

To summarize the scope and interests of the faculty is a difficult task and it is best to proceed alphabetically, letting the grouping and overlapping of research areas become evident as we go.

ARIS is interested in any problem that yields a significant mathematical structure and more generally in the whole question of how physical systems may be modeled intelligently. With CARR he shares an interest in continuous chromatographic reactors of rotating or counter-current design. Of course, Carr's interests in kinetics go far beyond this area of joint investigation reaching to the kinetics of reactions among species having nonequilibrium energy distributions and to multiphoton infrared photochemical reaction engineering. Atomic and radical reactions, particularly those occurring in the atmosphere and in combustion, are also one of Carr's interests and he has investigated large kinetic systems using sensitivity analysis.

CUSSLER brings an interest in the mass transfer processes of biological systems and this includes work on corrosion of ionic materials as well as problems in membrane diffusion. With EVANS he explores the kinetics of detergency, especially of the bile which is the human body's detergent. His interests even extend into the psychology of perception, for, in food development, the understanding of the impact of food texture can only be understood by a combination of engineering and psychology. Cussler is one of the keenest runners in the University and has actually participated in the Boston marathon; with Evans and Griffin, Tirrell and Macosko we can field a formidable team.

DAHLER, who also has an appointment in Chemistry, has research interests that encompass a broad spectrum of problems in nonequilibrium statistical mechanics and in the theory of atomic and molecular collisions. DAVIS also comes from a background in chemical physics and has applied this in several engineering contexts as well as having continued his work in the theory of liquids. Thus, with Scriven and others

he has looked into some questions of interfaces, micelles, thin films, microdispersions and emulsions and their applications to enhanced oil recovery. Percolation theory has been one of his tools and this has recently led to an analysis of some problems in surface diffusion connected with catalysis. With Evans and Tirrell he has an interest in the study of transport processes and the statistical mechanics of diffusion relaxation and flow. Evans studies micelle formation under unusual conditions ranging from those that form in low melting fused salts to those in aqueous solutions up to 200°C. Using a Taylor dispersion technique he has also done much work in determining the diffusion coefficients of small solutes and works with Davis to link these determinations up with the basic theory. In collaboration with Cussler he is trying to understand why organosilicon films are so effective in inhibiting corrosion.

FREDRICKSON has the reputation of being of that select band of teachers who can make thermodynamics both interesting and understandable. It is to be hoped that he will have time to get his text out soon but as Director of Undergraduate Studies and Editor of Chemical Engineering Science he has his hands more than full. Besides all this he has a very active research program in the dynamics of bacterial populations and, in particular, of mixed cultures and the dynamics of competition and predation.

GERBERICH is an expert in the fields of flow and fracture, studying hydrogen embrittlement, polymer fracture, elastic-plastic fracture mechanics and fatigue crack growth. GRIFFIN joined the department in 1980 after a post-doctoral stay at the Surface Science Division of NBS and his doctorate at Princeton. His research interests are in the fields of heterogeneous catalysis and surface chemistry with particular emphasis on the reactions that involve oxide catalysts. He uses in-situ measurement techniques such as infrared spectroscopy to examine the catalyst under reaction conditions. His interests link most closely with Schmidt's and he is one of a group, with Jensen and Aris, which, under Schmidt's leadership, looks at various aspects of catalysis and its applications in chemical engineering.

ISBIN, the doyen of the department in virtue of his more than 30 years of service, is a well-known nuclear and chemical engineer and, for many years, a member of the Advisory Committee on Reactor Safeguards. His expertise on two-phase flow and transport has spread now to the problems involved in the design of solar boilers while his experience in reactor safeguards had led him to a more general concern with risk analysis. When JENSEN came from Wisconsin in 1980 he brought with him an interest both in chemical reaction engineering and in process control. In the first area his projects concern the fundamental reaction and transport phenomena of catalytic coal gasification and the chemical deposition of microelectronic materials. He is also investigating the problem of multiple steady states, oscillations and pattern formation in combustion and heterogeneous catalysis. In the control area, he is our expert on development of algorithms and real time experiments with the department's PDP 11/60 mini-computer.

Before his elevation to the academic vice-presidency, KELLER, besides heading the department, conducted a research program in various biomedical areas, particularly those involving blood flow and its relation to artificial organ design, thrombogenesis and arteriosclerosis. MACOSKO, the first monomeric unit of the polymer bridge, is interested in all aspects of polymer processing. This includes models for processes that involve network polymerization and relating the reaction kinetics to the development of network structures and to the physical properties that result from these. He is also bringing his rheological interests to bear on one of Scriven's main concerns, that of coating flows with non-Newtonian fluids. In ORIANI we are fortunate in having a man of extensive industrial background who took early retirement from U.S. Steel to become the first Director of the Corrosion Research Center. RANZ has applied his understanding of fluid mechanics and his great skill and feeling for the order of magnitude of different physical effects to a number of rather difficult fluid mechanical and mass transfer problems. His particular emphasis is now concentrated on new models of laminar and turbulent mixing with chemical reaction in one and two phase systems, but aerosol technology continues to be an active subject for him. As one of the leaders, with Amundson, in the development of team teaching 20 years ago his influence and example are still most valuable.

SCHMIDT, one of the five members of the department whose primary training was in chemistry, came from the University of Chicago in 1965. He leads a very active group of students in research on many aspects of surface science and catalysis. He uses techniques, such as Auger and photoelectron spectroscopy, to characterize reactions on single and polycrystalline surfaces of transition metals. The dynamics of both natural and forced oscillations of catalytic reactions is another of the things he has looked into both experimentally and theoretically and on which a natural collaboration with Aris has developed. Schmidt's is the initiative behind an informal center for catalysis that has grown up to use the mutually interlocking interests of Griffin, Jensen and Aris with his own.

Of SCRIVEN's interests a complete article could be written in itself. His work on porous media has covered both the application to enhanced recovery and to the properties of catalysts pellets, packed beds and foodstuffs; some of this is being done in conjunction with Davis. A second area covers micro-structured fluids either in thin films or at interfaces or in dispersions. The need for computational results has led him to pioneer the application of finite element methods and to develop a range of computer-aided analytical techniques which allow the generation of numbers to assist, rather than obscure or dominate, the insight that can be obtained through mathematical analysis. SIVERTSEN's current research interest has centered on the relationship between the structure and various physical properties of bulk and magnetic thin film solids, especially the oxide analogs of the alkali halides.

TIRRELL, who also serves as the Director of Graduate Studies in the Department, is very active in many areas of polymer science. These include the control and

design of polymerization reactors where experimental studies are coupled with appropriate mathematical models. Of particular interest is the copolymerization of many components where temperature and mass transfer, reaction kinetics and reactor design all influence the composition and molecular weight distributions and properties of the product. He also studies high conversion free radical polymerization both theoretically and experimentally and is using dynamic scattering techniques to develop and apply modern theories of polymer diffusion in concentrated systems. Another area of interest is the influence of hydrodynamics on the kinetics processes involving macromolecules. These influences are exerted through induced conformational changes which in turn affect some of kinetic processes. TSUCHIYA came to the department in 1956 as the forefront of the development of interest in biological and bacteriological matters. He still is very interested in the role of metabolic products in the growth of microorganisms and in the development of continuous processes. On the materials science side, WALLACE uses positron probing to investigate the microstructures and substrates of metals and alloys. He has a considerable knowledge of the history of metallurgy and has taught an Honors Seminar in that area. WELLINGHOFF is interested, amongst other things, in polymers which normally crystallize very slowly in solution by chainfolding but can exhibit a fine spinodal phase separation along with rapid formation of fringed micelle crystals to provide the crosslinks for an extended elastic network. The interaction of flowfields upon polymer solvents is another part of his research, as is the kinetics and morphology of polymer phase separation in blends of polymers and the exciting new area of conducting polymers.

It would be futile to try and indicate the range of the papers published by members of the department for at the last count that the Dean required of us there were over a hundred papers published last year and almost as many the year before. It may, however, be germane to point out that several earlier contributions to this journal have reflected the approach of the department to the enjoyment of chemical engineering and have discussed various aspects of its program.* For some strange reason the department used to have a reputation for being dominantly theoretical. This was never really accurate, for there has always been a predominance of experimental programs. What we have tried to cultivate is the lively interaction of theory and experiment that is the hallmark of fruitful research. How well we have attained this balance is for others to judge.

*See II, 36-39; III, 48-52; VII, 19-40; X, 2-5; X, 114-124; XI, 68-73; XII, 148-151; Profiles of faculty are at V, 104-106 1971; XI, 50-52 1977; XIII, 8-12 1979. Light-hearted ephemera appear at IX, 118-119 1975 and XV, 12 1981.

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J. D. Seader of Utah

A. D. BAER AND VICKIE JONES

University of Utah

Salt Lake City, UT 84112

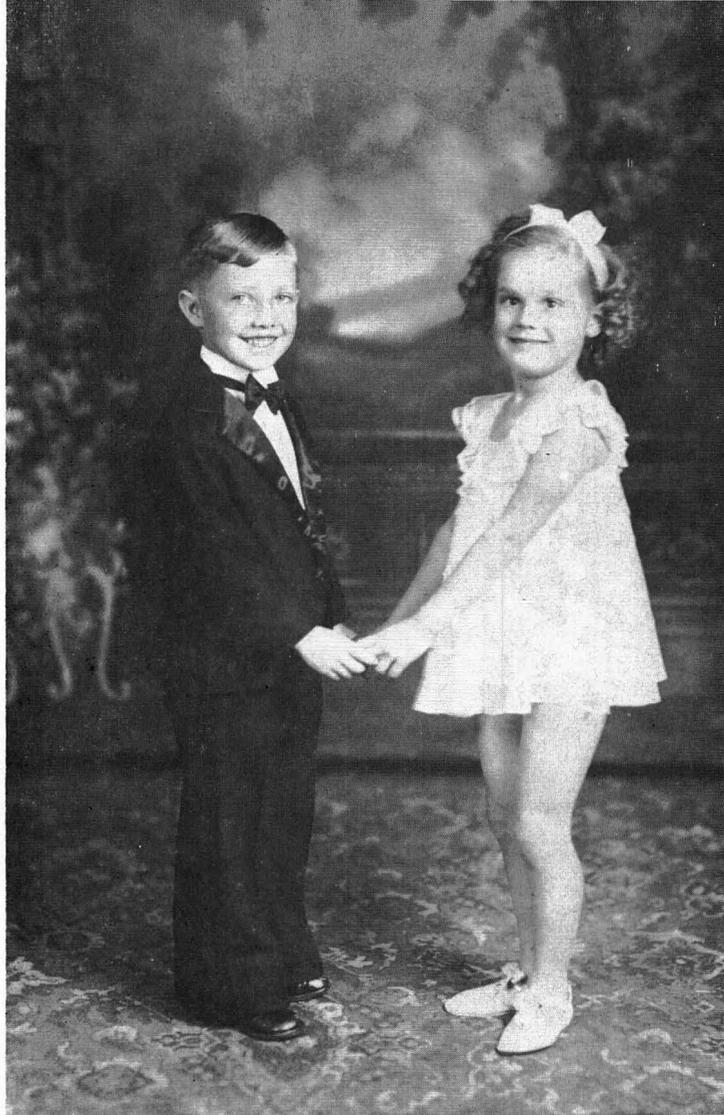
"BOB" SEADER WAS BORN IN San Francisco three months after Lindbergh's flight across the Atlantic. Being raised in the Bay Area in the 30's and 40's was a plus for any young man since it was then possible for a bright student of limited means to aspire to and receive an outstanding technical education. The Lindbergh flight signaled a public awareness of our developing, high technology, society and Bob has been both fascinated by and a contributor to the development of that society.

After graduating from high school and spending one semester at City College of San Francisco, Bob (at 17 years of age) enlisted in the Navy a few months before VJ Day. When the war was over, the Navy reneged on its promise to train Bob as an electronic technician and put him in charge of a demobilization interviewing team at Treasure Island in San Francisco Bay. Once Bob learned how the system worked, however, he arranged his own discharge in time to return to college in the fall of 1946. His C.O. and the Navy are still trying to understand his ploy, and the story illustrates why it can be undesirable to have enlisted men in the Navy who are too bright.

Bob's father wanted his son to be an entertainer (and perhaps enter politics) and in his pre-teen years Bob performed as a tap-dancer, an actor,

... he had the experience of seeing his designs built and operated. His most satisfying project was a 100-plate, 215-foot tall, 10 foot diameter deisobutanizer ... which was the largest distillation column built by Chevron at that time.

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Bob and a dancing partner, 1935

and a boy soprano in such prestigious and diverse places as the War Memorial Opera House in San Francisco and at San Quentin Prison in Marin County. When his voice changed, however, he decided that it would be best to confine his singing to the shower and instead began to pursue a life-long interest in athletics. He had lettered in basketball in San Francisco but later decided that desire and a competitive spirit were not enough for a successful career in sports. Thus, the father's and son's separate aspirations were now compromised to consideration of a career in science or engineering.

A word of explanation is required to explain how the nickname "Bob" comes from the initials J. D. By use of the peculiar thinking that only a parent naming a son can understand, Bob's father selected the name "Junior" since he didn't like his own first name (George) but did want to name a son after himself. However, Junior is not a name to be known by on the streets of San Francisco. The middle name DeVere likely comes from his

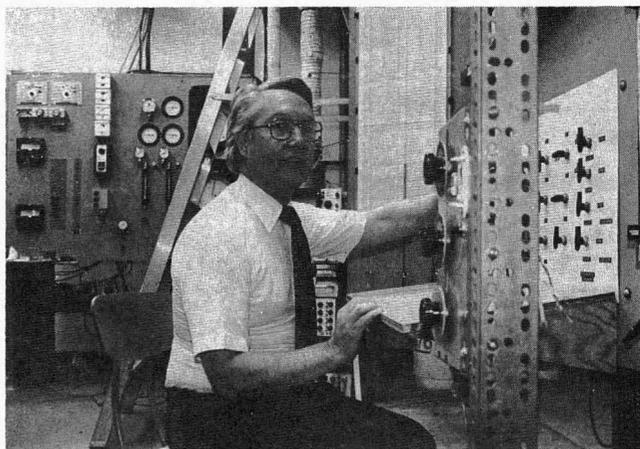
mother's Mormon heritage, and is a name to be used only in Utah. So, with the help of some of his peers in high school, the nickname Bob was selected out of desperation, and it stuck.

After an additional year at City College of San Francisco, Bob completed his sophomore year and transferred to the chemical engineering department at Berkeley, graduating at the top of his class in 1949. He spent an additional year at U.C. and received the M.S. degree in chemical engineering while working as the first graduate student for Charles Tobias. In the fall of 1950, Bob and his good friend Robert "Bob" Brodkey (now a professor at Ohio State) both left Berkeley and went to the University of Wisconsin in pursuit of the PhD degree. At Wisconsin, Bob worked for W. R. Marshall as one of Marshall's 16 PhD candidates. Seader had seldom seen snow in California, and the winters of 1950-51 and 1951-52 along Lake Mendota motivated him to complete his dissertation on drying in as short a time as possible so that he could return to sunny California. He maintains that he considered jobs with only two companies after completing his work at Wisconsin. The companies, both in the San Francisco Bay area, were Shell Development (then at Emeryville) and Chevron Research at Richmond. Since Chevron offered \$1 more a month than the competition, Bob reported to Richmond in September of 1952 and spent seven years at that location, involved in research and process design. In 1959, the lure of the unknown and the adventure of our manned space program attracted him to the aerospace industry. He joined the Rocketry Division of North American Aviation, Inc., at Canoga Park in Southern California to work on problems associated with the development of very large liquid-fueled rockets.

His friends in Northern California couldn't understand how he could leave the culture of that area for the "playground" of Southern California. However, while at Canoga Park Bob met his future wife, Sylvia, and they were married in 1961. They have four children; Suzanne, age 19, Robby, age 16, Kathleen, age 13, and Jennifer, age 7. Bob also has four older children, Steven, Clayton, Gregory, and Donald (two sets of twin boys), from a previous marriage.

When he left Wisconsin, Bob's original intention was to work for seven years in industry and then become a professor; but 13 years later he found himself still working in industry. Characteristically, he decided that it was time to

get back to his original plan and seek a position at a university. He decided to look outside of California (but not outside the Western States) and he subsequently accepted a position at the University of Idaho. In September of 1965, Bob arrived at the University of Idaho with the intention of spending the rest of his days there. But fate, in the form of a fortune cookie, intervened. At a Chinese restaurant in Moscow, Bob read that he was to receive an important telephone call in three days; and, sure enough, three days later, E. B. Christiansen (who had been Chairman of the Chemical Engineering Department at the University of Utah since 1947) called with an offer for a Professorship. Chris had heard from Bob Marshall that Seader was looking around, and he



"Where is the computer?"

finally tracked him down in Moscow. Bob was reluctant to leave his new friends at Idaho; but being a fatalist and not wishing to alienate the Chinese, he agreed to join the department at the University of Utah in the fall of 1966. Even though Salt Lake City is the headquarters of the LDS (Mormon) Church, he maintains that was not a factor in his decision. He is an active member of the LDS Church and has served in several important positions in the lay clergy of the church.

Seader was then the sixth member in the department at Utah, and his many talents and varied background really strengthened the faculty. In 1975, he became Departmental Chairman, succeeding Christiansen, who had been in that position for 28 years. Bob served as chairman for a single three-year appointment and then stepped down with the comment that it was too easy to become corrupt in that position, although it is hard to see

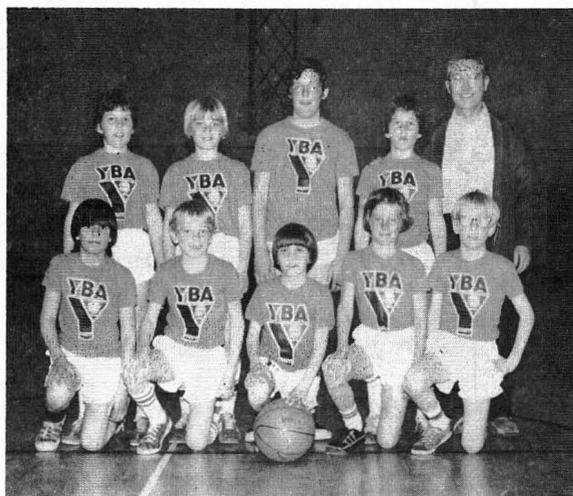
what could be gained in an academic department even if one were corrupt. In fact, Bob really wanted to spend all his time with his first loves, research and teaching. His most significant accomplishment as chairman was to succeed in adding three new members to the departmental staff with a budget increase for only one new member. This accomplishment still baffles the University administration, and it remained for later chairmen to reconcile the budget; but through this maneuver, the department was well staffed at the time of the recent enrollment surge.

