



CHEMICAL ENGINEERING DIVISION OF AMERICAN SOCIETY FOR ENGINEERING EDUCATION

GRADUATE EDUCATION ISSUE

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- COAL SCIENCE AND TECHNOLOGY . . **WHEELOCK**

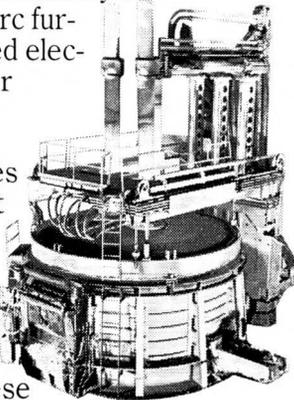
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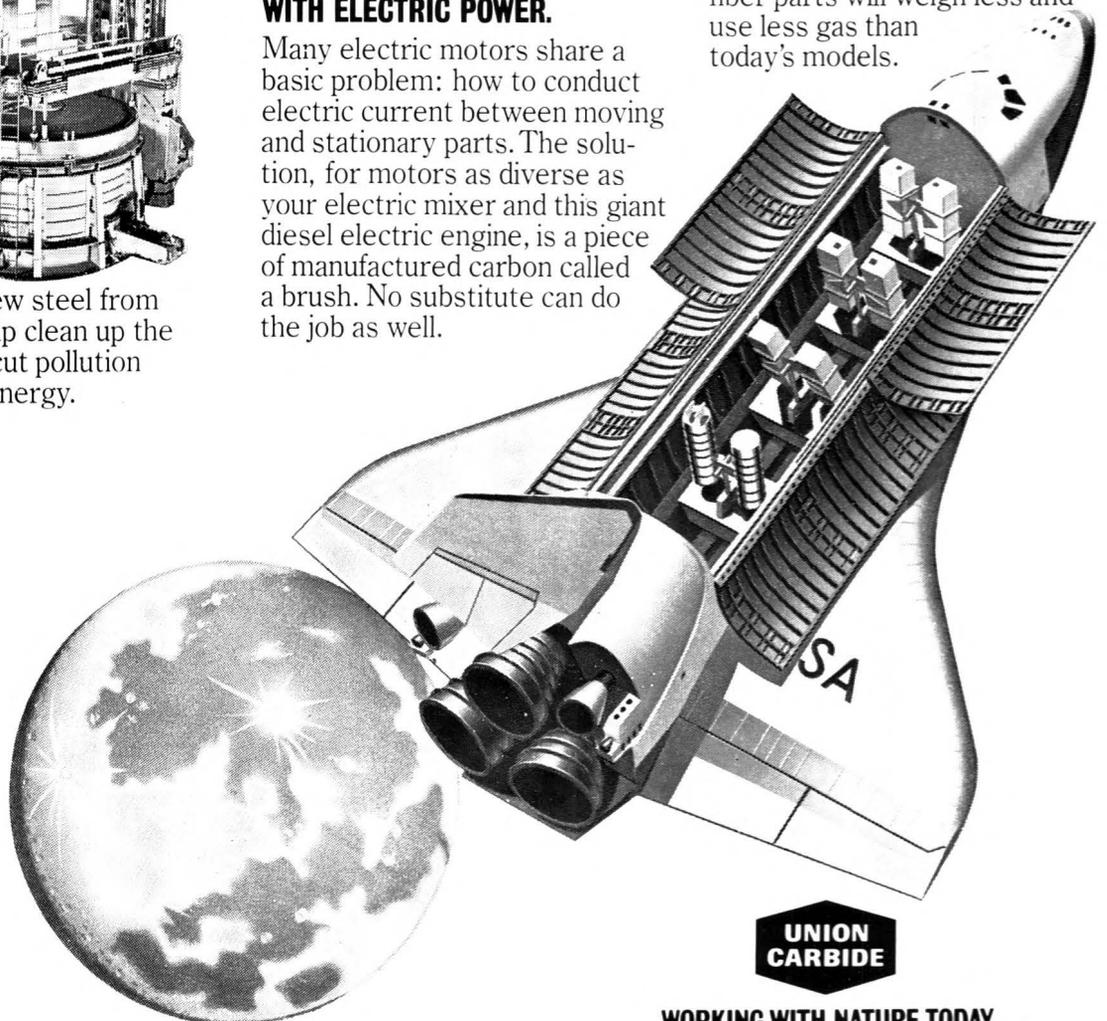


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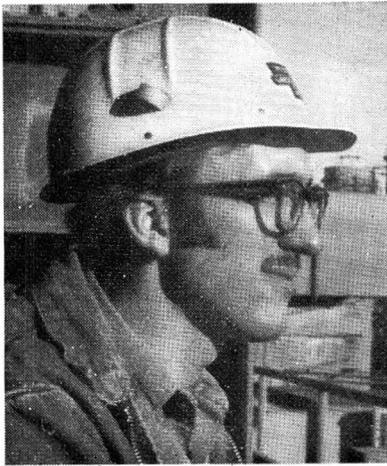
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Loren Schillinger

B.S.Ch.E. from Montana State University in 1975 . . . joined FMC's Industrial Chemical Group plant at Pocatello as a process engineer in the technical department . . . involved in pilot project working with a fluid bed dryer to see whether a byproduct from the plant's production process could be used to fuel this vessel . . . worked with production, maintenance and engineering groups to gain better production efficiency throughout plant . . . promoted to unit foreman, supervised hourly workers in the preparation department . . . now planning analyst in the Phosphorus Chemical Division at Industrial Chemical Group headquarters . . . responsibilities include working on economic analyses of plant expansion to ensure that they are consistent with the Division's long-range plan; also conducts feasibility studies on the effect of proposed marketing changes on plant production equipment . . . says, "What really impresses me about FMC is the fact that a person is judged both on technical competence and on ability to work with others."