Bob Seader's work has been at the forefront of the major thrusts in chemical engineering for the past 30 years. It was planned that way, and he is fond of setting objectives and then making sure that the objectives are achieved. A good illustration of his approach and use of objectives occurred when he was informed that he had been selected to coach his then-12-year-old son's basketball team. He accepted the challenge but quickly recognized that there were no budding Julius

While at Richmond, he helped develop and publish the "Chao-Seader" correlation for distillation K values. He is "that" Seader.

Irving in the group. However, he could teach his four- to five-foot tall charges something about man-to-man defense; and the objective was set to prevent opposing teams from scoring. His success was almost fatal for the league. In the 11-game season his team completely shut out the opposition three times (this was basketball, not baseball!); and during the first half of one game, the opponents never got the ball out of their backcourt. The league rules were changed the following week to disallow the backcourt press.

One of Bob's favorite hobbies is to harrass Jerry Pimm, the coach of the University's "Running Utes" basketball team. He firmly believes that if the coaches had listened to him, the University of Utah would have been national champions in 1981, when they started two senior All-Americans. Pimm good naturedly answers Seader's letters and, if pressed, might concede that Bob could be right. In spite of Seader's interests in athletics, none of the several skiers in the department have been able to get Bob on skis. He is indifferent to all sports having to do with ice and snow.



"Don't let the other team score!"

At the time Bob worked for Chevron, the petrochemical industry was in a period of very rapid growth, and he was involved in promoting that growth. During one year he worked with Wayne Edmister in developing the "Standard of California" data books. Many of the projects that originated in his process design group resulted in completed plants, and he had the experience of seeing his designs built and operated. His most satisfying project was a 100-plate, 215-foot tall, 10-foot diameter deisobutanizer for the El Segundo refinery, which was the largest distillation column built by Chevron at that time. A picture of this unit is shown in the frontispiece of his book (with E. J. Henley) entitled *Equilibrium-Stage Separation Operations in Chemical Engineering*. Bob reads all accounts of L.A. earthquakes closely to make sure that the unit still stands. While at Richmond, he helped develop and publish the "Chao-Seader" correlation for distillation K values. He is "that" Seader. Bob suspects that his reputation is occasionally enhanced by being in a profession influenced by another Seider (Warren D.) with whom he has written books and given short courses.

He also learned something of the pitfalls in solids handling when he designed a system consisting of a high-speed vacuum rotary filter feeding a rotary steam-tube dryer, which in pilot tests performed very well when fed with a filter cake. How was he to know that, during plant startup, lack of attention to operation of the filters would permit them to feed a slurry instead of a cake to the dryer? The slurry set up like cement in the dryer and plugged it so badly that the tubes

His colleagues consider Bob as a "super-star." Some of the secretaries have referred to him as "Super-Seader" or "Dr. Dynamo." He does everything well, and it is a humbling experience to see him work. He appears to be able to master tough technical material after only one reading . . . he requests six to eight papers from the weekly Current Contents in widely varying fields.

had to be completely replaced. His experience at Chevron is unique among current-day engineering professors and, even when his research becomes very mathematical and abstract, he is able to draw on that background to relate his results to the real world. In the current vernacular, "he has been there."

While with Standard of California, Bob championed the then-unreliable digital computer for design and control applications. In 1958, he directed the development of Chevron's first process simulation and distillation computer programs. His "love affair" with the computer has never diminished. He was a charter member of the CACHE committee and is currently the Executive Officer and Treasurer for that group. With that committee, he was instrumental in making the arrangements for chemical engineering departments to use the FLOWTRAN process simulation program written by Monsanto.

The attraction of Rocketdyne and the aerospace industry in the 1960's was simply that "that was where the action was." The aerospace industry was an ideal place for high technology work. Bob enjoyed the excitement of the goals of that time and recalls with wonder how he and his colleagues would attend night classes or lectures at UCLA where the materials at the frontiers of science and applied mathematics were taught and then try to apply the information the next day to solve real problems. There was always enough money to do the job right, and teams of dedicated and outstanding engineers and scientists were assembled to accomplish the impossible. Seader claims that he lost a lot of his "chemical engineering provincialism" while working with so many competent people from so many other disciplines. His own work included fundamental studies of heat transfer to cryogenic fluids (for which he received a NASA Tech Brief Award in 1971), applications of computers for data acquisition, control and real-time analysis, and a wide range of heat, mass, and momentum transport and fluid dynamics problems. He became a recognized authority in the area of ablative materials and of theories of charring-ablation heat transfer.

His research interests at the University of Utah have been of broad scope and, as usual, have been in the mainstream of chemical engineering work. In the latter half of the 1960's, he concentrated on kinetics and transport phenomena in curved tubes. In the early 1970's, when the vogue was on relevance of research, he served as co-director of and supervised research in the Flammability Research Center at the University of Utah. His primary efforts dealt with characterization of the smoldering properties of synthetic and natural polymers and the smoke generated by pyrolysis and combustion in catastrophic fires. In 1975 he teamed with Alex Oblad and Wendell Wisler of the College of Mines and Mineral Industries at the University in support of efforts



CACHE Committee receiving grant from Monsanto, 1976.

to produce liquid coal and to develop processes for recovery of oil from the unique tar sands formations in the state of Utah. He is co-inventor of a promising patent for a tar sands thermal recovery process that represents a novel application of heat pipes. As usual, he continues to find new applications for the digital computer. A major interest of his is computer-aided synthesis of separation sequences using artificial intelligence. Currently he has a student developing methods for design of coupled systems of separators. He is not only conversant with computers but also communicates

with mathematicians. Bob quickly recognizes and uses applied mathematical achievements that have engineering applications.

While at the University of Utah, Bob has been a very effective industrial consultant, and he is popular as a lecturer. Since 1974, with Dick Hughes and Warren Seider, he has conducted AIChE Continuing Education Courses in computer-aided design and in mathematical modeling. He has lectured in "Spanglish" in Puerto Rico, Mexico, Brazil (in broken Portugese), Chile, and Peru. Often, after a lecture tour, he is followed

Seader claims that he lost a lot of his "chemical engineering provincialism" while working with so many competent people from so many other disciplines.

from South of the Border by exceptionally capable graduate students. In an unguarded moment, most of these students will admit that Bob's mathematics is easier to understand than his Spanish.

His colleagues consider Bob as a "super-star." Some of the secretaries have referred to him as "Super Seader" or "Dr. Dynamo." He does everything well, and it is a humbling experience to see him work. He appears to be able to master tough technical material after only one reading. Typically, he requests six to eight papers from the weekly Current Contents in widely varying fields and when the articles are received, he reads each one carefully. Anyone answering his request for a reprint can be sure that the paper will be read; and if there are errors, one can expect to hear from him. He has a reputation as an outstanding reviewer of technical material, and several standard texts have benefited from his comments. He swears that he will review no more texts, but he intends to write more books. His latest book, to be published by the MIT Press, deals with the thermodynamic efficiency of chemical processes.

Bob is one of the most effective and likely the best-liked teacher in the department and in the Engineering College. He received the University of Utah Distinguished Teaching Award in 1975 and has always been very popular with students. His lectures are concise, well organized, and almost totally free from distractive, trivial mistakes. His presentations always include many references to recent practical applications of the

material in areas of immediate interest to the students. He is a master of bringing material from his research activities into his courses at all levels. In addition to carrying a regular teaching assignment in the department, he has developed a unique and popular second-year graduate course in advanced concepts of reactor design, which is based on his experience at Chevron and at Wisconsin. His senior-level course in computer-aided design (FLOWTRAN based) draws students from many disciplines on campus. He works pretty much in a one-on-one basis with his graduate students and has a weekly conference with each student in which it is well understood that some progress in the last week had better be reported. Somehow he gets an enormous amount of work out of all students, but no one ever complains. There are no threats, no posturing; and he is neither a hard nor an easy grader. All students simply like to work hard for him.

The opinion held by people who have worked with Bob for many years is best expressed by a comment whose source has been forgotten, "It is almost too bad that Bob is such a nice guy; if he were real nasty, I could at least feel superior to him in something." □

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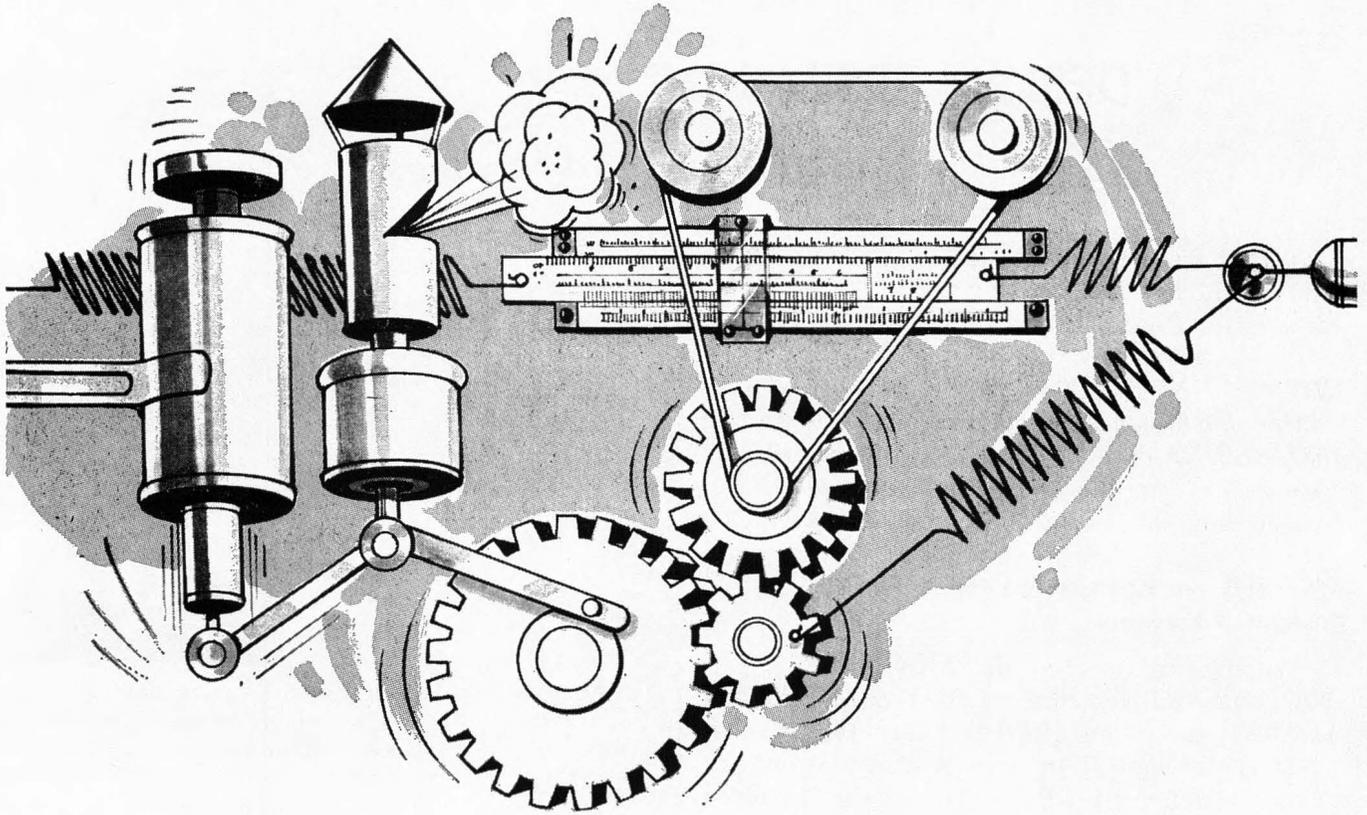
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Award Lecture

DESIGN RESEARCH

Both Theory and Strategy

ARTHUR W. WESTERBERG
Carnegie-Mellon University
Pittsburgh, PA 15213



Arthur W. Westerberg received his degrees in chemical engineering at Minnesota, Princeton, and Imperial College, London. He then joined Control Data Corporation in their process control division for two years. In 1967 he joined the University of Florida where he remained for nine years. In 1976 he joined the faculty at Carnegie-Mellon University. He was Director of the Design Research Center from 1978 to 1980 and just became Head of Chemical Engineering this January.

EDITOR'S NOTES This is the second and concluding installment of Professor Westerberg's 1981 ASEE Award Lecture. The first installment appeared in the Winter 1982 issue of Chemical Engineering Education (Vol. 16, No. 1, page 12).

ASCEND-II: An Analysis Aid for Arbitrarily Configured Processes

We shall move off on an entirely new tack at this point and describe briefly the ASCEND-II flowsheeting system (Locke, et al (1980)) that we are developing in my research group at Carnegie-Mellon University. The persons involved are Michael Locke (Locke (1981)), Selahattin Kuru (Kuru (1981)), Peter Clark (Clark (1980)), Dean Benjamin and Andrew Hrymak. The messages to be conveyed by this example are two: the breadth of research activities which support this project and a description of the use of this system to develop a working analysis model for a process in a manner which is consistent with the design strategy that has been the main theme of this paper.

To examine ASCEND-II we need first to es-

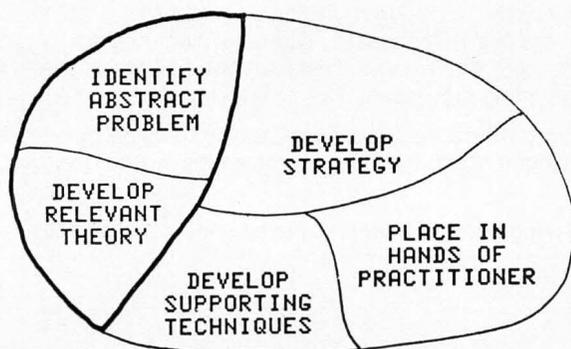


FIGURE 4. Aspects of Design Research.

tablish what we mean by analysis. We include the following types of analysis for a given but arbitrarily configured process flowsheet.

- 1) **Simulation.** The inputs to the process, the temperature and pressure levels at which to operate and the equipment sizes are fixed. The calculation is to discover how the equipment performs, a rating calculation.
- 2) **Design.** Some outputs from the process and some intermediate stream variable values may be specified in exchange for calculating an equal number of the inputs, levels of operation and/or equipment sizes.
- 3) **Dynamics.** The dynamic behavior of a process may be required.
- 4) **Optimization.** We may wish to optimize the process over the set of continuous variables that describe equipment sizes and process operating levels.

Fig. 4 illustrates the breadth of questions which one can address in the area of design research. Many persons identify design research

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Unlike conventional flowsheeting systems, each unit with a flowsheet can be tested by itself in ASCEND-II, permitting a bottom up solving of the units at any time. In this mode and using the simple model as the base case design, much testing can be done to see where to add complexity, and where perhaps to remove complexity.

with only the two aspects highlighted with a dark line: 1) Identify Abstract Problem and 2) Develop Relevant Mathematical Theory. We have been arguing all along about the importance of developing a correct design strategy. Support techniques are often shrugged off as not fundamental enough, but, if not done correctly, the implementation of the theory will likely prove too complex to be practical. Finally one should not overlook the problem of placing sophisticated tools into the hands of unsophisticated users. There is research lurking there too.

The abstract problem for developing ASCEND-II is how to solve large sets of simultaneous nonlinear, sparse algebraic, ordinary and partial differential equations, perhaps subject to inequality constraints and perhaps containing discrete variables. There is certainly enough of a problem here to require considerable effort.

Relevant theory includes convergence proofs, analysis techniques to take advantage of structure and Lagrange theory. We have already discussed strategy ideas at length. The supporting techniques include consideration of data structures, problem decompositions (see Westerberg and Berna (1978), Berna, et al (1980), Clark (1980)), data bases and use of network computing. Finally the ideas involved in placing the tools into the hands of the practitioner include language design, level of interaction, online documentation system design and use of graphics. We are making considerable progress at dealing with the above ideas and others in the development of ASCEND-II.

Fig. 5 illustrates the underlying evolutionary aspect of ASCEND-II.

ASCEND-II is intended to help a process engineer "design" a computer model for his process, using the available building blocks provided within the program. "Design" here refers to finding and solving a model of the needed complexity to answer the questions being asked of the process, where the engineer is learning both about the questions he should ask and about the model as he proceeds. We could broaden the meaning of design to that of designing the process for which the model is being developed, a task for which ASCEND-II is also well suited, but we want to

limit ourselves here to the narrower model design problem.

The axes in Fig. 5 are axes along which the model design can evolve. Model complexity can evolve from simple to complex, where simple models consist of only a few units and the use of the simplest of physical property models; e.g., a flash unit using constant relative volatilities.

With each model a range of analysis types can be performed, starting with simulation, moving to design and finally (when ASCEND-II is further developed) to optimization. Simulation is intuitively the easiest mode to use for the engineer. In that mode he can usually establish a

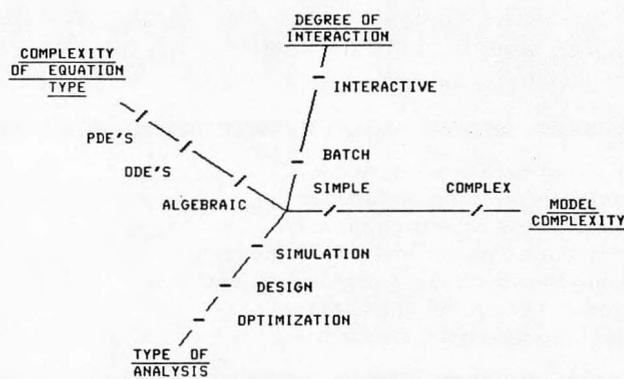


FIGURE 5. The ASCEND-II Flowsheeting System.

set of specifications which will lead to a solution for the remaining variables. For example, one has some confidence that, if he fixes the feed stream to a flash unit, fixes the fraction of the feed which will vaporize and the flash pressure, then the flash unit will have to operate and so will the corresponding calculation. Why not allow the user to start then with this "comfortable" calculation? Once he can simulate the flash unit ASCEND-II allows him to alter the set of variables to be specified. For example, he could require that the recovery fraction of one of the components be specified and that the pressure be calculated. If the trade is illegal, he will be warned immediately.

Running through a few design calculations will acquaint him with the shape of the solution space and when he gets near to a good solution,

he can switch into doing an optimization calculation.

Once this sequence is solved using simple algebraic models, he can selectively add more complexity to the model by adding more units and/or more sophisticated physical property calculations and continue.

A type of complexity which can be added is to broaden the type of equations which are used to model portions or all of the process, i.e., by allowing models involving ODE's (Kuru (1981)) and PDE's to be introduced. With ODE's and PDE's one can consider doing dynamic studies.

The last axis is that reflecting the degree of interaction ASCEND-II will have with the user. In ASCEND-II a standard command file can be created which will attempt to solve any model once it is set up. Invoking this "standard" file is like running the problem in batch mode on a computer. At the other extreme, the commands can be executed interactively one at a time in fairly arbitrary order. (The computer is a DEC-20 which provides a very friendly interactive environment.)

Examples of the types of commands available

The heat exchanger network synthesis problem epitomizes the effective use of approximate criteria to locate excellent final network designs. Using thermodynamic arguments, one can predict a priori the least amount and kind of utilities needed.

are 1) to input some more structure to the flowsheet, 2) to delete some of the existing structure, 3) to save and retrieve variable values, 4) to initialize variable values (selectively), 5) to change the set of variables whose values are to remain fixed, 6) to cause variables and equations to be rescaled to reflect current variable values, 7) to do one or more Newton-Raphson iterations, 8) to determine the constrained derivative of one variable with respect to another, 9) to display variables selectively, and 10) to display equation errors selectively.

With this structure for ASCEND-II, the user can "drive" his computation around computational obstacles much as he drives a car and can become very effective at getting solutions quickly, even for stubborn problems.

We have set the stage now to argue that ASCEND-II allows the model for a given process to be designed using our earlier guidelines.

Clearly the first guideline is dealt with: evolving from simple to complex. The depth first strategy can be followed by developing first a simple model for the entire process.

Unlike conventional flowsheeting systems, each unit within a flowsheet can be tested by itself in ASCEND-II, permitting a bottom up solving of the units at any time. In this mode and using the simple model as the base case design, much testing can be done to see where to add complexity, and where perhaps to remove complexity. Answers can be obtained to a simpler version of the problem to use as a starting solution point for the more complex versions, a strategy often needed when solving highly nonlinear equations. The notion of developing and using approximate criteria is also possible. One usually gets a solution to the equations, perhaps far from the desired solution point. This solution may be from doing a simulation rather than the desired design calculation. Not unlike the idea behind a continuation method, the calculation can be converted to the desired design calculation in terms of which variables are specified. Then one can move to the solution point desired through a series of small steps, converging to the solution at each step.

While it is obvious that much of the power of a program like ASCEND-II comes from its being interactive, it is equally as obvious when using it that the ability to find a base case solution and then to move from that solution in almost any manner desired (top down/bottom up, simulation/design, etc.) is the heart of the rest of its power. It is the learning that can occur which helps to decide the nature of the next calculation, to see its impact and to alter one's path as a consequence, that makes ASCEND-II so useful. Traditional flowsheeting systems (and for that matter, traditional equation solving packages) do not offer the flexibility provided by ASCEND-II for this approach.

ASCEND-II has been designed under the assumption that calculations will often fail until one learns about the problem. Diagnostic tools are thus provided to allow the user a chance to detect where the failures are occurring. As mentioned only briefly before, these include interactive access at any time to *every* variable in the problem by a convenient name and similarly to every *equation error*. This latter access allows one to note, for example, that the phase equilibrium equations on stage 3 of the diethyl ether column are not converging. The variables around that stage can

"Design" here refers to finding and solving a model of the needed complexity to answer the questions being asked of the process, where the engineer is learning both about the questions he should ask and about the mode as he proceeds. We could broaden the meaning of design to that of designing the process for which the model is being developed, a task for which ASCEND-II is also well suited, but we want to limit ourselves here to the narrower model design problem.

then be examined to see if one is perhaps too large or worse yet, negative. Having located the problem, the user can then start to work on correcting it.

Interestingly, the current version of this system is a third generation version. We designed ASCEND-II following our guidelines by prototyping it twice, at each step improving the design based on the previous version. This was and remains a deliberate policy for creating ASCEND-II.

Heat and Power Integration of a Process

THE LAST PROCESS PROBLEM to be considered is to integrate the heat and power requirements

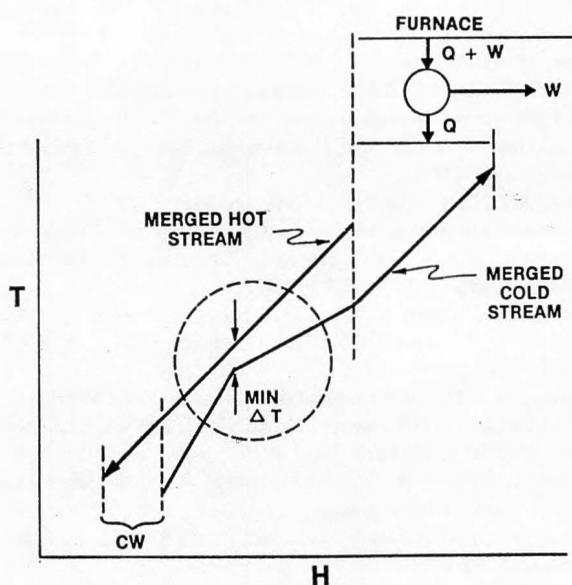


FIGURE 6. Minimum Utility Calculation. Upper right illustrates how to extract "work" efficiently from process.

for a process for which one has just set temperature and pressure levels for each of the units and has solved the process heat and material balances (using ASCEND-II for example). Great progress has been made for solving this problem. The heat integration portion is usually called a heat exchange network synthesis problem. See Nishida et al (1981) for an extensive review of the heat exchanger network synthesis problem.

The heat exchanger network synthesis problem epitomizes the effective use of approximate criteria to locate excellent final network designs. Using thermodynamic arguments, one can predict a priori the least amount and kind of utilities needed to solve this problem. Also using graph theoretic ideas one can guess the fewest number of heat exchanger units likely to be needed. Experience has shown that the better designs meet these goals, or come very close to meeting them. Finally, effective design techniques exist to aid one to find such designs.

In preanalyzing the heat integration problem, one discovers for most problems a bottleneck will occur to further heat integration in the form of a temperature pinch. Fig. 6 illustrates the way Hohmann (1971) located this pinch. He merged all hot streams into a single "super" hot stream and all cold into a single "super" cold stream. Placing them as illustrated on a temperature versus total enthalpy diagram reflects the opposing hot and cold stream temperature profiles one would see if these super streams met in a single counter current heat exchanger. The pinch is the point which precludes further integration. Cerda (1980) from our group and, in parallel, Mason and Linnhoff at ICI recently developed an approach which generalizes this minimum utility calculation.

Umeda et al (1979) have exploited the pinch to aid in locating where in a process the re-establishing of temperature and pressure levels will permit more heat integration. Very recently Linnhoff and coworkers (Townsend and Linnhoff (1981), Dunford and Linnhoff (1981)) have shown how to exploit large temperature differences between these super streams which occur either entirely above or entirely below the pinch. They show how to convert heat entirely to mechanical work or obtain some "free" separation work within a process. For example, the upper right part of Figure 6 shows how one can place a turbine to get 100% of the thermal energy which must be added into the process converted to the desired mechanical work. The cost is the degrading of the thermal energy which enters and is later rejected by the turbine. If that energy can be degraded

and still be rejected at a temperature where it is useful as heat input to the process *and* if that heat can be extracted and rejected entirely above or entirely below the pinch, then 100% of the extra energy added to drive the turbine is converted to work.

The design strategy is to establish first a process design not yet heat integrated. Then by examining the process, one finds the pinch temperature and predicts the minimum utility costs associated with the process. Next one can modify the process near the pinch if further heat integration is desired. Finally one can place some turbines if possible so they degrade thermal energy either entirely above or below the pinch. The design can then be reassessed and improved from this thermally integrated base case.

PROVING THE STRATEGY ITSELF

How would one "prove" that the design guidelines are basically sound? That problem is itself a design problem and should be (if we are correct) solved using a strategy consistent with the guidelines themselves. The concept should be recursive. In our case it is leading to the design and testing of the ASCEND-II system. We are only at present proving we are right by demonstrating how rapidly one can put together a working computer model for a process using this system. In one example a model was constructed using a conventional flowsheeting system and the exercise took two full time days. Using ASCEND-II, it took two hours.

Since teaching these guidelines to our students in the undergraduate design course, we see a noticeable reduction in the time needed to get realistic designs.

IN CONCLUSION

The guidelines suggested to aid one to do design more efficiently have been illustrated on several diverse problem types. Only qualitative "proof" exists as to their correctness. If correct a principal use can be to examine a proposed or existing design tool (or design effort) to see if it abides by them. Where it fails should suggest modifications to the tool which could significantly change its effectiveness. Designers have to make a conscious effort to stick to the guidelines as

they do not always coincide with the most natural approach. They can be taught; we try to do so in the undergraduate design class. □

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CHEMICAL ENGINEERING DIVISION ACTIVITIES

SUMMER SCHOOL 1982

The Summer School for Chemical Engineering Faculty is organized by the Chemical Engineering Division of the American Society for Engineering Education and is held every five years. The 1982 Summer School, ninth in a series begun in 1931, will be held August 1-6 at the University of California in Santa Barbara and has been generously supported by industrial concerns. Its purpose is to acquaint faculty with new developments in chemical engineering education and to provide for personal interaction with other faculty and representatives from industrial firms concerned with the educational process. The 1982 Summer School

is being co-chaired by T. W. Fraser Russell and Stanley I. Sandler of the University of Delaware.

In February of 1982, program and registration information was mailed to chemical engineering department chairmen in the United States, Canada and Mexico. Attendance at the Summer School must be limited due to constraints on both classroom space and living accommodations and the Chemical Engineering Division has elected to have each chairperson select an attendee from their department.

Summary information concerning the topics to be covered at the Summer School is shown in Figure 1 below.

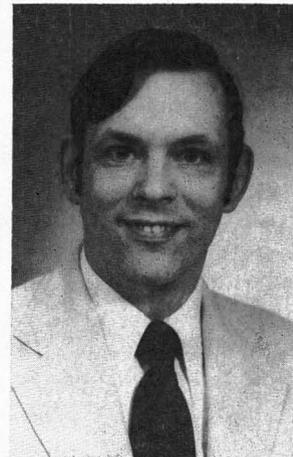
FIGURE 1

PROGRAM SUMMARY CHART

BLOCK SESSION	BLOCK 1 NEW TECHNICAL DIRECTIONS IN CHEMICAL ENGR T. J. Anderson	BLOCK 2 EXPANDING ROLE OF COMPUTERS IN CHEMICAL ENGR EDUCATION T. F. Edgar	BLOCK 3 CHEMICAL ENGINEERING IN THE CLASSROOM AND LABORATORY & A SPECIAL POSTER SESSION ON CHEMICAL ENGR TEACHING G. M. Howard	BLOCK 4 INDUSTRIAL/UNIVERSITY INTERACTIONS W. S. Kemp	BLOCK 5 THE SOCIAL RESPONSIBILITIES OF THE ENGINEER B. J. Lubersoff P. V. Telo	BLOCK 6 CHEMICAL SCIENCES & CHEMICAL ENGR G. L. Schrader
SUNDAY EVENING	SOCIAL EVENT					
MONDAY 9:00 am	OPENING REMARKS					
MONDAY MORNING	Biomedical Engineering I	Computer Graphics & Modular Instruction I	Problem Solving I	The Senior Design Course I	Statement of the Problem	Catalytic Chemistry and Surfaces I
MONDAY EVENING	Biomedical Engineering II	Computer Graphics & Modular Instruction II	Problem Solving II	The Senior Design Course II	The Law and its Implementation	Catalytic Chemistry and Surfaces II
TUESDAY MORNING	Biotechnology	Use of Computers in Teaching Process Design I	Undergraduate Laboratory Instruction	University-Academic Personnel Interchange	Can Big Be Beautiful?	Applied Thermodynamics I
TUESDAY EVENING	Process Synthesis Development	Personal Computing	Managing Large Classes	Intern & Co-op Programs	Separate Together?	Applied Thermodynamics II
WEDNESDAY MORNING	Solid-State Processing	Use of Computers in Teaching Process Design II	Updating Process Dynamics and Control Education	Academic-Industrial Perceptions of Engr Education	Social Implication: Two Views	Industrial & Engineering Chemistry
WEDNESDAY AFTERNOON	3-M AWARD LECTURE					
WEDNESDAY EVENING	SOCIAL EVENT					
THURSDAY MORNING	Polymer Science and Engineering	Microcomputers in CHE Laboratories I	Oral & Written Communication Skills	Financial Aid	Relating to the Market	Food Processing & Food Science I
THURSDAY EVENING	New Separation Techniques	Teaching of Process Synthesis in Design	Course Design & Evaluation of Learning I	Role of Industrial Advisory Boards	Two Successful Courses	Food Processing & Food Science II
FRIDAY MORNING	Pulp and Paper Technology	Microcomputers in CHE Laboratories II	Course Design & Evaluation of Learning II	How to Conduct A Short Course	Tie-Up	Electrochemistry & Corrosion

CHEMICAL PROCESS SYNTHESIS

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PROCESS SYNTHESIS IS THE specification of chemical and physical operations and the selection and interconnection of equipment to implement these operations to effect desired chemical processing transformations. Synthesis is the first of an iterative set of process design activities which also includes analysis, evaluation, and optimization. Significant progress has been made, particularly since the advent of the digital computer, in the development of a more scientific and less empirical framework for modeling, simulating, and improving equipment and operating parameters for a given design. However the necessarily prerequisite invention of the design, the generation of the processing structure represented as a flowsheet, remains largely a creative art. Economic competitiveness has demonstrated the importance of correct structural choices in meeting process objectives. This realization has led to present efforts to investigate the possibility of formalizing the synthesis activity. The ultimate goal is not just to invent technically feasible designs, but to produce structural configurations that when analyzed, evaluated, and optimized will prove by design objective criteria to be superior to (possibly all) other structural arrangements.

Inventing flowsheets is, of course, not new and some guidance embodied in design rules-of-thumb based on experience developed through trial and error has existed for many decades. However, formal consideration of structural generation

The ultimate goal is not just to invent technically feasible designs, but to produce structural configurations that when analyzed, evaluated, and optimized will prove by design objective criteria to be superior to . . . other structural arrangements.

J. J. Siirola received his B.S. from the University of Utah and his Ph.D. from the University of Wisconsin-Madison in 1970 where he developed the AIDES process synthesis system and coauthored the introductory text, *Process Synthesis*. Besides a continuing involvement in synthesis technique development, implementation, and application, his research interests also include simulation and optimization aspects of computer-aided design, non-numeric programming, artificial intelligence, and technology assessment. He is currently a Research Associate in the Eastman Chemicals Division of Eastman Kodak Company.

dates only from the late 1960's. Some investigators studied the general overall invention of complete flowsheets, while others concentrated on specific process synthesis subproblems such as reaction paths, reactor network configurations, separation train systems, energy recovery networks, fault trees, and safety and control systems. Several excellent reviews with extensive bibliographies [(Hendry, Rudd, and Seader (1973), Hlavacek (1978), Westerberg (1980), and Nishida, Stephanopoulos, and Westerberg (1981)] chronicle the developments and progress made in these areas to the present time. Here we will consider some of the underlying paradigms which have been suggested for continuous process synthesis.

SYNTHESIS IN DESIGN

Process synthesis has been defined as the invention of the process structure. This definition can be extended to include invention of associ-

ated control and safety systems, development of steady state and transient (start-up and shut-down) operating procedures, and other similar design specification activities. Synthesis should be differentiated from 'flowsheeting,' a term which refers to the simulation, often by computer, of an existing structure.

The number of tasks that must be performed to convert available raw materials into desired products and environmentally acceptable by-products may be quite large. Even given the concept of unit operations, the wide range of existing technologies capable of accomplishing these tasks and the multitude of ways in which these technologies can be interconnected to achieve the design objectives with varying efficiency leads to synthesis problems characterized by discrete decisions and combinatorial difficulties. Furthermore, although the existence of some feasible processing structure is usually not in question, the multivariable and sometimes subjective nature of the design objective criteria (safety, reliability, operability, environmental impact, feedstock security, quality, resilience, familiarity, experience, as well as capital investment, operating expense, etc.) makes it difficult to quantify the concept of 'optimum.' Often it is desirable to generate a series of structural alternatives judged to be nearly optimal by some economic criteria for further subjective evaluation.

Despite the fundamental importance of synthesis in chemical process design, few existing design texts give more than passing reference to the necessity for first establishing a workable manufacturing process for producing the desired product, preferring instead to concentrate on the more deductive and quantitative aspects of analysis, evaluation, and (parameter) optimization. When mentioned at all, more is noted about such attributes as experience, self confidence, constructive discontent, open mindedness, and demonstrated intuition and common sense of engineers who appear to be successful at synthesis than about invention techniques themselves. However, some qualitative concept discovery aids do seem to be used by successful designers. The most basic of these is historical information from such sources as engineering textbooks, handbooks, catalogs, proprietary company reports, commercially available comparative process analyses, and open scientific and patent literature, experience, and rules-of-thumb. Design concepts have also been discovered through individual or group creative

**Often more than merely
the invention of a feasible design,
process synthesis involved an optimization
over structure.**

efforts. These include functional and morphological analyses (mechanical schemes for forcing associations among desired design goals), imitation of nature, analysis of models of other designs, and brainstorming. These methods and aids rely heavily on analogies with or adaptations of past working designs and none have explicit provisions for generating optimal structural arrangements.

Are there attributes specific to the synthesis problem that should be exploited and developed into solution procedures not necessarily resembling techniques now employed by successful designers? Are there aspects of 'artificial intelligence' research, a relatively new branch of computer science concerned with understanding and simulating intelligent problem solving, that might contribute to a formalism for process invention? Early in systematic process synthesis research, optimization, evolution, and decomposition emerged as potential invention approaches. These remain the dominant framework for synthesis development today.

OPTIMIZATION APPROACHES

Often more than merely the invention of a feasible design, process synthesis involves an optimization over structure. A natural approach, and in fact one of the earliest proposed, is to combine structural optimization with equipment and operating parameter optimizations now routine because of recent advances in computerized numerical methods. In fact, the synthesis problem has been formally defined as a nonlinear mixed integer and continuous variable optimization problem. Equipment selection, interconnection, and other discrete decisions are represented by integer variables (often zero or one) and constraints among these variables. The difficulty is that no code exists to solve this generally exceedingly large mixed optimization problem.

One approach is to invent a superstructure in which all technologies under consideration and all their possible interconnections are embedded. Associated with each branch of an interconnection leading from one item of equipment to several

others is a 'structural parameter,' a continuous variable which represents the fraction of flow to be split to each of the alternate destinations. As fractions, structural parameters are constrained to be non-negative and to sum to unity for all branches from a junction. These structural parameters are included with other equipment and operating parameters in an overall design optimization. Should a structural parameter be optimized to zero, the corresponding interconnection is deleted from the superstructure, and should all flows associated with an item of equipment be zero, it too is deleted from the structure. In effect, the discrete decision making aspects of

Considerable savings may result if pairs of complementary heating and cooling tasks can be made to drive each other rather than require the use of auxiliary utilities.

process synthesis are replaced by a continuous nonlinear constrained optimization for which solution techniques exist.

Unfortunately, the method does not provide guidance for the initial generation of the superstructure. The larger the superstructure, the greater will be the number of structural parameters and the size of the corresponding optimization. The problem of assuring that the optimal structure has been included within a given solution formulation is one which arises repeatedly in process synthesis research. In the present case, human experience, rules-of-thumb, and other design aids are used to select the equipment and interconnections to be included in the superstructure.