Mary Ann Pizzolato

B.S.Ch.E. from Rutgers University in 1976 . . . joined Industrial Chemical Group's Carteret plant as a process engineer . . . worked as engineer for the acid plant—did troubleshooting, process review and some pilot and new project work . . . promoted to assistant area supervisor in production department . . . works directly with area supervisor to ensure high quality and maximum production levels . . . likes having the opportunity to gain experience working with management and hourly workers . . . believes that "with the pressure to get production out as scheduled, you have to learn to work well with these groups—it's the best kind of on-the-job-training."

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A Letter to Chemical Engineering Seniors

This is the tenth Graduate Issue to be published by CEE and distributed to chemical engineering seniors interested in and qualified for graduate school. As in our previous issues we include articles on graduate courses that are taught at various universities and ads of departments on their graduate programs. In order for you to obtain a broad idea of the nature of graduate course work, we encourage you to read not only the articles in this issue, but also those in previous issues. A list of these follows. If you would like a copy of a previous Fall issue, please write CEE.

Ray Fahien, Editor CEE

AUTHOR	TITLE
	Fall 1977
Dumesic	"Fundamental Concepts in Surface Interactions"
Jorne	"Electrochemical Engineering"
Retzloff	"Chemical Reaction Engineering Science"
Blanch, Russell	"Biochemical Engineering"
Chartoff	"Polymer Science and Engineering"
	Fall 1976
Alkire	"Electrochemical Engineering"
Bailey & Ollis	"Biochemical Engr. Fundamentals"
DeKee	"Food Engineering"
Deshpande	"Distillation Dynamics & Control"
Johnson	"Fusion Reactor Technology"
Klinzing	"Environmental Courses"
Lemlich	"Ad Bubble Separation Methods"
Koutsky	"Intro. Polymer Science & Tech."
Reynolds	"The Engineer as Entrepreneur"
Rosner	"Energy, Mass and Momentum Transport"
	Fall 1975
Astarita	"Modern Thermodynamics"
Delgass	"Heterogeneous Catalysis"
Gruver	"Dynamical Syst. & Multivar. Control"
Liu	"Digital Computations for ChE's"
Manning	"Industrial Pollution Control"
McCoy	"Separation Process"
Walter	"Enzyme Catalysis"
	Fall 1974
Corripio	"Digital Computer Control of Process"
Donaghey	"Solid-State Materials and Devices"
Edgar	"Multivariable Control and Est."
Gates, et al.	"Chemistry of Catalytic Process"
Luks	"Advanced Thermodynamics"
Melnyk & Prober	"Wastewater Engineering for ChE's"
Tavlarides	"Enzyme and Biochemical Engr."
Theis	"Synthetic & Biological Polymers"
Hamrin, et. al.	"Energy Engineering"
Sherwood	"History of Mass Transfer Theory"
	Fall 1973
Merrill	"Applied Chemical Kinetics"
Locke & Daniels	"Corrosion Control"
Moore	"Digital Computer Process Control"
Wei	"Economics of Chem. Processing Industries"
Hopfenberg	"Polymers, Surfactants and Colloidal Materials"
Fricke	"Polymer Processing"
Tierney	"Staged Separations"
O'Connell, et. al.	"Application of Molecular Concepts of Predicting Properties in Design"
	Fall 1972
Bell	"Process Heat Transfer"
Chao & Greenkorn	"Equilibrium Theory of Fluids"
Cooney	"Biological Transport Phenomena and Biomedical Engineering"
Curl & Kadlee	"Modeling"
Gainer	"Applied Surface Chemistry"
Slattery	"Momentum, Energy and Mass Transfer"
Kelleher & Kafes	"Process and Plant Design Project"
Douglas & Kittrell	"Engineering Entrepreneurship"
Wei	"How Industry Can Improve the Usefulness of Academic Research"
Tepe	"Relevance of Grad. ChE Research"
	Fall 1971
Reid & Modell	"Thermo: Theory & Applications"
Theofanous	"Transport Phenomena"
Weller	"Heterogeneous Catalysis"
Westerberg	"Computer Aided Process Design"
Kabel	"Mathematical Modeling . . ."
Wen	"Noncatalytic Heterogeneous Reaction Systems"
Beamer	"Statistical Analysis and Simulation"
Himmelblau	"Optimization of Large Scale Systems"
	Fall 1970
Berg	"Interfacial Phenomena"
Boudart	"Kinetics of Chemical Processes"
Koppel	"Process Control"
Leonard	"Bioengineering"
Licht	"Design of Air Pollution Control Systems"
Metzner & Denn	"Fluid Mechanics"
Powers	"Separation Processes"
Toor & Condiff	"Heat and Mass Transfer"
Tsao	"Biochemical Engineering"
	Fall 1969
Amundson	"Why Mathematics?"
Churchill	"Theories, Correlations & Uncertainties for Waves, Gradients & Fluxes"
Hanratty	"Fluid Dynamics"
Hubert	"Stat. Theories of Particulate Systems"
Lightfoot	"Diffusional Operations"
Lapidus	"Optimal Control of Reaction Systems"
Prausnitz	"Molecular Thermodynamics"
Dougharty	"Reactor Design"