Because of the size of the optimizations required, the structural parameter method has been applied primarily to smaller synthesis sub-problems (generally fewer than ten interconnections) such as reactor and distillation networks. Several solution techniques have been investigated including simultaneous and sequential optimization of the structural parameters and other design variables by a variety of codes. The feasible region is often multimodal and search methods starting from different points may be required to find a global optimum. The convergence rate of nonlinear constrained optimization is often slow, and transformations have been suggested to eliminate constraints on the structural pa-

rameters. However, inequality constraints on design variables may result in a discontinuous feasible region boundary necessitating discrete decisions the structural parameter method was developed to circumvent. Inequality constraints associated with equipment deleted from the superstructure during structural parameter optimization can force constrained behavior in the remaining structure. For many problems a completely continuous formulation may not be possible.

The optimal assignment formalism from operation research is another optimization approach that has been applied to the synthesis of heat integration networks. This synthesis sub-problem concerns the heating and cooling tasks which must be performed within a process. The problem statement includes a complete description of the streams to be heated or cooled, descriptions of auxiliary utilities capable of performing the required tasks, and descriptions and design equations for equipment (furnaces, reboilers, condensers, and other heat exchangers, etc.) useful for implementing the tasks. The object is to synthesize a scheme to accomplish these tasks in some optimal manner, for example at minimum net present cost. Considerable savings may result if pairs of complementary heating and cooling tasks can be made to drive each other rather than require the use of auxiliary utilities.

The discrete process of selecting the sequence of energy interchanges among streams and utilities to be heated and cooled is accomplished by dividing the heat loads of these streams into suitably small, equal-size elements. Subject to thermodynamic temperature constraints, a cost can be associated for the 'allocation' (effected by a tiny exchanger) of heat from any element of a stream or utility to be cooled to a suitable element to be heated. If it is assumed that these costs are independent of each other, then linear programming can be employed to perform an optimal allocation. Later, if multiple adjacent elements for two streams are found to be paired, the tiny exchangers are merged into a larger countercurrent unit. In this manner, the amount of heat to be transferred in each exchanger in the structure has also been made discrete.

Different kinds of structures can be synthesized depending on whether the original streams are divided into elements sequentially, or partly in parallel resulting in stream splitting, and also on how exchangers are merged. In fact, networks that involve minimum total exchanger area can be

synthesized graphically without linear programming by recognizing that maximum thermodynamic efficiency for the total network results when the temperature driving force is minimized in individual exchangers.

In addition to problems related to choosing the size and division of the heat load elements, the principal difficulty with the optimal assignment approach is that the synthesis problem is not linear and the match costs are not independent of each other. Large merged exchangers cost less per unit area than small ones. Near-minimum area networks generated by this method are characterized by a large number of small exchangers, whereas minimum cost networks tend to have much fewer exchangers. Furthermore, some versions of the method automatically exclude the warmest portions of the streams to be heated and the coolest parts of the streams to be cooled from integration, assigning them immediately to an auxiliary heating or cooling utility which, however, might not be the optimal policy where multiple utilities of varying cost are available.

Recently, it has been suggested that process synthesis problems be solved by mixed-integer linear programming techniques. Discrete variables not only indicate the existence of specific equipment and interconnections but also make possible very good approximations of many nonlinearities inherent in real systems such as fixed plus variable operating costs. Mixed-integer linear programming codes, which generally use branch and bound algorithms to handle the discrete variables, exist which can handle quite large problems of this type. The question remains whether it is more efficient to let such a generalized algorithm blindly find appropriate values for numerous discrete variables or whether specific features of the synthesis problem and other external procedures should be utilized to set combinations of variables known in advance to be feasible and expected to be near-optimal.

EVOLUTIONARY APPROACHES

Another class of process synthesis approaches attempts to systematize the methods and aids that many successful engineers are thought to use to improve upon initial design concepts. These approaches assume the existence of a feasible design and examine it for evolutionary improvement opportunities. The initial design may be a com-

mmercial, laboratory, or literature scheme for the same or similar product or process, or it may have been obtained by the application of a series of design rules or by some other synthesis technique. Some methods use cost and functional analysis or thermodynamic analysis to detect weaknesses and suggest structural modifications, whereas others concentrate on systematic reordering of design rules, or processing tasks. Two-level Lagrangian analysis can confirm the advantage of an evolutionary change, sometimes without requiring a complete optimization of the revised design.

Evolutionary methods for structural improvement are quite appealing, possibly because they resemble much historical process development. They have been applied to almost all synthesis subproblems including heat integration, separation systems, and even entire flowsheets. These methods, like the embedded superstructure optimization approaches, are concerned with the structural optimization aspects of process synthesis. Their success depends critically, as do most gradient-type searches in highly irregular

Evolutionary methods for structural improvement are quite appealing, possibly because they resemble much historical process development.

domains, on the nature of the starting point. Given a poor initial design, they will rarely evolve to a truly novel globally optimal flowsheet.

SYSTEMATIC GENERATION APPROACHES

To find new, less prejudiced, or more creative solutions for synthesis problems, it may not be desirable to use existing designs singly as the starting point for evolutionary approaches or in combination for embedded optimization approaches. Yet efforts to invent new designs face enormous combinatorial difficulties arising from the large number of processing tasks that may be required and technologies available to perform them. Recognizing that it is generally not possible to consider all possible equipment arrangements simultaneously, a synthesis approach based on a decomposition was proposed whereby any design problem for which a solution is not known is broken into smaller subproblems. Such a de-

Continued on page 96.

CHEMICAL PROCESS DESIGN*

An Integrated Teaching Approach

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THE EFFECTIVE TEACHING OF design to chemical engineering seniors often presents a challenge for many chemical engineering faculties. Philosophically, the senior design project should integrate flow sheet generation, chemical engineering sciences, transport and reaction equipment design skills, and engineering economics. The problem should be structured to emphasize group problem solving, project organization and planning, and effective communications. Further, the problem should be an "as realistic as possible" industrial design problem requiring synthesis of a final process. One way to create an appropriate environment is by combining the design and laboratory courses, thereby relating the design project to real facts, real chemicals, real alternatives, and involving industrial practitioners.

For the past several years we have conducted our senior plant design course as a combined one semester five hour design/laboratory course. Typical design projects have included:

- polymerization of DMT to polyester [1]
- manufacture of acetic anhydride from acetic acid
- design of a yeast plant
- design of a coking wastewater treatment plant

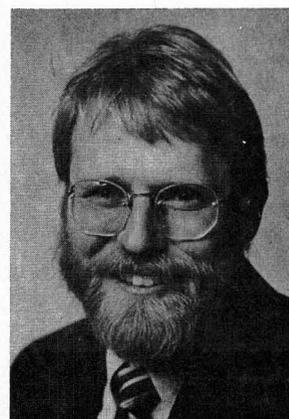
These projects have been carried out with the aid of engineers in industry.

In the early stages of the design course/laboratory development, real problems were encountered with obtaining the necessary commitment from industry. The proprietary information hurdles were almost insurmountable. Many projects involved hazardous chemicals and hazardous processes. They also quickly involved

*A preliminary version of this paper was presented at the 73rd Annual AIChE meeting, November, 1980.



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Kenneth A. Debelak is an Assistant Professor of Chemical Engineering at Vanderbilt University. He received his B.S. (1969) in Chemical Engineering from the University of Dayton and M.S. (1973) and Ph.D. (1977) from the University of Kentucky. He has had industrial experience with General Motors and governmental experience with the Environmental Protection Agency. His research interests are in coal kinetics, process control and synthesis, and physical-chemical processes for industrial waste water treatment. (R)

considerable expense both for chemicals and experimental equipment. We have found that the use of an energy or environmental design problem provides a solution to many of these difficulties.

COURSE STRUCTURE

THE STUDENTS ARE GIVEN THE design problem during the first week of class. They are assigned to individually synthesize a process to achieve the design objective. The class as a group then decides the process alternatives it wishes to consider in detail. Interaction and limited direction from the course instructors, other faculty,

and industrial consultants are essential throughout this process.

The class is organized as a company. A Project Manager and Research Director are nominated by the class and selected by the course instructors. The class is then divided into research/design groups with one member assigned as group leader. These groups develop design methods and cost curves; they also design, execute and conduct experiments to supplement the data and information in the literature. Since some students take only the three hour design course (non-chemical engineering graduate students and selected senior project students), they participate only in development of the design methods and cost information but not the laboratory.

A portion of the classroom time is devoted to a series of formal lectures on

- cost estimation and engineering economics
- related topics (i.e., corrosion, materials selection, patents, the technical library, statistics)
- supporting technical topics pertaining to the major design problem.

Additional homework assignments are made, primarily using Peters and Timmerhaus [2] as a text. One individual short design problem is assigned. Problems are also assigned covering cost estimations, economics, and statistics. One day a week is reserved for discussion of the major project and dissemination of data. Outside speakers are used extensively for the appropriate areas of expertise. The Project Manager, Research Director, and group leaders meet weekly with the course instructors to report on the week's activities and to plan for the next week. A major design report is required from each design group (3-4 persons). Weekly laboratory reports and a final report are required of the laboratory groups.

THE DESIGN PROBLEM

THE SELECTION OF AN appropriate problem is most crucial. It must be challenging but must also have good chances for successful completion. It must be common enough so that there is literature available and also require experimental work to supplement existing data. To actively involve local industries it must not include proprietary information. In the past this has been a serious problem in enlisting industrial support. Two types of problems seem to overcome many of these difficulties—those concerned with energy or environment. These are topical problems and

The choice of an environmental process design requires that the student become familiar with a new area, one which has its own terminology and language but which is based on chemical engineering principles.

have been enthusiastically supported by both industry and student involvement.

For the past two years we have focused on the design of wastewater treatment facilities for coal conversion processes. Industrial assistance from the Chemical Technology Division of Oak Ridge National Laboratory (ORNL) and Alabama By-Products Corporation (ABC) has been obtained. The group at ORNL has been responsible for the design of wastewater treatment facilities for coal gasification processes, while Alabama By-Products Company is a coking operation which has had to meet increasingly stringent discharge requirements from the EPA.

The choice of an environmental process design requires that the student become familiar with a new area, one which has its own terminology and language but which is based on chemical engineering principles. We feel that this is a common experience for graduating chemical engineers since they will be required to learn the specific terminology as they take their places in the specific industries.

DESIGN PROJECT EXAMPLE

THE FOLLOWING IS THE statement of the design of a coking wastewater treatment plant:

• • • •

VANDERBILT ENGINEERING COMPANY INTEROFFICE MEMO

TO: ChE Project Staff

FROM: Design/Laboratory Instructors

Our firm has been retained as consulting engineers to design a wastewater treatment facility for the Tennessee Coking Company, Cumberland Plant. The attachment shows the coking process and characterization of the raw waste load (influent). You are asked to complete a detailed estimate design for the wastewater treatment facility.

Data not available in the literature or uncertain will be determined in the laboratory. Effluent limitations are to be based on Tennessee standards, assuming that this plant will be constructed on the Cumberland River.

The final formal report is due_____. This report will include cost estimates as well as process design. Attach as an appendix your calculations and the source

of your data. You will be supplied the basis for cost estimation.

• • • •

The chemical engineering faculty were available as consultants. The industrial participants were also available to answer questions. The State Environmental Agency was contacted for technical information on waste treatment processes and for discharge requirements the plant would have to meet. Class lectures were presented as requested by the students on the following: biological waste treatment, liquid extraction, sludge dewatering and disposal, carbon adsorption, equilization, clarifier design. A number of textbooks, EPA documents and manuals, and training manuals were made available from the library or from individual faculty.

Biological waste treatment emerged as the cornerstone of the treatment scheme. One group was assigned to investigate this process. For ammonia removal, air stripping and steam stripping appeared as viable processes. Groups were assigned to each of these processes. The remaining laboratory groups were organized for this project as shown in Fig. 1. Each group was re-

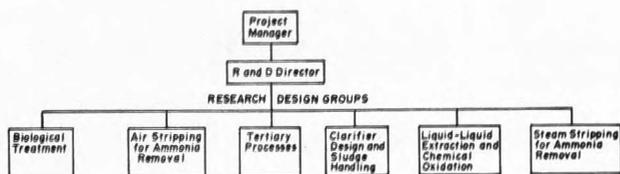


FIGURE 1. Student Organization.

sponsible for establishing the appropriate analytical tests. Members from other groups were instructed on the tests by the group that established the procedure.

Before entering the laboratory each group submitted a pre-experimental plan outlining their experiments and analytical tests. Also included in the plan was a time-table for completion of the work. These plans were reviewed by the Research Director, Project Director, and instructors. The final laboratory report presented design data and methods and a solved example of a design using design data and equations. A recommendation as to the feasibility of each process was made. Each group also presented an oral report to the entire class. The final reports along with any other information were made available to all class members.

LABORATORY

A SAMPLE OF PROCESS wastewater and sludge was obtained from ABC. Typical laboratory data needs for this project included:

- rate constants for decomposition of phenol by activated sludge
- sludge settling data for clarifier design
- neutralization curves
- chemical oxidation rates for phenol
- carbon adsorption data.

Bench scale studies were conducted on the activated sludge process in a completely mixed stirred tank reactor (CSTR). Two activated sludge reactors were operated. After flow rates were established for the influent, the process was allowed to reach steady state. Samples were collected over a period of several hours and stored at 0°C until the analyses were made. Kinetics for the removal of Chemical Oxygen Demand (COD), phenol, and cyanide were determined by varying the retention time for each run. Once the reaction rate constants were determined for each pollutant, the retention time for the limiting pollutant could be calculated and the size of the aeration basin determined. The group also determined the amount of excess sludge produced, and made recommendations for oxygen and nutrient requirements. An example of their laboratory data is shown in Fig. 2. This group established analytical procedures for COD, phenol and total cyanides in accordance with Standard Methods. Other groups were instructed in these methods.

The process wastewater obtained from ABC had already been treated to remove ammonia. It was necessary to make a synthetic waste for these experiments. The removal of ammonia by air stripping consisted of the following steps: pH adjustment, air stripping, ammonia adsorption of off gas in dilute sulfuric acid. The last step was then extended to recover the resulting ammonium sulfate, a by-product used for fertilizer. The group determined kinetic data to size the pH adjustment vessel. Mass transfer coefficients were determined for both stripping and absorbing the ammonia.

Not all of the lab groups were totally successful in completion of their assigned tasks. There are numerous reasons for the wide variation in performance among the groups. Some groups had a better understanding of their goals and objectives and better understanding of the processes they were investigating. Some groups just had people who were more motivated and enthusiastic about the project and worked more diligently to

achieve their goals. Some of the experimental problems were much more difficult, either because of inherent complexity, lack of equipment, or time constraints when supplies were not readily available.

FINAL DESIGN

THE END PRODUCT OF THE design course is the final report. We have required both individual final reports and 3-4 person group reports. This report is a formal report using the format as recommended by Peters and Timmerhaus [2]. To maintain some measure of uniformity, common economic parameters such as amortization rates, percentage of administrative costs, and other pertinent fixed-capital investment and production costs are specified. Common equipment/process cost curves are used. These are developed by the appropriate laboratory/design groups. There are nevertheless a wide number of options open to the design groups. We have also found that presentation of results by the groups to a joint faculty-industrial audience enhanced interest.

For grading, we heavily weighed peer evaluations for the group laboratory reports and the group design reports.

EVALUATION

FOR THE PAST EIGHT YEARS we have taught our senior design course as an integrated design laboratory course. The students have responded very well to this approach. They perform their work in a mature and professional manner and can see the results of their efforts. This experience forces the students to organize their efforts; make engineering judgments along the way; obtain, find and evaluate data; and organize an experimental program. We feel we have been successful in achieving an atmosphere similar to an industrial situation in which the interaction of a number of groups is necessary for the completion of a project.

We do not wish to gloss over the pitfalls of this approach, for there are several. Advanced planning is necessary. The faculty must develop some feel for the problem since there are an extensive number of student questions and problems which arise. It is important that equipment, reagents, and supplies be on hand before the beginning of the semester. During the first several weeks there is considerable chaos. Students are often unsure of what is expected of them. It is

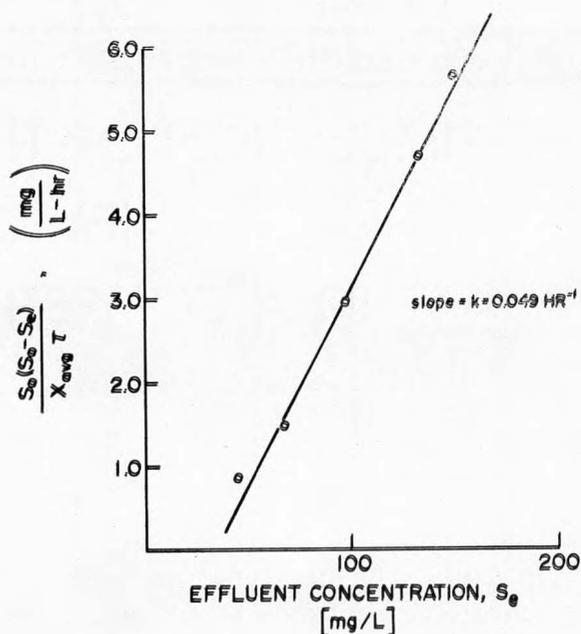


FIGURE 2. Phenol Biodegradability.

imperative that a timetable be established to keep the project moving forward. We found that a good approach to this problem was to encourage the Project Manager, Research Director, and group leaders to apply group pressure to their peers. Most students accept the challenge and are responsible. It is occasionally possible for a student to slide by with minimum effort. To counteract this, the peer evaluations are quite effective. For the most part, we find the students evaluate each other honestly.

This approach to design in the chemical engineering curriculum has been quite effective. We believe it comes close to providing a realistic experience for the student and a professional challenge for the student and the faculty. We heartily endorse this approach for a more effective design experience. □

ACKNOWLEDGMENTS

We would like to thank Jerry Klein, Oak Ridge National Laboratory; John Koon, AWARE, Inc.; and Moyer Edwards and John Shores, Alabama By-Products Corporation, for their time and assistance.

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SIMULATION OF THE MANUFACTURE OF A CHEMICAL PRODUCT IN A COMPETITIVE ENVIRONMENT

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and R. L. McCULLOUGH
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A MAJOR CHALLENGE FACING engineering educators is the infusion of notions of competition, uncertainty, and risk-taking into the deterministic methods traditionally used in the instruction of engineering students. An educational tool was described in a previous article [1] which utilized computer simulation techniques to provide an evaluation of a process design in a more realistic fashion than the usual procedure of "grading" a design report. In this article, we describe an advanced simulation which illustrates how basic engineering skills can be combined with economic considerations and risk-taking judgments in order to effectively design and operate a chemical processing unit in a competitive environment.

For this advanced simulation, data are provided to establish a design concept, capital cost, and operating cost. The completion of the design requires the specification of the production capacity (or "size") of the plant. This crucial decision is left to the participants and is based on their judgments concerning the uncertainty of market projections as well as their appraisal of the behavior of the competition. This decision is further confounded by the the availability of other options which compete for the limited funds available (\$9 million). Research and development programs are proposed which may have potentially high returns. However, the commitment of funds to these high risk projects reduces the funds available to build the processing plant and leaves open the possibility of not being competitive in an established market place. Information concerning the estimated risks involved in the research and

**The completion of the design
requires the specification of the production
capacity (or "size") of the plant. This
crucial decision is left to
the participants . . .**

development programs is provided so that rational qualitative judgments can be made concerning the disposition of limited funds. These elements of risk associated with the pay-off from the research and development projects along with possible fluctuations in the market and the uncertainty associated with the actions of competitors are intended to illustrate the difficult conditions under which many important engineering decisions are made.

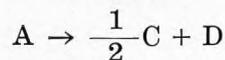
This simulation has been used as one of five projects in Technical Project Management, a course of the Chemical Engineering Department of the University of Delaware. This course is open to advanced seniors, graduate students, and practicing engineers. Their enthusiastic response to the simulation project has provided the motivation for this article.

DESCRIPTION

The participants are grouped into four competing teams with 4 to 5 members per team. Each team is provided with technical, marketing, and economic information in the form of memoranda in order to familiarize the participants with this important form of communication. The central theme of the project is the design and operation of a plant for the manufacture of a primary product "D". A by-product "C" is produced that can be a potential source of profit. Each group is allotted an initial sum of \$9 million to finance the project.

The first simple task involves the determination of the rate constant from concentration-time

data for the catalytic decomposition of raw material "A" into the product "D" and by-product "C" via the reaction:



A simple process with an isothermal continuous flow stirred tank reactor and distillation column can be used to manufacture "D" and "C". The process flow diagram is shown in Fig. 1 and described elsewhere [2]. Relationships that can be used to estimate the capital cost, operating cost, and materials cost are given in the memoranda. The information contained in these various memoranda can be easily formulated into an economic model for the process unit cost as a function of plant capacity by procedures described in engineering textbooks [3].

Estimates for the total demand and associated selling price for the primary product "D" are provided for a ten year period with the caution that these estimates may be in error by approximately 15%. The price-quantity data given are thus in the form of a standard demand curve used by the microeconomist. The marketing data for "D" provide a basis for judgments concerning the specification of plant capacity (reactor

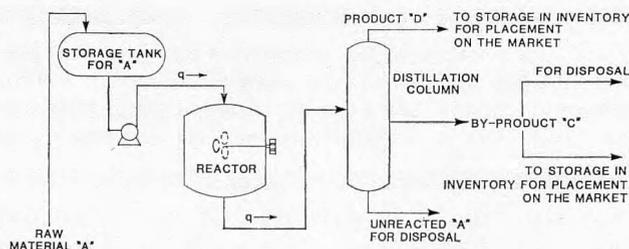


FIGURE 1. Process flow diagram

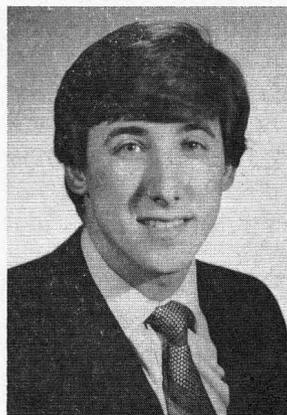
size, distillation column capacity). This crucial decision requires judgments concerning (i) the market share that can be obtained in relationship to the possible strategies and behavior of competing teams, and (ii) the uncertainty of the market projections.

The processing unit size and capital cost decision is made more difficult by the availability of options, all of which require funds which could be used for plant construction. As one option, data concerning improvements in process efficiency and the related cost are given which can be used as a basis for a "cost-benefit" analysis. These data are constructed to illustrate the option for an optimum investment in process related research. In a second option, a research and development program is proposed which could lead to the potential com-

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R. L. McCullough, Professor of Chemical Engineering and As-



sociate Director of the Center for Composite Materials at the University of Delaware, received his undergraduate chemistry training at Baylor University, and was awarded a Ph.D. in Chemistry by the University of New Mexico, while employed by the Los Alamos Scientific Laboratories. Prior to his appointment at the University of Delaware in 1971, he was associated with the Boeing Company as a Senior Research Scientist and Acting Director of Materials Science Laboratory; and the Chemstrand Research Center, Monsanto Company, as Group Leader and Acting Manager of the Fiber Science Section. Dr. McCullough has published technical papers and organized symposia in the areas of polymer structure, molecular mechanics, structure-property relations, and composite materials and is the author of several books. (R)

Upon specification of the production capacity (i.e. the anticipated share of the markets), some simple calculus can be used to obtain an optimal conversion of reactant. The distillation column is constrained by a maximum design flow rate since a flow in excess of the design limit will result in entrainment and loss of proper product specifications.

mercialization of by-product "C" and attendant new sources of income. This R&D program is a "high-risk" venture with no guarantee of success and requires an initial commitment of \$2 million for pilot plant capital and then additional support each year for a research staff. The allocation of the support funds is described in terms of "normal", "crash", and "minimal" programs. "Case studies" are given to illustrate the probabilities of success under these various levels of funding. For example, under the "crash" program it is projected that a 50% chance exists for marketing "C" in Year 2 and there is a 95% chance that "C" can be sold in Year 3. For a "normal" schedule, there is a 50% chance that "C" can be sold in Year 4 and a 95% chance that "C" will be on the market by Year 6. Other case studies are given to illustrate the effects of erratic funding patterns. Again, demand and price projections for "C" are given with the caution that these projections could be in error by approximately 20%. The diversion of funds to these alternate projects reduces the capital available to build the plant and therefore reduces the capacity for producing product "D".

The development of a strategy is further complicated by a provision which allows for an expansion of production facilities in the fifth year of the simulation. In order to accomplish this expansion, the team must have generated sufficient funds from the sale of "D" (and possibly "C") in the prior years to cover the capital cost of the expansion. A team with a large R&D effort (and a small capacity plant) could accumulate sufficient funds from the early sale of "C" for a large scale expansion in Year 5. This could allow them to dominate the future market for both "C" and "D". Alternately, a team which foregoes research could build a production facility capable of generating sufficient funds, solely from the sale of "D", to finance an expansion that could maintain their domination of the "D" market.

Upon specification of the production capacity (i.e. the anticipated share of the markets), some simple calculus can be used to obtain an optimal conversion of reactant. The distillation column is constrained by a maximum design flow rate since

a flow in excess of the design limit will result in entrainment and loss of proper product specifications. The teams may elect to "oversize" the distillation column (relative to the size dictated by the optimum conversion) to gain flexibility in developing a production strategy.

Each team submits proprietary reports for the initial design specifications, operating conditions, and research strategies (Fig. 2). The data for all teams are submitted to the simulator. Internal checks are conducted to identify trivial errors such as those resulting from unit conversions, etc. If design errors have been made, the value leading to a lower production rate is selected. Errors in operating conditions are adjusted to meet the design constraints, such as the flow limit on the distillation column. If the capital or research funds are allotted in excess of the current cash balance, the funds will be reduced to give a current cash balance of zero. Funds for plant construction are given priority over research funds.

In each period a random number generator is used to establish deviations away from the projected demand. The sampling procedures are de-

Initial Report

Company _____ Designation _____
 Names _____ (to be filled in by the
 _____ operator of the simulator)

Initial Design and Operating Strategy (year 1):

QPSR Volume _____ liters
 Design Flowrate (Q_D) _____ liters/minute
 Operating C_A/C_{AF} _____
 Total Capital Outlay _____ dollars
 (do not exceed \$9,000,000)

Amount of "D" to be stored in Inventory
 _____ Kg. moles

Optional Research Programs

Funding for Product R & D
 Capital Allocation (\$2,000,000)
 + Support Allocation _____ dollars
 Funding For Process R & D _____ dollars

FIGURE 2. Input to simulator: Initial team report

signed so that random fluctuations of $\pm 15\%$ (or less) and $\pm 20\%$ (or less) may occur from the yearly market projections for "D" and "C" respectively. The selling price is established from the actual values of the market sizes through the "demand-curve" relationships. These fluctuations can have a significant effect on the teams' cash flows. The assignment of market share is biased in favor of the teams with large capacity and large inventories. The specific relationship used to establish this bias is not made available to the participants.

Progress toward the R&D breakthrough is determined by a Monte Carlo procedure which operates by sampling at random, but with the frequency of a "research probability function". The "spread" of the research probability function is established by the funding levels and patterns as reflected by a "Case Studies Summary". Although each team can influence the "odds" for a breakthrough by modifying research strategies, the breakthrough time remains an unpredictable (stochastic) event within the limits described in the "Case Studies Summary".

The inventory of the primary product, "D", is controlled by the simulator. Any unsold "D" will be stored automatically and placed on the market (along with past inventories and current production) in the following year. No provisions are available for dumping "D" so that large inventories and high inventory cost can accumulate. Deposition of the secondary product, "C", is controlled by the team, and "C" can be dumped or retained in inventory. The product "C" can only be sold from inventory. If a new product research "breakthrough" occurs and no "C" is in inventory, no revenue will be generated from the sale of "C". The amount of "C" to be placed on the market in a given year must be specified by the team.

At the end of each period of operation performance summaries are returned to each group. An income statement is provided which gives information on revenue from sales of "D" and "C", cost of material sold, gross profit on sales, operating expenses (including plant depreciation), general expenses (including inventory charges and R&D expenditures), interest from unspent funds, and net profit. A balance sheet lists the company's current assets, plant and equipment, and liabilities and equity. In a marketing report the market fractions of "D" and "C" captured, the product selling prices, product costs, and the

amount of product produced in inventory and sold are reported. Operating conditions for the year are listed in a plant operations report and an R&D status report is given. This includes a projection of the year in which the sale of "C" will begin (at the 95% confidence level) if a program has been initiated, and the plant is operating efficiently. These reports are treated as proprietary for each company. In addition to supplying essential information, these reports provide experience in analyzing accounting statements.

Production facilities may be expanded at the beginning of Year 5 if sufficient funds have been generated from the sale of the primary product "D" and possibly the sale of "C" resulting from a research breakthrough. Design specifications for

Progress toward the R&D breakthrough is determined by a Monte Carlo procedure which operates by sampling at random, but with the frequency of a "research probability function."

any expansion (consistent with the available funds) are submitted for the beginning of Year 5. Increased production will begin in Year 5 so that increased sales can contribute to the revenues reported for the fifth year. The simulation is repeated through Year 10. The performance of each group is evaluated on the basis of the return generated from the initial \$9 million investment.

CLASS EXPERIENCE

The simulation has been performed at various stages of evolution six times in the course CHE 691, Technical Project Management, offered in the Department of Chemical Engineering at the University of Delaware. The current form has been used for three classes of CHE 691 and has been tested in three additional exercises with volunteer groups. Student time to complete the game varies from 25 to 35 hours and some 3 to 5 hours are required for class discussion and presentations. The results summarized in Tables 1 through 3 and Fig. 3 are typical results from a simulation carried out in the fall of 1978.

The plant capacities specified by each team before and after expansion are summarized in Table 1. In this particular simulation two teams (III and IV) elected to pursue the R&D programs for the commercialization of the by-product "C" while teams I and II built large production facili-

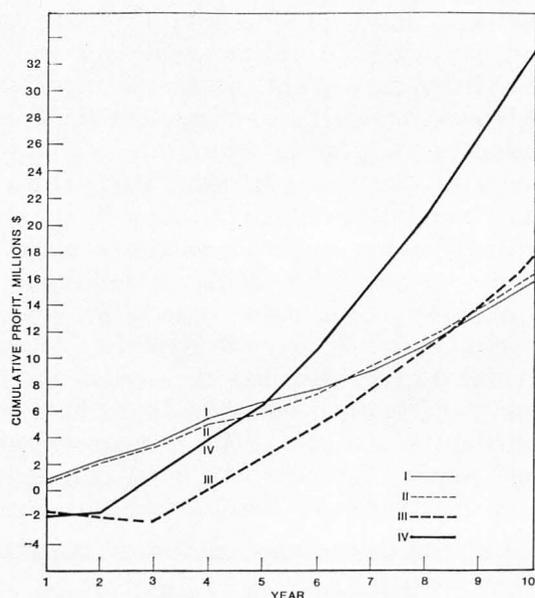


FIGURE 3. Trends in cumulative profit over the ten-year game.

ties in an effort to capture the established market for the primary product "D". The initial production capacities of the teams conducting research were about 40% smaller than the teams that declined the research program.

Team I elected to build a large capacity distillation column in order to insure flexibility of pro-

duction rates. Due to the high cost of the column relative to the reactor, they were forced to construct a smaller reactor to stay under the \$9 million limit. Team II also elected to construct an oversized distillation column. Team III constructed a more modest column which could handle a flow 20% in excess of the optimum flow rate. Team IV tightly designed the distillation column to match the optimum flow rate from the reactor.

The teams that elected not to support the R&D program designed their processing units to provide about 40% of the projected demand for product "D" in Year 3. Teams III and IV built the maximum capacity facilities possible with the funds remaining after the commitment to the R&D program.

The sensitivity of the outcome shown in Fig. 3 to competitive interactions is illustrated by the results summarized in Tables 1 through 3. Teams I and II built large production facilities by foregoing research. As a result, they captured a large percentage of the market for product "D" and acquired relatively high cumulative profits during the first three years while Teams III and IV carried out product "C" research. When Teams III and IV made product "C" research breakthroughs in Year 3, their profits began to swing upwards from the increased revenues. Team IV went on to accumulate the most profit by a great margin

TABLE 1
Summary of Facilities

INITIAL	I	II	III	IV
Reactor Size, in m ³	45.1	50.0	50.3	50.5
Reactor Cost, in \$ x 10 ⁶	1.74	1.91	1.92	1.93
Distillation Column Design Limit, in Kg-"D"/yr x 10 ⁵	6.7	5.6	4.2	3.8
Distillation Column Cost, in \$ x 10 ⁶	6.79	5.89	4.94	4.64
Initial Capital Investment (year 1), in \$ x 10 ⁶	8.53	7.80	6.86	6.57
R&D Investment (year 1), in \$ x 10 ⁶	0.00	0.00	2.00	2.00
Maximum Capacity, in Kg-"D"/yr x 10 ⁵	6.7	5.6	4.2	3.8
EXPANSION				
Reactor Size, in m ³	45.1	67.5	30.2	54.6
Reactor Cost, in \$ x 10 ⁶	1.74	2.50	1.22	2.07
Distillation Column Design Limit, in Kg-"D"/yr x 10 ⁵	6.7	6.6	2.2	6.8
Distillation Column Cost, in \$ x 10 ⁶	6.79	6.34	3.50	6.64
Total Capital Investment in Expansion (year 5), in \$ x 10 ⁶	8.53	8.84	4.72	8.71
Overall Capital Investment in Equipment, in \$ x 10 ⁶	17.06	16.64	11.58	15.28
R&D Investment (year 1), in \$ x 10 ⁶	0.00	0.00	2.00	2.00
Total Maximum Capacity, in Kg-"D"/yr x 10 ⁵	13.4	12.2	6.4	10.6

TABLE 2
Distribution of Market Share (%)

Period (Year)	"D" Team				"C" Team	
	I	II	III	IV	III	IV
1	31	30	19	20	—	—
2	35	30	14	21	—	—
3	37	30	12	21	15	85
4	35	29	16	20	53	47
5	34	30	16	20	45	55
6	28	31	17	24	37	63
7	29	30	15	26	37	63
8	31	29	15	25	37	63
9	32	28	15	25	37	63
10	32	28	15	25	37	63

by the end of the simulation. This one-sided outcome was due in part to mistakes in judgment made by the other teams.

Team III did not initiate a "crash" research program until the second year; nonetheless, they managed to achieve a "breakthrough" in the same period (Year 3) as Team IV (Table 2). Unfortunately, Team III did not anticipate such an early breakthrough and had not built up sufficient inventories of "C" by storing product made in prior periods. Consequently, Team IV captured 85% of the "C" market in Year 3 simply because they had the product available for sale. Team III responded by increasing production to generate more "C" (Table 3). At this point both Team III and IV began to view product "C" as their primary product with "D" relegated to the role of a by-product. Table 2 shows the results of this strategy.

Team III's fear of high inventory cost is reflected in their production strategies for the primary product "D". The mandatory accumulation of inventories of "D", that resulted from the small market share (19%), contributed to a deficit of \$1.6 million for Team III in period 1. In order to avoid additional inventory costs, they drastically reduced production in Year 2 (see Table 3). This caused a further decline in the market share for "D" that led to a cumulative deficit of \$1.9 million. As shown in Table 3, Team III increased production slightly in Year 3. Shored up by the breakthrough into the "C" market, Team III became more aggressive in Year 4. Unfortunately for Team III, the past production strategies left them with inadequate funds for a significant expansion in Year 5 so that Team IV gained and maintained control of the "C" market

for the remainder of the simulation.

Team I elected to allocate all the available funds to the construction of facilities for the production of the primary product "D". The decision to build an oversized distillation column to provide flexibility in operation introduced a significant penalty by reducing the funds available for the construction of the reactor. As a consequence, Team I had the largest capability for producing "D" but was penalized by having the smallest reactor (see Table 1). The small reactor led Team I to operate at a conversion of 71%—well below the optimum conversion of 85%. Team II also emphasized flexibility in operating conditions by building an oversized column which they consistently operated at an off-optimum conversion of 78%. Neither Team I nor II used the flexibility in production rates that had been so dearly purchased. Both teams tended to operate at the non-optimal maximum production rate throughout the simulation. This operating strategy led to a reduced return on the capital investments. In order to meet demands, all teams ran their facilities at the maximum production rate in the latter periods of the simulation.

Team IV operated close to the optimum conversion level consistently and stored a large

TABLE 3
Summary of Operating Strategies

Period (Year)	Conversion (%)				Production of "D" (kg/yr x 10 ⁵)			
	I	II	III	IV	I	II	III	IV
1	75	78	86	85	5.8	5.5	3.5	3.8
2	71	"	93	"	6.7	"	1.8	"
3	71	"	91	"	6.7	"	2.3	"
4	71	"	84	"	6.7	"	4.2	"
5	71	"	84	"	6.7	"	4.2	"
6	80	"	84	"	4.7	"	4.2	"
7	71	"	84	"	6.7	"	4.2	"
8	71	"	84	"	6.7	"	4.2	"
9	71	"	84	"	6.7	"	4.2	"
10	71	78	84	85	6.7	5.5	4.2	3.8

amount of by-product "C" in inventory in anticipation of a research breakthrough. This strategy gave them the highest cumulative profit at the end of the simulation. However, had Teams I and II operated their facilities closer to optimal and had Teams III and IV been in closer competition

Continued on page 87.