HORSES OF OTHER COLORS - SOME NOTES ON SEMINARS IN A CHEMICAL ENGINEERING DEPARTMENT

RUTHERFORD ARIS

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Minneapolis, Minnesota 55455

ONE OF THE STAPLES of the graduate curriculum in a ChE department is undoubtedly the ChE seminars that the students would attend during their graduate career. Their range and quality as an index of the quality of the department and their value, both to faculty and students, is unparalleled. Though the stringent budgets of recent years have often forced departments to cut back on the number of outside speakers they can afford to bring in, most departments make every effort to introduce as many and varied speakers as possible. Nor are the resources of industry to be overlooked, for often an industrial speaker can, with a good talk, give the students a much better idea of the uses to which their ChE training will be put than is possible under the pressures of classroom curriculum. But there is also a case for the student hearing an occasional seminar on something even more interesting than ChE. This can be accomplished by asking a speaker from another department of one's own university or, on occasion, by getting an outside speaker. There is also the possibility of devoting the seminars of a whole quarter or semester to subjects other than ChE itself and this we have tried about every third year at Minnesota. Arvind Varma has recently organized such a series at Notre Dame and the Editor thought that the idea might be worth general mention.

RANDOM LECTURE TOPICS

THE FIRST SUCH SERIES that we tried at Minnesota was, like many other good things here, started with the blessing and encouragement of Neal Amundson. It was held during the Winter Quarter of 1964 under the general title of "A Broader View of Research at the University." This series was deliberately discursive though it started with a hop, step and jump from classical times

into current research topics. It had the incomparable advantage of being launched by the late Mr. Douglas Cuthbert Coloquon Young, the Reader in Greek at St. Andrews University, who was spending a sabbatical at Minnesota. A redoubtable scholar of immense height and doughty mien, he was quite liable to wear the kilt to a seminar, though he did not, unfortunately, for his talk to us on "How the Greeks Started in Science and Why They Stopped." Commenting that one of the earliest works of Greek Science was Hesiod's "Works and Days," a work in verse, he remarked that "It would be a hardship for a modern scientist to have to present his Ph.D. thesis in verse. But such compulsory academic verse might not sound much worse than most modern scientific prose, nor indeed worse than much modern poetic verse." The second talk was on medieval scholasticism and the third, on modern philosophy of science, was given by Herbert Feigl, one of the last surviving representatives of the Vienna circle. From this three-stage launching the series became quite discursive, ranging from archaeology and physiology to mathematics and economics. The Vikings as poets were discussed by one speaker and the structure of theoretical physics by another.

In the Fall of '66 we had another series of random topics under the title of "The Scope of Scholarship." These ranged from ocean engineering and architectural design to the preservation of organs and the plays of August Strindberg.

Skip Scriven suggested a series on "Aspects of Technological Development and Social Change." . . . thanks to Scriven's vision we were also able to bring in people from outside. These included a director of a multinational corporation, an international economics consultant and a State Department man from Washington . . .



After a few years in chemical industry and a brief spell teaching mathematics at the University of Edinburgh, Aris came to the University of Minnesota in 1958 and has been in its Department of ChE ever since. He particularly appreciates the lively intellectual atmosphere of the department and the excellent quality of students that it serves and has endeavored to make some contribution to its good repute. His research has centered on the mathematical models of chemical engineering, particularly those of chemical reactors. He is currently Regents' Professor of ChE at the University of Minnesota.

Two would have needed audiovisual aids for a proper record. One on the ethnomusicology of Ecuador was enlivened by some excellent recordings, while another on the history and technique of stage movement was dramatically illustrated by the gambollings of the speaker. Walter Heller had recently returned from his service in Washington and was kind enough to speak on the "New Economics."

Under the rubric of "Varieties of Academic Experience" another series was launched in the Winter of 1970. This again was a series of diverse and disconnected topics ranging, this time, from ecology and cellular engineering to symmetry and the psychology of speech perception. We again had some classical archaeology from our Regents' Professor of that predilection, William McDonald. He had introduced the subject in 1964 and it was to his kind interest that we had been indebted for the suggestion of several speakers. We even had a Vice-President for administration speak on the perils, promise and perplexities of program planning budgets.

This illustrates one kind of seminar series that can be tried, namely the random or desultory. The essential thing is to find out who are the most likely and interesting speakers on campus and to give them their head as to the choice of topic. It need hardly be added that this criterion must be guarded with a sense for true scholarship, for there are on many campuses a number of quite

lively, but perhaps more superficial, individuals who from time to time surface with a great splash. These will be heard in any case by those who wish to and it is no service to the student to provide a forum for anything less than that which can pass the most exacting scholarly standards.

GENERAL THEME TOPICS

THE OTHER FORM OF seminar series is that which embroiders the talks around a general theme. Thus one quarter we had a series called "Research in the Industrial Context" in which we deliberately tried to give the graduate students a sense for the different conditions under which many of them would operate in their research once they found a job in the chemical industry. Here we were fortunate in being able to attract some of the top people of the profession such as Tom Baron of Shell and Vern Weekman from Mobil, but we were less fortunate in being able to get manuscripts from them and so make a permanent record of the series. Perhaps this was as well, for the impact on the current student body was the main intention and our industrial visitors were

"It would be a hardship for a modern scientist to have to present his Ph.D. thesis in verse. But such compulsory academic verse might not sound much worse than most modern scientific prose, nor indeed worse than much modern verse."

able to speak more freely and refer to more current topics when they were neither recorded nor asked to provide a full script.