ON THE TENSORIAL NATURE OF FLUXES IN CONTINUOUS MEDIA

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IT IS A CURIOUS CIRCUMSTANCE that while courses in fluid mechanics or transport phenomena invest special care to establish the tensorial integrity of the stress system in a fluid, quite often the status of a vector is nonchalantly offered to the mass and energy fluxes. The usual scenario begins with the instructor identifying a point in the fluid continuum, isolating a direction which orients an infinitesimal area dA normal to it and asking for the traction vector representing the net surface force per unit area of dA . The infinite multiplicity of directions at a point leads to the customary despair about its implications to the characterization of surface forces until their redemption through the gift of a second order tensor by the joint effects of the momentum principle and the continuum postulates.

Indeed the foregoing exercise is a healthy one, for the simplicity of description of fluid stress by a second order tensor is not one to be taken for granted. The motivation for this article is the extension of the same considerations to the mass and energy fluxes in a fluid: their claims to being *vectors* is a matter to be established by argument. More generally, the primitive instruments of

The infinite multiplicity of directions at a point leads to the customary despair about its implications on the characterization of surface forces until their redemption through the gift of a second order tensor by the joint effects of the momentum principle and the continuum postulates.

transport phenomena are orientation-dependent variables, which are an extraordinary encumbrance to mathematical treatment. The central issue here is the replacement of such primitive variables by substitutes that have *no* orientation-dependence for the price of a unit increase in tensorial order. This is a considerable bargain, in the realization of which the conservation laws are intimately involved. Of course, it is not that the dependence of the said primitive variables on orientation has been entirely eliminated but rather that it has been reduced to one of homogeneous linearity. The entire procedure as applied to the traction vector has been called Cauchy's fundamental theorem.[†]

If it is admitted that the velocity v is a vector, then it would instantly follow that the mass flux ρv is a vector and no further 'proof' would be called for. On the other hand, an independent definition of point velocity in a deforming continuum does not build on a limiting procedure of a collapsing mass, a requirement basic to proper definitions of "point" quantities. The alternative is then to seek a suitable definition of something related to velocity (such as mass flux) from which the velocity may be obtained as a derived quantity. The choice falls somewhat naturally on mass flux which, as mass flow rate per unit area, could depend on the orientation of the area. This complex situation is alleviated by the fact that the mass flux turns out to be a vector. Similar considerations also hold for the energy flux. Before demonstrating these results for mass and energy fluxes, it is instructive to review the derivation of Cauchy's fundamental theorem for stress, which is related to the modeling of mechanical interactions within a material continuum.

[†]See for example, "The Elements of Continuum Mechanics," by C. Truesdell, Springer Verlag, New York, Inc., 1965.



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The authors recall the many pleasant years of their interaction during their early academic careers at the I. I. T., Kanpur, where the academic environment was extraordinary. The present article grew out of an evening's discussion many years ago. (R)

THE STRESS TENSOR

At a point $\mathbf{x} = [x_i]$ in a continuous body consider a small area dA whose orientation is determined by its unit normal $\mathbf{n} = [n_i]$. Then, the mechanical action of one part of the body on its neighborhood across dA can be represented by a force density \mathbf{t} such that $\mathbf{t} dA$ gives the force exerted on the area dA . Because of the nature of force \mathbf{t} is a vector, called the traction vector, which has the dimensions of stress-force per unit area. Besides being a function of the position \mathbf{x} and

time t , the traction vector $\mathbf{t} = \mathbf{t}(\mathbf{x}, t; \mathbf{n})$ is also a function of the orientation \mathbf{n} of the area dA . As a result, the traction vector is not suitable for purposes of analysis, even though it is the primitive variable of interest. Cauchy's fundamental theorem guarantees the existence of a second order tensor $\mathbf{T}(\mathbf{x}, t) = [T_{ij}]$, called the stress tensor, such that

$$\mathbf{t}(\mathbf{x}, t; \mathbf{n}) = \mathbf{n} \cdot \mathbf{T}(\mathbf{x}, t) \quad (1)$$

or

$$t_i(\mathbf{x}, t; \mathbf{n}) = n_j T_{ji}(\mathbf{x}, t), \text{ summation over } j$$

The proof of this result is in two steps. First we show that $\mathbf{t}(\mathbf{x}, t; -\mathbf{n}) = -\mathbf{t}(\mathbf{x}, t; \mathbf{n})$. This follows from an application of Euler's first law of motion (the rate of change in linear momentum of a body is equal to the total force applied to the body) to a thin cylindrical disk of thickness dl and cross-sectional area dA , as shown in Figure 1, which results in the equation of motion

$$\rho(dl dA) \mathbf{a} = dA[\mathbf{t}(\mathbf{x}, t; \mathbf{n}) + \mathbf{t}(\mathbf{x}, t; -\mathbf{n})] + dl \int_c \mathbf{t}(\mathbf{x}, t; \mathbf{s}) ds + \rho(dl dA) \mathbf{f}(\mathbf{x}, t)$$

where \mathbf{a} is the acceleration of the material disk, ρ is the density of the material, the line integral along the contour c gives the contribution to the force due to the stress vector $\mathbf{t}(\mathbf{x}, t; \mathbf{s})$ acting on the

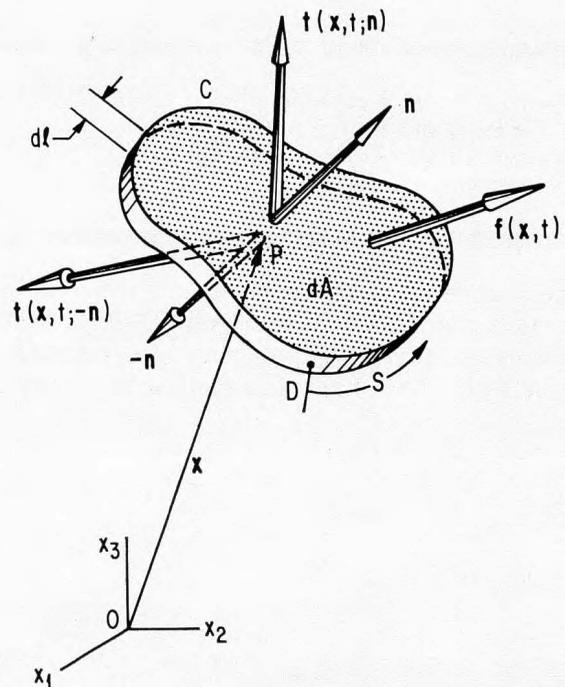


FIGURE 1. Traction vectors acting on a thin disk.

cylindrical surface of the disk, and the last term is the contribution due to the body force. Taking the limit $dl \rightarrow 0$ in Eq. (1) and dividing the resulting equation by dA yields

$$\mathbf{t}(\mathbf{x}, t; -\mathbf{n}) = -\mathbf{t}(\mathbf{x}, t; \mathbf{n}) \quad (2)$$

Next we consider the motion of the small material tetrahedron, PABC, at the point \mathbf{x} , as shown in Fig. 2, whose edges are along the orthogonal unit vectors \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 , and where face ABC has an area dA and normal $\mathbf{n} = [n_i]$. The areas of the faces with normals $-\mathbf{e}_r$ are then given by $dA_r = n_r dA$, $i = 1, 2, 3$. Let the distance of P from the face ABC be ds . Then, an application of Euler's first law of motion to the material tetrahedron results in the equation

$$\rho \left(\frac{1}{3} ds dA \right) \mathbf{a} = dA \left[\mathbf{t}(\mathbf{x}, t; \mathbf{n}) + \sum_{r=1}^3 n_r \mathbf{t}(\mathbf{x}, t; -\mathbf{e}_r) \right] \quad (3)$$

$$+ \rho \left(\frac{1}{3} ds dA \right) \mathbf{f}(\mathbf{x}, t)$$

Division of Eq. (3) by dA , followed by taking the limit as $ds \rightarrow 0$, and the use of Eq. (1) then gives

$$\mathbf{t}(\mathbf{x}, t; \mathbf{n}) = \sum_{r=1}^3 n_r \mathbf{t}(\mathbf{x}, t; \mathbf{e}_r). \quad (4)$$

This equation shows that if the traction vector \mathbf{t} is known at a point on three mutually orthogonal

The same procedure could be used for mass and energy fluxes, both of which arise from orientation dependent scalars.

planes (here \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3), then it can be determined on any plane \mathbf{n} at that point. We can reduce this result further: Let the components of $\mathbf{t}(\mathbf{x}, t; \mathbf{e}_r)$ along the axes \mathbf{e}_1 , \mathbf{e}_2 and \mathbf{e}_3 be given by

$$\mathbf{t}(\mathbf{x}, t; \mathbf{e}_r) = \sum_{s=1}^3 T_{rs} \mathbf{e}_s.$$

Then Eq. (4) becomes

$$\begin{aligned} \mathbf{t}(\mathbf{x}, t; \mathbf{n}) &= \sum_{r=1}^3 \sum_{s=1}^3 n_r T_{rs} \mathbf{e}_s \\ &= \mathbf{n} \cdot \sum_{r=1}^3 \sum_{s=1}^3 T_{rs} \mathbf{e}_r \mathbf{e}_s \end{aligned}$$

Thus

$$\mathbf{t}(\mathbf{x}, t; \mathbf{n}) = \mathbf{n} \cdot \mathbf{T}(\mathbf{x}, t), \quad (5)$$

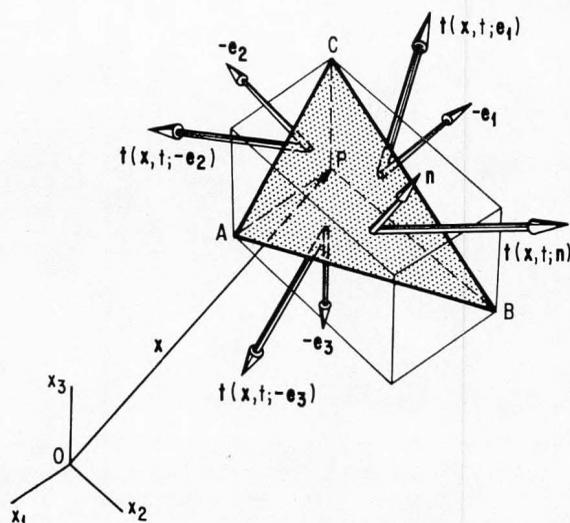


FIGURE 2. Traction vectors acting on a infinitesimal tetrahedron.

where \mathbf{T} is the dyadic

$$\mathbf{T} = \sum_{r=1}^3 \sum_{s=1}^3 T_{rs} \mathbf{e}_r \mathbf{e}_s.$$

If Cartesian tensors are used, with summation implied over a repeated index, then this equation can be written alternatively as

$$t_i(\mathbf{x}, t; \mathbf{n}) = n_r T_{ri}(\mathbf{x}, t)$$

Let us summarize what we have so far. We started with a primitive variable of interest—the traction vector which is orientation dependent. By using a physical principle, here Euler's first law of motion, we were able to establish the existence of a second order tensor—the stress dyadic $\mathbf{T}(\mathbf{x}, t)$, which is a point function and which factors out the dependence of \mathbf{t} on \mathbf{n} .

The same procedure could be used for mass and energy fluxes, both of which arise from orientation dependent scalars. Application of physical laws—here conservation of mass and the first law of thermodynamics, respectively, would result in suitable point functions that are vectors which factor out the dependence of the primitive scalars on the orientation \mathbf{n} . In each case the desired result would be obtained because, in the equation which results as a consequence of the application of the physical principle, the volume dependent terms vanish faster than the surface dependent terms in the limit when one of the dimensions of the body approaches zero—just as

in the derivation of Eqs. (2) and (5). Instead of going through this exercise individually for each case, it is useful to formalize this property in the form of a theorem that is discussed in the following section. Since the result applies to tensors of all orders, it is more descriptive to use Cartesian tensors rather than Gibbsian dyadics and polyadics. However, each result will also be presented in its Gibbsian polyadic form.

A THEOREM FOR TENSOR FIELDS

Consider a cartesian tensor *field* of order p (the case of $p = 0$ represents a scalar and that for $p = 1$ represents a vector), $\mathbf{b} = [b_{i_1 i_2 \dots i_p}]$, whose components at time t depend not only on the spatial coordinates $\mathbf{x} = [x_i]$ of the point, say P at which they are considered but also on a specified orientation $\mathbf{n} = [n_i]$ at P . The foregoing dependence on spatial coordinates and orientation is presumed to be *continuous* and we write

$$b_{i_1 i_2 \dots i_p} = b_{i_1 i_2 \dots i_p}(\mathbf{x}, t; \mathbf{n})$$

or

$$\mathbf{b} = \mathbf{b}(\mathbf{x}, t; \mathbf{n})$$

Before we state the theorem of interest, some preparations are essential. At *any point* P in the continuum we identify a volume V bounded by an area A enclosing P . The surface integral

$$\frac{1}{A} \iint_A b_{i_1 i_2 \dots i_p}(\mathbf{x}, t; \mathbf{n}) dA$$

or

$$\frac{1}{A} \iint_A \mathbf{b}(\mathbf{x}, t; \mathbf{n}) dA$$

where \mathbf{n} is everywhere *normal* to area A and pointing *outwards*, is defined for every volume enclosing P and in fact, through the mean value theorem, equals the value of the integrand somewhere on the area A . It is now possible to take the limit of this surface mean by contracting the volume to zero around P .

The theorem concerned states that there *exists* a tensor of order $p + 1$, denoted by $\mathbf{B} = [B_{j i_1 i_2 \dots i_p}(\mathbf{x}, t)]$ such that

$$b_{i_1 i_2 \dots i_p}(\mathbf{x}, t; \mathbf{n}) = n_j B_{j i_1 i_2 \dots i_p}(\mathbf{x}, t), \text{ summation on } j, \quad (6)$$

which is $\mathbf{b}(\mathbf{x}, t; \mathbf{n}) = \mathbf{n} \cdot \mathbf{B}(\mathbf{x}, t)$ in Gibbsian notation, *if and only if*

$$\lim_{V \rightarrow 0} \frac{1}{A} \iint_A b_{i_1 i_2 \dots i_p}(\mathbf{x}, t; \mathbf{n}) dA = 0$$

i.e.

$$\lim_{V \rightarrow 0} \frac{1}{A} \iint_A \mathbf{b}(\mathbf{x}, t; \mathbf{n}) dA = 0 \quad (7)$$

Note in particular that the new tensor $\mathbf{B}(\mathbf{x}, t) = [B_{j i_1 i_2 \dots i_p}]$ is not a function of the vector \mathbf{n} .

The proof of this theorem is straightforward.

Thus the conservation principles are themselves responsible for "fluxes" being vectors or tensors, a result of tremendous significance in the investigation of the mechanics of continua.

To prove the 'only if' part we assume that Eq. (6) is true. Thus we establish Eq. (7) by

$$\begin{aligned} & \lim_{V \rightarrow 0} \frac{1}{A} \iint_A b_{i_1 i_2 \dots i_p}(\mathbf{x}, t; \mathbf{n}) dA \\ &= \lim_{V \rightarrow 0} \frac{1}{A} \iiint_V \frac{\partial}{\partial x_j} [B_{j i_1 i_2 \dots i_p}] dV = 0 \end{aligned}$$

where we have used (i) the divergence theorem, (ii) the summation convention on index j and (iii) the assumption that the divergence $(\partial B_{j \dots} / \partial x_j)$ is continuous and bounded. For the converse, we start from Eq. (7). By taking V to be a right cylinder of infinitesimal cross-section dA with its normal along \mathbf{n} , as shown in Figure 1, and contracting the cylinder along its axis to a section passing through \mathbf{x} , we conclude that

$$b_{\dots}(\mathbf{x}, t; -\mathbf{n}) = -b_{\dots}(\mathbf{x}, t; \mathbf{n})$$

or

$$\mathbf{b}(\mathbf{x}, t; -\mathbf{n}) = -\mathbf{b}(\mathbf{x}, t; \mathbf{n}) \quad (8)$$

where for simplicity the indices have been replaced by dots. Next, at any point \mathbf{x} (position vector referred to some origin) and orientation \mathbf{n} , we apply the result of Eq. (7) to a sequence of tetrahedra such that each of them has a vertex at \mathbf{x} and the face opposite is *normal* to \mathbf{n} , which points *out* of the tetrahedron (see Figure 2). The other faces are formed such that the edges passing through \mathbf{x} lie along three mutually perpendicular lines chosen to be a set of cartesian coordinate directions. The normals pointing out of these faces are the unit vectors $-\mathbf{e}_1$, $-\mathbf{e}_2$ and $-\mathbf{e}_3$ re-

spectively. The application of Eq. (7) to this collapsing sequence together with Eq. (8) gives

$$b_{...}(\mathbf{x}, t; \mathbf{n}) = n_j b_{...}(\mathbf{x}, t; \mathbf{e}_j), \text{ summation over } j, \quad (9)$$

or

$$\begin{aligned} b(\mathbf{x}, t; \mathbf{n}) &= \sum_{j=1}^3 n_j b(\mathbf{x}, t; \mathbf{e}_j) \\ &= \mathbf{n} \cdot \sum_{j=1}^3 \mathbf{e}_j b(\mathbf{x}, t; \mathbf{e}_j) \end{aligned}$$

Since $b_{...}(\mathbf{x}, t; \mathbf{n})$ and n_j are tensors of orders p and 1 , respectively, it follows from the quotient law that $\sum_{j=1}^3 \mathbf{e}_j b(\mathbf{x}, t; \mathbf{e}_j)$ is a tensor of order $(p+1)$. Thus the theorem is proved with

$$B_{j...}(\mathbf{x}, t) = b_{...}(\mathbf{x}, t; \mathbf{e}_j)$$

or

$$\mathbf{B}(\mathbf{x}, t) = \sum_{j=1}^3 \mathbf{e}_j b(\mathbf{x}, t; \mathbf{e}_j)$$

MASS FLUX IS A VECTOR

At any point \mathbf{x} in the deforming continuum, given a direction \mathbf{n} it is possible to define a mass flow rate per unit area (a continuum postulate!) across an area normal to \mathbf{n} . Denoting this by $m(\mathbf{x}, t; \mathbf{n})$, we obtain the mass flow rate through dA by $m(\mathbf{x}, t; \mathbf{n})dA$. Conservation of mass for a volume V bounded by A gives

$$\frac{d}{dt} \left\{ \int_V \rho dV + \int_A m(\mathbf{x}, t; \mathbf{n}) dA \right\} = 0 \quad (10)$$

where ρ is the fluid density. If Eq. (10) is divided by A and we let $V \rightarrow 0$, the continuum postulate that $\partial\rho/\partial t$ be continuous on V and A leads to the result

$$\lim_{V \rightarrow 0} \frac{1}{A} \int_A m(\mathbf{x}, t; \mathbf{n}) dA = 0$$

which is precisely the condition given by Eq. (7) so that the theorem just discussed leads to the existence of a *mass flux vector* $\mathbf{M}(\mathbf{x}, t)$ such that

$$m(\mathbf{x}, t; \mathbf{n}) = n_j M_j(\mathbf{x}, t)$$

or

$$m(\mathbf{x}, t; \mathbf{n}) = \mathbf{n} \cdot \mathbf{M}(\mathbf{x}, t)$$

Thus the mass flow rate through area $dA \equiv \mathbf{n}dA$ is given by $dA \cdot \mathbf{M}$. The point velocity vector is now readily defined by $\mathbf{v} = (1/\rho)\mathbf{M}$. In an n -component mixture, the mass flux of the k^{th} com-

ponent of mass fraction ω_k is defined $\mathbf{M}_{(k)} = \mathbf{M}\omega_k$, from which its velocity is defined by $\mathbf{v}_{(k)} = (1/\rho_k)\mathbf{M}_{(k)}$.

STRESS IS A SECOND ORDER TENSOR

Although the stress tensor has been covered earlier, the repetition here will serve this tutorial well by reinforcing the result as a fallout from the generalized theorem above.

A momentum balance for the volume of fluid V bounded by A must account for the traffic of momentum across A because of mass flow, body forces throughout V and surface forces along the entire surface A . The traction (force per unit area) on an area dA , located at \mathbf{x} on A , with normal \mathbf{n} (directed out of V) is denoted by $[t_i(\mathbf{x}, t; \mathbf{n})]$. For the i^{th} component one has

$$\begin{aligned} \frac{d}{dt} \left\{ \int_V \rho v_i dV + \int_A v_i M_j dA_j \right\} \\ = \int_V \rho f_i dV + \int_A t_i(\mathbf{x}, t; \mathbf{n}) dA \end{aligned} \quad (11)$$

where $[f_i]$ represent components of the body force. Dividing Eq. (11) by A and letting $V \rightarrow 0$, the volume integrals are readily seen to vanish. Since we have shown that \mathbf{M} is a vector, $[M_j v_j]$ transforms as a vector for each fixed i and the theorem is applicable to the second term on the left hand side of Eq. (11). Thus we obtain

$$\lim_{V \rightarrow 0} \frac{1}{A} \int_A t_i(\mathbf{x}, t; \mathbf{n}) dA = 0$$

so that the theorem is again applicable, and yields second order tensor $[T_{ji}(\mathbf{x}, t)]$ such that

$$t_i(\mathbf{x}, t; \mathbf{n}) = n_j T_{ji}(\mathbf{x}, t)$$

or

$$\mathbf{t}(\mathbf{x}, t; \mathbf{n}) = \mathbf{n} \cdot \mathbf{T}(\mathbf{x}, t)$$

The surface force on an area $dA \equiv \mathbf{n}dA$ has for its i^{th} component $dA_j T_{ji}$.

ENERGY FLUX IS A VECTOR

By energy flux here we mean that which occurs by molecular conduction.[†] Of course energy is transported by fluid motion but since this is associated with the mass flux vector the resulting energy flux is already known to be a vector. Thus our con-

[†]Radiative transport through weakly absorbing media would require a slightly more elaborate treatment.

cern here belongs to the energy transported by conduction per unit area across an area located at \mathbf{x} and normal to \mathbf{n} , denoted by $q(\mathbf{x},t;\mathbf{n})$. The first law of thermodynamics applied to volume V bounded by A , gives

$$\begin{aligned} \frac{d}{dt} \iiint_V \left[\hat{u} + \frac{1}{2} v^2 \right] dV + \iint_A \left[\hat{h} + \frac{1}{2} v^2 \right] M_j dA_j \\ = \iint_A dA_j T_{j,i} v_i + \iiint_V \rho f_i v_i dV - \iint_A q(\mathbf{x},t;\mathbf{n}) dA \end{aligned} \quad (12)$$

The interpretations of the various terms in Eq. (12) are available in any standard textbook. In view of the pattern already set before we are able to conclude that

$$\lim_{V \rightarrow 0} \frac{1}{A} \iint_A q(\mathbf{x},t;\mathbf{n}) dA = 0$$

so that there exists an energy flux vector $[Q_j(\mathbf{x},t)]$ such that

$$q(\mathbf{x},t;\mathbf{n}) = n_j Q_j(\mathbf{x},t)$$

or

$$q(\mathbf{x},t;\mathbf{n}) = \mathbf{n} \cdot \mathbf{Q}(\mathbf{x},t)$$

Thus the conservation principles are themselves responsible for "fluxes" being vectors or tensors, a result of tremendous significance in the investigation of the mechanics of continua. It is a fact that deserves mention in courses on fluid mechanics and transport phenomena.

ACKNOWLEDGMENT

Personal discussions have borne out that the issues raised in this paper are a routine matter to many. The authors would like to specially acknowledge Professors L. E. Scriven at the University of Minnesota and Stephen Whitaker at the University of California, Davis. In particular, Professor Whitaker was kind enough to provide evidence that the contents of this paper are not common knowledge and represent useful information. □

COMPETITIVE ENVIRONMENT

Continued from page 81.

for product "C", Team II could have gained the largest profits.

Upon the completion of 10 operating periods, a year by year summary of the performance of all teams is made available to the participants. Each

team is asked to prepare a report to analyze their performance and identify the important decisions and actions that led to their relative position in the competition. Although the simple "return on investment" is suggested as a possible economic evaluator of performance, the teams are at liberty to select alternate evaluators; e.g., "internal rate of return" (the interest rate that makes the cumulative discounted cash flow equal to zero) or "borrowing power". As would be expected, those groups that make significant profits in the early periods of the simulation tend to base comparisons on the "internal rate of return". The use of these alternate measures of performance can cause reversals in the relative positions established by comparisons based on "net profit" or the simple "return on investment" criteria.

CONCLUSION

Student response to this project has been enthusiastic. The immediate consequence of their decisions provides a sense of realism for the interplay between technical, marketing, and economic factors. The computer simulator, the package of memoranda, and instruction manual are available at a total cost of \$275.00 from Engineering Educational Materials, 805 Baylor Drive, Newark, Delaware 19711. □

ACKNOWLEDGMENTS

We would like to thank all those who have helped us in the development of this educational tool. Mr. R. N. Pratt, Engineering Computation Specialist in the College of Engineering at the University of Delaware, has been most helpful in setting up and modifying the computer program for the simulation. His efforts in running the simulation are also greatly appreciated. Student feedback from experiences in playing the game was essential to proper game development and their input is gratefully acknowledged.

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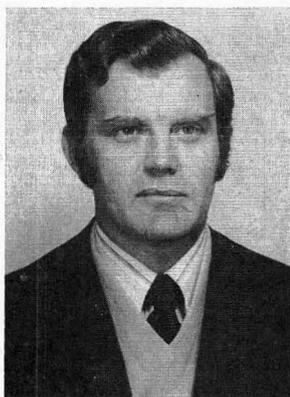
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THE INTEGRATION OF ENERGY CONSERVATION PRINCIPLES INTO A COURSE ON STAGED OPERATIONS

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MY INTERESTS IN ENERGY conservation began with a one credit special topics course which involved studying our local ice rink to suggest energy conservation measures [8]. The course was very successful and student enthusiasm was high. The motivating factors were that we were working on a real system, we had to define the problem, and that energy conservation was topical. After the course the Department of Energy awarded a contract to develop the class' results into a technology transfer manual which was recently published [1].

The Department of Energy's technology transfer series covers a wide range of topics such as energy conservation in distillation, evaporation, and the use of computers for energy conservation. Staged operations in general and distillation in particular are prime areas for energy conservation. It has been reported [9] that 3% of the



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TABLE 1
 Course Outline—Staged Operations

- I. Vapor Liquid Equilibrium Review
- II. Enthalpy Concentration Diagrams
- III. One Stage Flash Calculations
- IV. Ponchon Savarit Method
- V. McCabe-Thiele Method
- VI. Design Considerations—Flooding, Weeping, Tray Efficiency
- VII. Shortcut Techniques
- VIII. Multicomponent Column Calculations
- IX. Energy Conservation

energy used in the United States goes into distillation. When I taught our senior course on staged operations I decided to integrate energy conservation into the course. About 25% to 30% of the course involved energy conservation. Again student interest and enthusiasm were very high.

There are two other benefits to including the energy conservation material. First, evaluating energy conservation measures forces one to focus on economics. Thus, the staged operations course reinforced the students' experience in their process design and evaluation courses. Secondly, energy conservation generally involves good, sound engineering. Invariably it only takes an undergraduate training to appreciate the conservation techniques. What students learn is that energy conservation measures already exist and the question of their use depends primarily on economics.

The purpose of this paper is to discuss how energy conservation can be integrated into a course on staged operations. Table 1 gives an outline of the material covered in the course. Topics I to V were taught in the usual way without consideration of energy conservation. Some energy conservation material was introduced in covering topics VI and VII. For the somewhat dry subject matter such as flooding, tray

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efficiencies, etc., the energy conservation implications of these topics helped greatly to motivate students. During the three week period when the students worked on a multicomponent computer project, lectures on energy conservation were given.

SOURCES OF ENERGY CONSERVATION MATERIAL

Essentially all of the energy conservation material that is required can be gotten from the literature. The two primary sources that were used are the Department of Energy (DOE) Technology Transfer Manual [10] and Shinskey's text on distillation control [11]. The DOE manual lists over 50 journal references. The Mix [9] article cited earlier is also useful and it presents a number of rules of thumb.

In the DOE manual and Mix article energy information is given on the 29 most important towers in the petroleum industry as well as for the 131 key towers in the chemical industry. This information includes the energy required/lb product, the number of trays, reboiler temperature and condenser temperature. The DOE manual divides energy conservation measures up into three broad categories: as shown in Table II.

TABLE II

Energy Conservation Measures In Distillation

- A. CHANGES IN OPERATING PROCEDURE
 1. Lower reflux operation
 2. Lower pressure operation
 3. Changing feed plate location
 4. Proper maintenance
 5. Reducing heat exchanger fouling
- B. MODERATE INVESTMENT MEASURES (up to \$50,000)
 1. Insulation particularly for valves and flanges
 2. Waste heat recovery
 3. Retraying for higher efficiency/lower pressure drop
- C. MAJOR INVESTMENT MEASURES (over \$50,000)
 1. Advanced instrumentation and control
 2. Heat pumping
 3. Intermediate condensers and reboilers
 4. Two stage condensation
 5. Multiple tower operation

At this point it is useful to discuss three typical examples that were used in the course. Other

examples are given in the DOE manual and homework problems can be developed from them.

Example 1: Lower pressure operation.

Fig. 1, taken from Shinskey's text [11], shows a typical operating window for a butane splitter with the various column constraints labeled. It is necessary for a column to operate within these constraints, or window as they are sometimes called. The dashed curves, labeled contours of constant separation, are for a fixed feed (F) and a fixed product split (x_D, x_B). It is possible to use Fig. 1 to show that minimum energy consumption corresponds to minimum pressure operation. Since coolant temperature sets column pressure, when favorable cooling conditions arise one should take advantage of them and minimize column pressure. This minimum pressure can be determined from the intersection of the condenser constraint and the appropriate contour of constant separation.

The calculation of the constraints and the contours of constant separation is straightforward and an excellent homework assignment. For

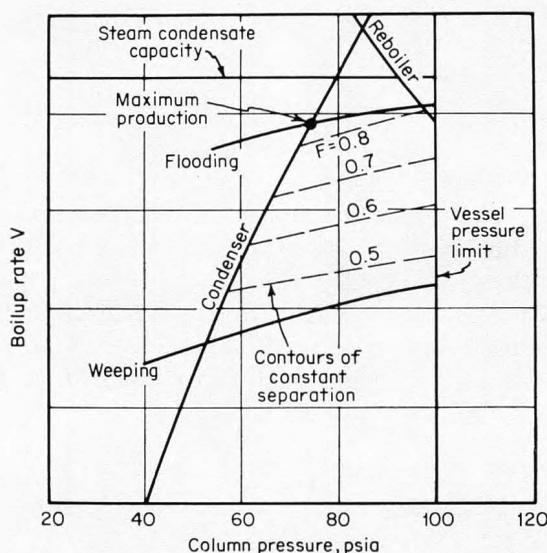


FIGURE 1. Typical operating windows for a butane splitter, illustrating that production may be maximized at the condenser constraint. (From "Distillation Control," by F. G. Shinskey, © 1977. Used with permission of McGraw-Hill Book Company.)

example, the flooding curve is a simple rearrangement of the standard flooding correlation given by Van Winkle [14]

$$V = A \left(\frac{\sigma}{20} \right)^{0.2} \sqrt{\rho_V (\rho_L - \rho_V)} f \left(\frac{L}{V} \sqrt{\frac{\rho_V}{\rho_L}} \right) \quad (1)$$

Similarly the weeping constraint can be calculated from standard correlations. The reboiler and condenser constraints are heat transfer constraints. For the condenser assume a constant coolant temperature, T_c , constant heat transfer coefficient, U , and fixed area, A . Changes in column pressure will change the temperature of the overhead product. For nearly pure products this temperature pressure relationship is given by the Clausius Clapeyron equation

$$P = P_o \exp \left[\frac{\Delta H}{R} \left(\frac{1}{T_o} - \frac{1}{T} \right) \right] \quad (2)$$

As P increases the temperature at the top of the tower increases and the amount of heat that can

As can be seen, lower pressure operation gives substantial energy savings. Such savings can occur at night, during the winter and during a rain storm for air cooled condensers.

be transferred increases. If this heat is assumed to be only latent heat then V and P can be related along the condenser constraint as

$$V = \frac{UA}{\lambda} \left[\frac{1}{\frac{1}{T_o} - \frac{R}{\Delta H} \ln \frac{P}{P_o}} - T_c \right] \ln \text{mean} \quad (3)$$

The reboiler constraint can be similarly calculated. The steam condensate capacity constraint and the vessel pressure constraint are self explanatory.

The contours of constant separation can be calculated using any of several shortcut techniques. The equation of Jafarey et al. [5] will be used.

$$N = \frac{\ln \left(\frac{x_D}{1-x_D} \cdot \frac{1-x_W}{x_W} \right)}{\ln \left[\frac{\alpha}{\left(1 + \frac{1}{R x_F} \right)^{1/2}} \right]} \quad (4)$$

For a fixed column separating a fixed feed into fixed products, Eq. (4) shows that the relative

volatility, α , and the reflux ratio, R , are related as

$$\frac{\alpha}{\sqrt{1 + \frac{1}{R x_F}}} = \text{Constant} \quad (5)$$

The reflux ratio and the vapor boilup are related as

$$V = (R + 1) F \left[\frac{x_F - x_B}{x_D - x_B} \right] \quad (6)$$

Assuming that the reboiler and condenser heat loads are equal and that only latent heat effects are important, the energy to run the tower is given as

$$Q = \lambda V \quad (7)$$

As tower pressure is lowered due to the availability of lower cooling conditions, several effects occur. Tray efficiency decreases and α and λ increase. Table III shows the results of using Eqs. (5)-(7) on Shinsky's butane splitter. The constant in Eq. (5) was calculated from Shinsky's values for a 120°F condensate temperature. The effects of tray efficiency are not included in Table III. As can be seen, lower pressure operation gives substantial energy savings. Such savings can occur at night, during the winter and during a rain storm for air cooled condensers. All of these cases result in a lower T_c in Eq. (3) and the condenser constraint is shifted to the left.

One of the interesting aspects of the calculations given in Table III is that relatively small increases in α are translated into relatively large decreases in energy consumption. Kister and Doig [6] [7] have published papers on the effect of pressure on column performance and these papers are useful supplements to Shinsky's text.

TABLE III
Energy Required to Separate Butanes
at Constant Feed Conditions

($x_F = 0.5$; 97-3 Split)

Cond. Temp °F	Tower P (psia)	α	λ (BTU/lb)	V/F	Q/F	Air Temp °F
120	95.2	1.32	129	5.00	645	76
100	71.9	1.35	135	4.09	552	61
80	53.1	1.38	140	3.48	487	45
60	38.1	1.41	145	3.03	439	28

Another important aspect of Fig. 1 is that it can be used to discuss the concept of maximizing throughput. For the butane splitter maximum throughput occurs at the intersection of the condenser and flooding constraints. For other systems maximum throughput can occur at the intersection of the reboiler and flooding constraints [11], [6], [7]. The slope of the flooding curve relative to the slope of the contours of constant separation determines the maximum throughput point. In going through either the minimum pressure analysis or maximum throughput analysis students see the importance of such mundane considerations as flooding.

Example 2: Retraying for higher efficiency.

In the DOE manual retrofitting old towers with more efficient trays is discussed. The example chosen for illustration is a naphtha debutanizer shown in Fig. 2. In calculating energy conservation results, the Eduljee [2] fit of Gilliland's [4] correlation is used

$$\frac{N - N_{\min}}{N + 1} = 0.75 \left[1 - \left(\frac{R - R_{\min}}{R + 1} \right)^{0.5668} \right] \quad (8)$$

The Underwood equation [12] [13] can be used to calculate R_m and N_m can be calculated from Fenske's equation [3]. By increasing tray efficiency, the number of theoretical plates N is increased and the reflux ratio R can be decreased.

To estimate energy savings assume that ΔN is the increase in N and that this produces a ΔL reduction in reflux. From Eq. (8) and the column material balance ΔL can be calculated. The resulting energy savings are approximately

$$\Delta Q = \Delta L \lambda \quad (9)$$

The results presented in the DOE manual are given in Table IV. The cost of new trays was estimated to be \$11,300 and the installation

TABLE IV
Retrofitting Trays for Naphtha Debutanizer

	Case 1	Case 2	Case 3
Increase Theoretical Trays by	2%	5%	10%
R (Gilliland)	2.12	2.04	1.94
Energy Savings, (10 ⁶ BTU/hr)	0.12	0.32	0.59
Annual Savings @ \$2.50/10 ⁶ BTU	\$2376	\$6369	\$11,682
Payout time (yrs) for \$16,950	7.1	2.7	1.5
Payout time (yrs) for \$22,600	9.5	3.5	1.9

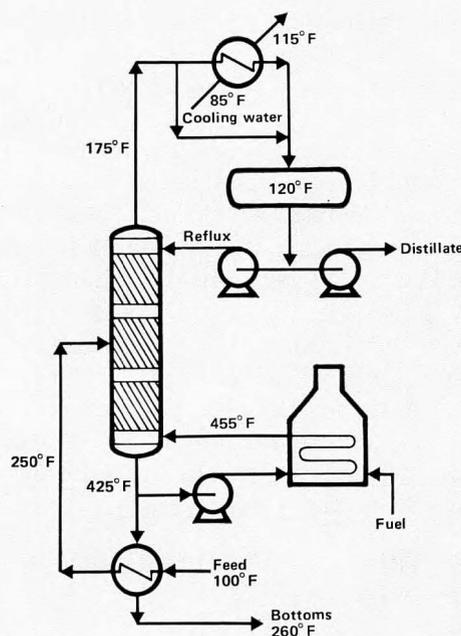


FIGURE 2. Naphtha Debutanizer [Taken from DOE Manual (1980)].

charges were estimated to be between 50% and 100% of tray costs.