In the Spring Quarter of 1974, Skip Scriven suggested a series on "Aspects of Technological Development and Social Change." This was even more thematic than anything we had attempted before, yet we wanted to be sure it would not be without its leaven of humanities. Our local expert on ethnomusicology [among other things, for he is a musicologist of vast range] Johannes Riedel came again to talk about music and social change and an anthropologist discussed the interaction of growth and no-growth cultures. One of our leading political scientists discussed the differences and similarities in economic development in England and France at the time of the Industrial Revolution and between China and Japan in more recent history. A geographer spoke of the changing metropolitan patterns of America while a visiting

professor discussed the interaction on aesthetics and politics in recent Latin American literature. But thanks to Scriven's vision we were also able to bring in people from outside. These included a director of a multinational corporation, an international economics consultant and a State Department man from Washington as well as Dr. Jayaragan Chanmugam, a chemical engineer, whose paper with George Box graces the first page of *I&EC Fundamentals* and who now works with the World Bank.

Last fall we again had a thematic series, though the theme was very lightly—even metaphorically—treated at times. The current interest in catastrophe theory seemed to be a good starting point and indeed we were launched with a splendid description of the elements of the mathematical theory by Larry Markus of our Mathematics Department. He was followed by Professor Holt, who had three years before told us about the politics of economic change and who now discussed his analysis of the beginnings of World Wars I and II in the light of the categories of catastrophe theory.

There is also the possibility of devoting the seminars of a whole quarter of semester to subjects other than ChE itself and this we have tried to do about every third year at Minnesota.

Apart from a final “wayside dandelion without the gate” which made some reference to catastrophe theory in the context of chemical reactors, there was little in the rest of the series which had anything to do with catastrophe theory as such. Instead the term was used in a variety of meanings and this freedom allowed us to invite an archaeological geologist to talk about Atlantis and an art historian to show how the eruption of Vesuvius in 1631 helped date some of Carracciolo's later frescoes. A classicist described the influence of the plague in Athens in 430 B.C. on the thought of Thucydides, while a psychologist talked of crisis intervention psychology. The Director of our Limnological Research Center raised the question of whether a catastrophe was necessarily a catastrophe by showing that forest fires had a definite value to the forest community in the longer perspective of the ecological cycle. The use of the term catastrophe was even more metaphorically used in a discussion of the rise of mounted shock combat as one of the chief instruments of feudal-

ism. Here the title “The Feudal Catastrophe” really referred to the commonly received opinion of our day that feudalism as such was a disaster. Very thought-provoking were the remarks of a Germanic philologist who suggested that in primitive societies nothing short of a catastrophe broke the chain of cyclical thinking and allowed man to recognize the essential difference between past and future. This linked catastrophe with the origin of history as a science.

SELECTION PROCEDURES

AS WAS MENTIONED above the great essential for all these enterprises is the choice of the liveliest and most vigorous of scholars, and the advantage of a major university is that there should be a sufficient number of these around. The other essential is that some one, or perhaps two, members of the ChE faculty should take it up as a positive commitment. They will certainly benefit from the suggestions of their colleagues, but it is fatal to try and get a series like this run by a committee. Since there is generally a very small budget for these things it is usually necessary to depend on colleagues within one's own university to whom one is not allowed to pay an honorarium and for whom no expenses are required. Obviously where there is money the series can be greatly enhanced by invitations to people from farther afield. It is generally well to line up the speakers at least nine months in advance. They are usually eminently pregnable when they think they can carry to full term, forgetting, as is so often the case, that the going may be more than a little laborious when their hour has come. Beyond the usual administrative reminders and provision of audiovisual equipment, the occasion of the seminar often gives an opportunity to get the faculty together for a lunch with the speaker beforehand.

If the speakers are not being offered an honorarium it is a little unfair to demand a manuscript, though there are always some who like to write out their talks. Thus, if a record of the seminars is thought desirable, one must be pre-

. . . . we had another series of random topics under the title of “The Scope of Scholarship.” These ranged from ocean engineering and architectural design to the preservation of organs and the plays of August Strindberg.

The second talk was on medieval scholasticism and the third, on modern philosophy of science, was given by Herbert Feigl, one of the last surviving representatives of the Vienna circle. From this three-stage launching the series became quite discursive, ranging from archaeology and physiology to mathematics and economics. The Vikings as poets were discussed by one speaker and the structure of theoretical physics by another.

pared to tape the lecture and transcribe from the tape. It is incredible how incoherent in transcript a perfectly good, or even really exciting, talk can be. It is absolutely fatal to show the raw transcript to the speaker. He or she will throw up their hands in horror and that is the last you will see of it. Therefore an intermediate stage of editing by the organizer of the seminars, or colleagues, is absolutely essential. Indeed it is this, and the preparation of suitable introductions for the speakers, that constitutes the major part of the labor of such a series. The burden of it is enormously lightened if one is blessed, as we have been at Minnesota, with highly intelligent secretaries. Marsha Riebe, Laura Muellenbach and others here have been able to produce transcripts that only take three or four hours to edit. Without such intelligent transcription it can take six or eight hours to turn into grammatical and continuous form the eloquent talk that one so much enjoyed when it was being given. There is an occasional speaker who transcribes into connected prose, such as the late Jacob Bronowski, but these are the exception rather than the rule and the labor of editing from transcript should not be underestimated in planning to make a record of such a seminar series. The edited transcript should then be typed up for the speaker to go over and the organizer's work then consists in hounding his speakers until the manuscripts are returned. There is of course no need to make a permanent record of such seminar series but we have found it a great pleasure to do so when funds permitted.

The publications have more value, too, than as a mere record and recollection of a series of enjoyable talks for they may be sent out with offer letters to prospective graduate students. Here they serve as a certain touchstone. If a student is put off by them, their irrelevance to ChE and lack of solemnity, then we are only too thankful—such a person would hardly take to the atmosphere of a good graduate school. On the other hand, if it tips the balance of the decision in the favor of Minnesota as a graduate school we are appropriately

grateful. Of one aspect there has never been any question: their popularity with the graduate students is immense. It is not just a relief from the strenuousness of ChE, but is a definite challenge and opening of windows on wider perspectives. To the faculty they also offer an opportunity for wider contact within the university and have been enthusiastically welcomed whenever we have been able to arrange them. □

ChE letters

RANKING OF DEPARTMENTS

Dear Sir:

In the spring issue of C.E.E. you have published an article by Professor Griskey that dealt with ratings of Chemical Engineering Departments. I will not deal here with the particulars of the article since several members of the profession have done so in statements accompanying it. The article, however, points unwittingly to two major aspects of the current state of chemical engineering education.

Indiscriminate comparisons of Chemical Engineering Departments without regard to their emphasis and direction is ludicrous. Today there are departments which resemble applied mathematics; other departments act as industrial appendices. Then we have those places which emphasize bioengineering, physical chemistry, theoretical chemistry, etc., etc. To rate all these together is like comparing "apples and oranges."

The second point of this letter derives directly from the above notion. It is high time, I believe, to reexamine the direction of the profession as an academic discipline. Crouched somewhere between tenure, publications, and personal prestige, we certainly need to rediscover relevance in both teaching and research.

Some of Griskey's "top rated" institutions seem to forget that we are an applied discipline; that not all graduates intend to pursue academic careers; that there is such a thing as undergraduate education. (Over 80% of the students terminate their academic careers at the B.S. level). Perhaps the accreditation of certain institutions which call themselves Chemical Engineering Departments need to be reexamined and reevaluated.

Michael Economides
Graduate Student
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CHEMICAL REACTOR ENGINEERING*

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THE DEVELOPMENT OF chemical reaction engineering as an identifiable area within chemical engineering has led to renewed interest and emphasis on courses dealing with chemical reaction kinetics and chemical reactor design. The basic issues concerning instruction in these areas are probably not much different from those involved in any other area of chemical engineering insofar as fundamentals vs. applications, extent of coverage, and similar factors. There is, however, a chemical factor involved in this area that may not appear quite so prominently in other endeavors, and instruction at the undergraduate level particularly may be sensitive to the contents of current offerings in chemistry courses.

Certainly there is no lack of literature on all aspects of the topic. In Table 1 is given an extensive (but by no means comprehensive) list of references dealing with chemical kinetics, engineering aspects of kinetics and reactor design, experimental methods, catalysis, and several specialized topics. Most of us are possibly familiar with the offerings listed under engineering aspects, and a quick glance at this tabulation might induce one to think there is an enormous variation in what individuals conceive to be useful components of an undergraduate course. It is interesting to see if this is really so. Let us do this by comparing the table of contents of three typical offerings from the list, as shown in Table 2. Two of the books, by Smith and Levenspiel, were chosen because they are perhaps the most widely used undergraduate texts. The third book, by Carberry, is a very recent addition to the kinetic literature. In each case the author has chosen to treat a number of funda-

mental topics, with more specialized applications in later chapters. Descriptive kinetics and data interpretation are, logically, accorded first place on each list, followed by introductory material on reactor design and analysis. The latter is largely limited to ideal reactor models; the effect of temperature is treated somewhat differently in an organizational manner by the three authors, but the level and extent of coverage is quite similar. Concepts of selectivity as well as rate and conversion are presented early in each case and maintained as an important factor in kinetics and reactor analysis throughout. Following this introductory material, each author then turns to problems associated with deviations from ideal reactor performance. Here somewhat more variation is apparent in organization and presentation but, again, the net coverage and information is quite similar.

The point is that, in terms of information which might form the core content of a typical



John B. Butt is presently a Professor of ChE at Northwestern University. He received his S.C. and B.S. from Clemson University and his M.Eng. and D. Eng. from Yale University. He has had industrial experience with Humble Oil, Chevron Research and Exxon Research Laboratories, and is presently a consultant for Argonne National Laboratory and Illinois Inst. of Tech. Research. He was the recipient of the AIChE Allan P. Colburn Award in 1968 and the AIChE Professional Progress Award in 1978. (L)

Gene Petersen did his undergraduate and masters work at the University of Washington and obtained his Ph.D. in Fuel Science at Pennsylvania State University in 1953. He joined the faculty at the University of California at Berkeley where he pursues research and teaches kinetics, catalysis and reaction engineering. (R)

*ASEE Summer School for ChE Faculty, Snowmass Resort, Colorado, August, 1977.

TABLE 1.
Selected References in Chemical Kinetics,
Catalysis and Reactor Design

Basic Material For Review:

- E. L. King, "How Chemical Reactions Occur", Benjamin, 1964 (Paperback).
- F. Daniels and R. A. Alberty, "Physical Chemistry", Wiley.
- Latham, J. L., "Elementary Reaction Kinetics", 2nd ed., Butterworths (1969).