The DOE manual estimates that a 3% increase in N is necessary to achieve a maximum reasonable payout time of 5 years. However, this estimate is based upon relatively cheap energy (\$2.50/10⁶ BTU) and therefore it should drop with increasing energy costs.

Example 3: Heat pumped towers.

In the DOE manual a propane/propylene splitter was chosen to illustrate heat pump economics. This system involves reboiler flashing, shown in Fig. 3. With reboiler flashing the bottoms product is used as the working fluid in the refrigeration loop. The economics for heat pumping the propane/propylene splitter are given in Table V. As can be seen, substantial energy and dollar savings can be realized by going to a heat pump design in this case.

The DOE manual gives calculation procedures for determining energy and dollar savings for all the examples discussed. Using these procedures the results in Table V can be calculated. In addition the manual gives detailed guidelines for application of each of the energy conservation measures. The most important guideline for heat pumping is that the ΔT between the condenser and reboiler should be less than 65°F. An interesting

homework problem can be given to illustrate this guideline. Suppose that two engineers decide to spend the same amount of money to reboil a tower. One buys low pressure steam at \$2.50/10⁶ BTU and uses this steam directly in the reboiler. The other buys high pressure steam at \$3.50/10⁶ BTU, and uses this steam to run a compressor in a heat pump arrangement. If the condenser temperature is 120°F at what ΔT between the reboiler and condenser will the heat pumped tower begin to be competitive with an ordinary tower? Assume reasonable efficiencies and neglect the added equipment costs for the heat pumped system. For 80% efficient compressor and a 33% efficiency for generating work from steam the answer can be calculated from the Carnot cycle equation as

$$\Delta T = (\$2.5/\$3.5) (0.33) (0.8) (580^\circ\text{R}) \quad (10)$$

$$= 109^\circ\text{F}$$

The difference between 109°F and the DOE recommendation of 65°F results from the added capital and maintenance costs for the heat pumped system.

SUMMARY

The three examples which have been presented are typical of those which can be incorporated into a standard staged operations course. More than enough material is available from literature sources to easily cover the subject of energy conservation. Because of the topical nature of the material student interest and motivation are high. Energy conservation involves good, sound engineering and it forces students to consider the economic aspects of their designs. Lastly, students

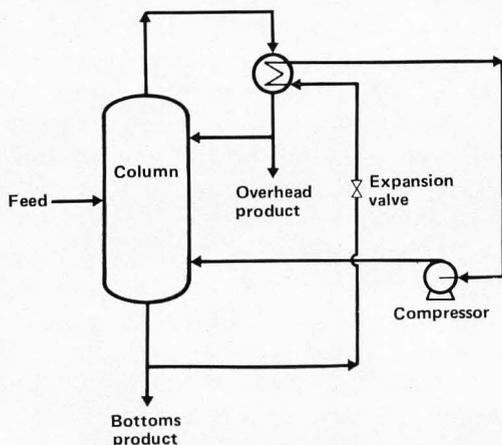


FIGURE 3. Reboiler Flashing [Taken from DOE Manual (1980)].

TABLE V
Economics for the Application of a Heat Pump
to a Propane/Propylene Splitter*

Operating and economic factors	Conventional tower design	Reboiler flashing as a retrofit	Reboiler flashing on a new column
Column pressure, psia	275	275	275
Overhead temperature, °F	115	115	115
Bottoms temperature, °F	135	135	135
Steam consumption, 10 ⁶ BTU/hr	101†	12‡	12‡
Cooling water, 10 ⁶ BTU/hr	101	6	6
Utility costs, 10 ⁶ \$/yr	3.06	1.10	1.10
Increased maintenance, 10 ⁶ \$/yr		0.28	0.28
Savings, 10 ⁶ \$/yr		1.68	1.68
Additional capital cost, 10 ⁶ \$/yr		3.44	2.04
Simple payout, yrs		2.1	1.2
After-tax ROI, %		24.4	41.2

*All costs are in 1978 dollars.

†Low-pressure steam (valued at \$2.50/10⁶ lb).

‡High-pressure steam (valued at \$3.50/10⁶ lb).

begin to learn about column operation. For all these reasons it is felt that energy conservation is a useful addition to any course, but in particular to one on staged operations. □

Nomenclature

A = Area	P = Pressure
C _p = Heat capacity	Q = Heat duty
f = Function	R = Reflux ratio
F = Feed flow	T = Temperature
H = Enthalpy	U = Heat transfer coefficient
L = Reflux flow	V = Vapor flow
N = Theoretical number of trays	x = Mole fraction

Greek Letters

α = Relative volatility	λ = Latent heat of vaporization
Δ = Difference	σ = Surface tension
ρ = Density	

Subscripts

C = Coolant	min = Minimum
D = Distillate	o = Base case
F = Feed	V = Vapor
L = Liquid	W = Bottoms

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ChE book reviews

TRANSPORT PHENOMENA IN LIQUID EXTRACTION

By G. S. Laddha and T. E. Degaleesan
McGraw-Hill, 1978, 485 pages

Reviewed by N. L. Ricker
University of Washington

From the title, one might expect this book to be confined to the study of theoretical and experimental developments in the field of transport phenomena. While this is the authors' main emphasis, they also give an overview of other important facets of the practice of liquid extraction. The general orientation is very similar to the well known book by Treybal (1963)*, and it seems appropriate to use Treybal's work as a frame of reference for this review.

**Liquid Extraction*, by R. E. Treybal, McGraw-Hill, 1963.

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Laddha and Degaleesan begin with a brief discussion of common industrial applications of liquid extraction, followed by chapters devoted to the fundamentals: phase-equilibrium thermodynamics, theories of diffusion and interphase mass transport, and calculational methods for stagewise extraction and countercurrent differential extraction. The material follows a logical sequence, and practicing engineers will be comfortable with the format, which emphasizes conventional graphical methods, overall NTU's and HTU's, etc. Treybal, however, covers much of the same material in more depth. Also, Laddha and Degaleesan fail to cite the more recent theories for the prediction of liquid-liquid equilibria, and they do not discuss the use of modern calculational methods for extractor design and simulation. There is an incorrect statement, repeated in several places, that the distribution coefficient is given by *slope* of the distribution curve, which is not true in general.

The next two chapters deal with the behavior of single drops and multiple interacting drops dispersed in a continuous phase, with an emphasis on the fluid dynamics and mass transfer characteristics of such systems. There is also a qualitative discussion of the important Marangoni effects. The material is presented in a unified form, whereas in Treybal it is much more scattered.

The next major section of the book begins with a description of the different types of extraction devices used in practice and gives a brief summary of the factors that might influence the selection of a device for a specific application. Following this, six common types of contactors: spray, packed, perforated-plate, rotary-agitated, and pulse-agitated columns, and mixer-settler extractors, are treated in individual chapters. Each chapter contains performance correlations and design criteria that can be used for the given contactor. These chapters comprise about one half of the book, and are perhaps its best feature.

The final chapter reviews the special problems that arise when extraction is accompanied by

Continued on page 96.

ChE class and home problems

The object of this column is to enhance our readers' collection of interesting and novel problems in Chemical Engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class or in a new light or that can be assigned as a novel home problem are requested as well as those that are more traditional in nature that elucidate difficult concepts. Please submit them to Professor H. Scot Fogler, ChE Department, University of Michigan, Ann Arbor, MI 48109.

ICE RINK PROBLEM

THOMAS J. McAVOY
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PROBLEM STATEMENT

In newer ice rinks a direct expansion refrigeration system is used to keep the ice frozen. A schematic of such a system is shown in Fig. 1.

In effect the ice and the pipe under it serve as the evaporator in the refrigeration loop.

Several different mechanisms contribute to the heat, Q , which has to be removed from the ice. First, the air in the building tends to heat up the ice and second, water vapor in the air tends to condense on the ice surface. Suppose that you are a rink owner and a salesman shows up claiming that a third mechanism is important as well. He claims that radiational heat transfer from the ceiling to the ice accounts for a significant fraction of Q . To solve the problem he will sell you a non-radiating ceiling which has an aluminized face. The non-radiating ceiling will be hung from the present ceiling if you decide to buy it. The installed cost of the ceiling is \$30,000. Using the data below estimate if the investment is worthwhile. Give any assumption that you make

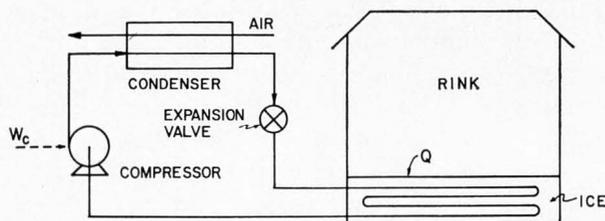


FIGURE 1.

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in calculating your answer.

DATA

Condenser temperature	90°F
Evaporator temperature	16°F
Ice temperature at surface	27°F
Ceiling temperature	65°F
W_c	55,000 kwh/month
Ceiling height	40 ft.
Ice length	200 ft.
Ice width	85 ft.

The ceiling area can be taken equal to the ice area. Use \$.05/kwh as a cost for electricity. The rink operates for 8 months during the year.

SOLUTION

Assume that the ceiling and ice are black bodies and that the side walls are adiabatic. Eq. (14.4-15) from Bird, Stewart, and Lightfoot [1] gives the radiant heat transfer from the ceiling to the ice as

$$Q_R = \sigma A \bar{F} (T_c^4 - T_i^4) \quad (1)$$

where

$$\begin{aligned} \sigma &= 0.1712 \times 10^{-8} \text{ BTU/hr ft}^2 \text{R}^4 \\ A &= 85 \text{ ft} \times 200 \text{ ft} = 17000 \text{ ft}^2 \\ T_c &= 525^\circ \text{R} \\ T_i &= 487^\circ \text{R} \end{aligned}$$

Since the length to width ratio of the ceiling is approximately 2.0, a value of \bar{F} can be estimated from curve 7 given in Figure 14.4-4 of Bird, Stewart and Lightfoot. The estimated \bar{F} is

$$\bar{F} = 0.75$$

The hourly rate of heat transfer can be calculated

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from Eqn. (1) as

$$Q_R = (0.1712 \times 10^{-8}) (17000) (0.75) \\ (525^4 - 487^4) = 4.31 \times 10^5 \frac{\text{BTU}}{\text{hr}}$$

If it is assumed that the new ceiling completely eliminates radiation to the ice then over an 8 month period the reduction in heat input to the ice can be calculated as

$$Q_R = (4.31 \times 10^5) (365 \times \frac{8}{12}) \quad (24) \\ = 2.53 \times 10^9 \text{ BTU}$$

Next the Carnot cycle equation can be used for the refrigeration system to calculate the work that is saved. This work is

$$W = Q_R \frac{T_{\text{cond}} - T_{\text{evap}}}{T_{\text{evap}}} \frac{1}{\eta} \quad (2)$$

where

$$\eta = \text{comp. efficiency (assume 0.80)} \\ T_{\text{cond}} = \text{cond. temp. (550}^\circ\text{R)} \\ T_{\text{evap}} = \text{evap. temp. (476}^\circ\text{R)}$$

Substituting for Q_R , T_{cond} , and T_{evap} , gives the work savings for the 8 month operating period as

$$W = (2.53 \times 10^9 \text{ BTU}) \left(\frac{550 - 476}{476} \right) \\ \left(\frac{1}{0.8} \right) (2.931 \times 10^{-4} \left(\frac{\text{kwh}}{\text{BTU}} \right)) \\ = 1.43 \times 10^5 \text{ kw hr}$$

The dollar savings can be calculated as

$$\text{\$ Savings} = 1.43 \times 10^5 \text{ kw hr} \times \frac{\text{\$.05}}{\text{kw hr}} = \text{\$7150}$$

The estimated payout time for the non-radiating ceiling is 4.2 years which is reasonable. Given the fact that energy costs are bound to rise, the ceiling is probably a good investment. \square

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ChE book reviews

WHAT EVERY ENGINEER SHOULD KNOW ABOUT ECONOMIC DECISION ANALYSIS

By Dean S. Shupe

Marcel Dekker, Inc., 1980. 136 pages

Reviewed by William G. Sullivan
University of Tennessee

This short book provides a concise treatment of many principles of engineering economic evaluation. It is full of good example problems to illustrate these principles, and it can be read and easily understood by the practicing engineer in a few hours.

Several topics are covered that one might not expect to encounter in a book of this length. For example, several examples deal with inflation and there are numerous solved problems related to solar energy applications. The subject of debt versus equity financing and how to handle it is also included in a separate chapter. Furthermore, several relatively advanced federal income tax provisions are illustrated very clearly in another chapter.

The book is ideal for review of engineering economy topics that appear on professional engineering examinations. In addition, it could serve well as a textbook for a shortcourse (1 or 2 days) on this subject. Because of its brevity in conceptual development regarding why various evaluation methods work the way they do, the book is not suitable as a text for a college-level course. No homework problems are included at the end of any of the eight chapters.

In Summary, *What Every Engineer Should Know About Economic Decision Analysis* should help engineers with no formal training in engineering economics to more fully appreciate the "how to," but not the "whys," of conducting studies of engineering alternatives. The book could make a valuable addition to the practitioner's bookshelf. \square

CHEMICAL PROCESS SYNTHESIS

Continued from page 71.

composition of the total flowsheet generation problem leads to the identification of many of the synthesis subproblems mentioned before such as heat integration, separations sequencing, etc. in which much progress has been made. The decomposition principle might also be applied recursively to the solution of each of these subproblems. A special case arises if the decomposition is done in such a manner that at least one of the resulting subproblems is recognized immediately as solvable by some available technology. If this process is repeatedly and successfully applied until no unsolved subproblem remains, the result is equivalent to the systematic specification of a finite sequence of technologies which together form a feasible design for the original processing problem.

The heat integration synthesis problem described previously is amenable to such a decomposition strategy. At each stage, a stream to be heated and another to be cooled (either two process streams or a process stream and a utility) for which required tasks remain are selected and, if thermodynamic or other constraints are met, simultaneously solved with immediately recognizable technology (an exchanger, furnace, etc.). Should this heat exchange match fail to perform the required task completely for a process stream (reach the desired final temperature or phase state), the remaining task, or 'residual', is simply included among the other as yet unsolved process heat transfer tasks for consideration in successive stages. With appropriate available utilities, this systematic generation scheme will produce a feasible design in a finite number of steps. Different designs result from alternative streams or possible portions of streams selected for each match and from how strictly the various task specifications and other constraints are met. The number of such designs for heat integration among M streams is on the order of $((M/2)!)^2$.

Specification of separation sequences for multicomponent mixtures is another synthesis subproblem for which systematic generation approaches have been proposed. The problem arises in reactor feed preparation, product purification, by-product recovery, waste treatment and other situations where the tasks of increasing concentration or component isolation are specified. In a simplified form, a mixture is to be separated into each of its components using a sequence of

technologies which sharply split a single multicomponent feed stream into two outlet streams, one containing some subset of the feed components and the other containing the remaining components. Differences in various physical properties of the components such as volatility or solubility are exploited by various technologies to effect the desired separations. If S different separation technologies are available (such as simple, azeotropic and extractive distillation, extraction, fractional crystallization, etc.), the number of different design sequences for the complete separation of an N -component mixture is on the order of $S^{N-1} (2N-2)! / (N!(N-1)!)$. □

EDITOR'S NOTES The concluding section of Dr. Siirola's lecture will be published in the next issue of CEE (Summer, 1982).

REVIEW: TRANSPORT PHENOMENA

Continued from page 93.

chemical reaction. This subject is only given a very brief treatment by Treybal. The theoretical discussion in the present work draws heavily from results obtained in studies of chemical absorption. Although there are a few data for liquid-liquid systems, there should be more. The presentation generally falls short of the state-of-the-art in this area.

Topics covered by Treybal but not discussed in the present work include calculational methods for multicomponent extraction, methods for laboratory and small-scale extractions, economics of extraction processes, and the competing factors involved in the selection of a solvent. In general, Treybal's book has the same theoretical basis, but a more practical, process-oriented flavor than the present work.

The subject material is probably too specialized for the book to find much use in the undergraduate chemical engineering curriculum. It seems better suited as a reference for students and industrial practitioners with a special interest in liquid extraction. It would have been more valuable in this regard had the authors included more references to the recent literature. Only 2% are from the period 1971-1978, with the most recent of these being from 1974.

A final minor criticism: the printing quality in the review copy was noticeably inferior to that found in most technical books printed in the U.S. The type was uneven and generally too light, and pages were often slanted from the verticle. □

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Hendrick C. Van Ness and **Michael M. Abbott**,
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Solutions Manual

This unique text—the *only textbook devoted entirely to the subject*—includes numerous worked examples and problems for solution. The book gives a systematic and comprehensive exposition of classical thermodynamics of nonelectrolyte solutions, including applications to the formulation and solution of problems in fluid-phase equilibria. In a thorough discussion of fluid properties and their interrelations, the authors include state-of-the-art methods for representing the properties of pure fluids and mixtures.

SYNTHETIC FUELS

Ronald F. Probstein, Massachusetts Institute of Technology, and Water Purification Associates; and **R. Edwin Hicks**, Water Purification Associates
1982, 496 pages
Solutions Manual

The first complete textbook covering a new and important field, presented here as a unified engineering subject. The text includes relevant chemical and physical fundamentals and develops the basic principles of each technology.

ENGINEERING EVALUATION OF ENERGY SYSTEMS

Arthur P. Fraas
1982, 720 pages (tent.)

A comprehensive study of all major energy systems, including—for each system—historical background, underlying theory, and a critical review of actual test experience that defines the practical limitations of the system. Early chapters are devoted to the *characteristics of basic components and problem areas* common to most types of energy systems. Includes summaries for all chapters and for most sections, and over 300 figures and tables.

PRINCIPLES OF POLYMER SYSTEMS, 2/e

Ferdinand Rodriguez, Cornell University
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Solutions Manual

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MOMENTUM, HEAT AND MASS TRANSFER, 3/e

Carroll O. Bennett, University of Connecticut; and **J.E. Myers**, University of California, Santa Barbara
1982, 848 pages (tent.)
Solutions Manual

This text is designed for chemical engineering students in the transport staged operations sequence. Changes for the third edition include: a general updating throughout; 50% SI units; chapter summaries; and additional problems.

MEASUREMENT AND DETECTION OF RADIATION

Nicholas Tsoulfanidis,
University of Missouri—Rolla
1982, 656 pages (tent.)

Covers all aspects of radiation measurement, using worked examples and problems to support concepts. The text includes the most current radiation detectors and techniques, teaching students to select the proper detector given the energy and type of particle to be counted and the purpose of the measurement.