Introductory Texts Emphasizing Chemical Aspects Of Subject:

- A. A. Frost and R. G. Pearson, "Kinetics and Mechanism", 2nd ed., Wiley, 1969.
- K. J. Laidler, "Chemical Kinetics", 2nd ed., McGraw-Hill, 1965.
- K. J. Laidler, "Reaction Kinetics", Volumes I and II, Pergamon Press, 1963 (Paperback).
- C. N. Hinshelwood, "Kinetics of Chemical Change", Clarendon Press, 1940 (Somewhat out of date, but contains a good qualitative discussion of basics).
- M. Boudart, "Kinetics of Chemical Processes", Prentice-Hall, 1968.
- I. Amdur and G. G. Hammes, "Chemical Kinetics", McGraw-Hill, 1966.

More Advanced Treatments:

- H. S. Johnston, "Gas Phase Reactions", Prentice-Hall.
- N. Semenov, "Some Problems in Chemical Kinetics and Reactivity", Vol. I and II, trans. by M. Boudart, Princeton Univ. Press, 1958, 1959.
- S. W. Benson, "Foundations of Chemical Kinetics", McGraw-Hill, 1960.
- V. N. Kondratiev, "Kinetics of Chemical Gas Reactions", 1958, trans. from the Russian, Pergamon Press, 1964.
- S. Glasstone, K. J. Laidler and H. Eyring, "The Theory of Rate Processes", McGraw-Hill, 1941.

Texts Emphasizing Engineering Aspects of Kinetics and Reactor Design:

- O. Levenspiel, "Chemical Reaction Engineering", 2nd ed., Wiley, 1972.
- J. M. Smith, "Chemical Engineering Kinetics", McGraw-Hill, 2nd ed., 1970.
- S. M. Walas, "Reaction Kinetics for Chemical Engineers", McGraw-Hill, 1959.
- O. A. Hougen and K. M. Watson, "Chemical Process Principles", Vol. III, Wiley, 1947.
- R. Aris, "Introduction to the Analysis of Chemical Reactors", Prentice-Hall, 1965.
- K. G. Denbigh, "Chemical Reactor Theory", Cambridge Univ. Press, 1966.
- H. Kramers and K. R. Westerterp, "Elements of Chemical Reactor Design and Operation", Academic Press, 1963.
- D. A. Frank-Kamenetskii, "Diffusion and Heat Exchange in Chemical Kinetics", Trans. Ed. John P. Appleton, 2nd ed., Plenum Press, 1969.
- G. R. Gavalas, "Nonlinear Differential Equations of Chemical Reacting Systems", Springer-Verlag, 1968.
- J. J. Carberry, "Chemical and Catalytic Reaction Engineering", McGraw-Hill, 1976.

- L. C. Lee and W. J. Thomas, "Chemical Engineering", Vol. III, edited by J. F. Richardson and D. G. Peacock, Chapters 1 and 2, Pergamon, 1971.
- C. G. Hill, Jr., "Chemical Engineering Kinetics and Reactor Design", Wiley, 1977.

Experimental Techniques:

- H. W. Melville and B. G. Gowenlock, "Experimental Methods in Gas Reactions", Macmillan, 1964.
- S. L. Friess and A. Weissberger (Editors), "Investigations of Rates and Mechanisms of Reactions", Volumes I and II (Volume 8, parts 1 and 2, of "Technique of Organic Chemistry"), Interscience, 1953 and 1963.
- R. B. Anderson, "Experimental Methods in Catalytic Research", Academic Press, 1968. Volumes I, II, and III.

Heterogeneous Catalysis:

- J. M. Thomas and W. J. Thomas, "Introduction to the Principles of Heterogeneous Catalysis", Academic Press, 1967.
- E. E. Petersen, "Chemical Reaction Analysis", Prentice-Hall, 1965.
- P. G. Ashmore, "Catalysis and Inhibition of Chemical Reactions", Butterworths, 1963.
- J. R. Anderson, "Structure of Metallic Catalysts", Academic Press, 1975.
- R. Aris, "The Mathematical Theory of Diffusion and Reaction in Permeable Catalysts", Volumes I and II, Oxford, 1975.
- C. N. Satterfield, "Mass Transfer in Heterogeneous Catalysis", MIT Press, 1970.
- G. C. Bond, "Heterogeneous Catalysis", Clarendon Press, 1974.
- G. C. Szabo (Editor), "Contact Catalysis", Elsevier, 1976, Volumes I and II.

Special Topics:

- J. Szekeley, J. W. Evans and H. Y. Sohn, "Gas Solid Reactions", Academic Press, 1976.
- D. Kunii and O. Levenspiel, "Fluidization Engineering", Wiley, 1969.
- D. F. Othmer, "Fluidization", Reinhold, 1956.

undergraduate course, there is considerable agreement on content and even order of presentation. This is not to say that these texts, or others, are all the same, for in the latter stages of each there appears considerable variation in content and organization, indicative of individual interests and perhaps specialized applications. The manner of presentation varies considerably to reflect the style of the author. This is shown in Table 3 which presents the content of the basic undergraduate courses at Berkeley and Northwestern. This diversity leads to what we believe to be a healthy variation in individual undergraduate courses around the country, in which the fundamentals are fairly well agreed upon but many different approaches exist within presentation and the use of

TABLE 2.
Tables of Contents of Basic Material from Three Texts on
Chemical Engineering Kinetics and Reactor Design

Levenspiel		Smith		Carberry	
1. Introduction	7	1. Introduction	32	1. Introduction	11
2. Kinetics of Homogeneous Reactions	33	2. Kinetics of Homogeneous Reactions	65	2. Behavior of Chemical Reactions	50
3. Interpretation of Batch Reactor Data	52	3. Design Fundamentals	33	3. Behavior of Chemical Reactors	66
4. Introduction to Reactor Design	4	4. Homogeneous Reactor Design: Isothermal Conditions	73	4. Conservation Equations for Reactors	51
5. Single Ideal Reactors	27	5. Temp. Effects in Homogeneous Reactors	40	5. Heterogeneous Reactions	50
6. Design for Single Reactions	39	6. Deviations from Ideal Reactor Performance	30	6. Gas-Liquid and Liquid-Liquid Systems	67
7. Design for Multiple Reactions	47	7. Heterogeneous Reactions	9	7. Fluid-Solid Non-Catalytic Reactions	47
8. Temp. and Pressure Effect	43	8. Heterogeneous Catalysis	47	8. Heterogeneous Catalysis and Catalytic Kinetics	100
9. Non-Ideal Flow		9. Kinetics of Fluid-Solid Catalytic Reactions	28	Total pages: 442	
10. Mixing of Fluids		10. External Transport Processes in Heterogeneous Reactions	42		
11. Introduction to Design for Heterogeneous Reacting Systems	8	11. Reaction and Diffusion Within Porous Catalysts: Internal Transport Processes	65		
14. Solid Catalyzed Reactions	77				
Total pages: 337			Total pages: 464		

specific examples to develop material beyond the entry level. Historically this situation may be the result of the fact that many current undergraduate courses in reaction kinetics and reactor analysis had their origins not too long ago at the graduate level. It is within recent memory that many undergraduate curricula contained no courses (or elective, at best) in this area.

KINETICS AND EXPERIMENTATION

THERE ARE SOME ASPECTS of undergraduate education concerning kinetics and reaction engineering that should be of current concern. Interestingly, most of them deal with kinetics. One has to do with the chemical part of chemical kinetics. In most cases this is not treated in any detail, if at all, with the result that the student's analysis of kinetics is based purely on phenomono-

logical rate laws with little understanding of their basis. Where does the Arrhenius law come from anyway? If we are careful to use activities in thermodynamic problems, shouldn't we use them in kinetics? Certainly all of us could formulate numerous questions similar to these and perhaps even admit that they are not addressed in our undergraduate course. Earlier, such problems may not have been of quite so much concern, but current undergraduate physical chemistry courses differ from those taught 20 years ago. Increased emphasis (if not total preoccupation) on spectroscopy and quantum theory has reshaped much of the course content and the student may come away with somewhat less chemical intuition regarding reaction analysis than was formerly the case.* A problem in developing suitable coverage is that text material is distributed over a wide range of sources, as indicated in Table 1.

A second factor of concern is the development of suitable laboratory experiments in the area. Too often relevant experimentation is found only as one or two entrees in the undergraduate chem-

..... we feel strongly that the undergraduate program in kinetics should not be devoid of relevant experimentation in an engineering context.

*Do you know what your Chemistry Department is doing tonight?

ical engineering laboratory menu, or an occasional experiment in introductory or physical chemistry laboratory. This is admittedly a difficult problem, since the timing sequence of courses in kinetics in many curricula does not make for convenient relation between classroom and laboratory experience. Unfortunately we have no general solutions to set forth for this problem, but we feel strongly that the undergraduate program in kinetics should not be devoid of relevant experimentation in an engineering context. In fact, experiments on non-trivial catalytic, kinetic and reactor design systems introduce the student to the real world and focus attention on the enormous difficulties associated with getting good data, interpreting them, and using them to predict reactor behavior. An undergraduate elective course, half lecture and half laboratory, is available at Berkeley. The course outline is shown in Table 4. A course with a similar objective was developed some years ago at Princeton and a laboratory manual detailing several excellent experiments was prepared by J. B. Anderson.

A second factor of concern is the development of suitable laboratory experiments in the area. Too often relevant experimentation is found only as one or two entrees in the undergraduate chemical engineering laboratory menu, or an occasional experiment in introductory or physical chemistry laboratory.

ENTRANCE-LEVEL COURSES

IT IS INTERESTING that an increasing number of schools throughout the country are offering two courses in this area at the undergraduate level, either as a Junior-Senior sequence or by making available the entering level graduate course as a second offering for qualified undergraduates. This, in turn, presents an interesting problem as to what to offer students entering a graduate program with such a background. Probably, any graduate program should include at least one course beyond the entering level, and many do considerably more. Often the advanced graduate

TABLE 3.
Undergraduate Kinetic Courses Compared

Northwestern University 4 hr/wk of lecture for 10 weeks		California, Berkeley 3 hr/wk lecture and 1 hr tutorial for 10 wks	
Week	Content	Week	Content
1	Introduction, definition of rate and extent of reaction Descriptive kinetics of simple and nearly complex reactions Elementary steps and chain reactions	1	Introduction to subject, references, purpose, relationship to other chemical engineering courses Stoichiometric equations, simple and complex reactions Extent of reaction, rate of reaction Elementary steps, sequences of reactions
2	Nonisothermal reactions Interpretation of kinetic data	2	Temperature coefficient, Arrhenius expression Theories of reaction—collision theory and transition state theory
3	Collision theory, Lindemann theory	3	Finish transition state theory Steady state approximation
4	Midterm I (basic kinetics) RRK theory, transition state theory	4	Rate limiting step—meaning and utility Examples of homogeneous and heterogeneous systems. HBr, HI, dehydrogenation of methylcyclohexane
5	Reactions on surfaces Mixing and segregation Age distributions	5	Plug flow reactor isothermal, adiabatic and non-isothermal
6	Midterm II (rate theories) Mixing models	6	Midterm CSTR equations for isothermal and non-isothermal
7	Mixing and ideal reactor models (PFR, CSTR)—conversion and selectivity	7	Multiple steady states in reaction systems
8	Temperature effects in ideal reactors Nonideal reactor models: mixing cell and dispersion	8	Examples of real reaction systems: Chlorination of Benzene Oxidation of naphthalene Ammonia synthesis
9	Temperature effects in nonideal reactors Reactions in two phases, mass transfer and reaction Midterm III (mixing and ideal reactors)	9	Residence time distribution function, its utility and short-comings Moving bed and fluidized reactors
10	Introduction to some detailed simulation methods Overview of course Industrial example, catalytic cracking Midterm IV (nonideal reactors) in lieu of final exam	10	External and internal diffusion in heterogeneous reaction systems.

... the student's analysis of kinetics is based purely on phenomenological rate laws with little understanding of their basis. Where does the Arrhenius law come from anyway? If we are careful to use activities in thermodynamic problems, shouldn't we use them in kinetics?

TABLE 4.
Undergraduate Course, "Catalytic Reactor Design and Catalysis", University of California, Berkeley 3 hr/wk for 10 weeks.

Week	Content
1	Course Organization Laboratory organization
2	Tutorials* Preparation of Catalysts
3	Preparation of Catalysts Physical Characterization of Catalysts
4	Reactor Design Principles
5	Tutorials* Reactor Design Problem
6	Reactor Design Problem Rate Expressions for Catalysts
7	Tutorials* Rate Expressions, contd.
8	Homogeneous Catalysis NO _x reduction
9	Tutorials* Fluidized Reactors
10	Liquid-Liquid and Gas-Liquid Reactors Student Reports

*Tutorials by appointment, individually arranged.

EXPERIMENTS*

- H₂-D₂ Exchange**
H₂-D₂ exchange is measured on a fresh Ni film in a bulb using mass-spectrometer to analyze the progress of the reaction in a batch reactor.
- Hydrogenolysis of Cyclopropane**
The kinetics of hydrogenolysis are studied in an integral packed bed reactor using Pt on γ -alumina catalyst. The objective is to determine experimentally reaction order and activation energy.
- Oxidation of Propylene**
The objective is to determine activation energy for reaction of a dilute mixture of ethylene in air to CO₂ and water on a Pt-alumina catalyst. This experiment is an idealized model of an automobile catalytic converter.
- Esterification of Butyl Alcohol with Acetic Acid**
The purpose of this experiment is to study the kinetics of esterification as affected by temperature, acidity, and effects of reversibility.
- Carbon-Carbon Dioxide Reaction**
The reaction between graphite rods and CO₂ is studied at atmospheric pressure and at very high temperatures in a glow-bar furnace. The objective is to show directly the non-uniform reaction within the carbon rod.
- Oxidation on a Platinum Foil**
The reaction of CO and O₂ is studied on an electrically heated platinum foil in a flow reactor. Reaction rates are determined from heat release on the catalyst. Reaction mechanism and activation energies are determined.

7. Catalyst Characterization
BET surface area. Metal surface area.

8. Catalyst Preparation
A typical catalyst is prepared by impregnating an alumina support with nickel salt. The nickel is reduced and subsequently the catalyst pellet is observed to establish the metal distribution.

*Students do 2 experiments plus a catalyst characterization in addition to a reactor design.

experience need not be in terms of formal lecture courses, but may be in the form of research or journal reading seminars, special topics courses (whose content may vary from one year to the next), intensive mini-courses, etc. It is perhaps less appropriate here to become involved in a discussion of details of graduate courses at any level, since these ordinarily are much more reflective of the interests and experience of the instructor, and variations in content within wide limits are possible. Nonetheless, when we originally compared notes concerning the content of the entering level graduate courses at Berkeley and Northwestern we were struck by their similarity. These courses are basically a continuation in depth of the undergraduate courses, assuming background in descriptive kinetics and some understanding of ideal (PFR and CSTR) reactor models. One unifying theme in both courses is the discard of pseudo-homogeneous approximations and extensive treatment of reactions involving two phases. Under this cover we discuss heterogeneous catalysis, gas-liquid reactions, heterogeneous (two phase) reactor models, and the theory of diffusion and reaction. To our additional surprise, we found that considerable effort is devoted in both Northwestern and Berkeley courses to discussion of what might be termed "industrial examples". At Berkeley these include analysis of a FCC reactor-regenerator system and a study of the chlorination of benzene; at Northwestern kinetic lumping and decay models for catalytic cracking are investigated. Both courses also include a "sampler" on reactor stability and parametric sensitivity and introductory material on two-dimensional modeling. A syllabus of the Berkeley course is given in Table 5.

TABLE 5.
Graduate Course, "Chemical Reaction Analysis",
University of California, Berkeley, 3 hr/wk
for 10 weeks.

Lecture	Content
1	Orientation, organization, goals
2	Stoichiometry, minimum independent variable in system
3	Conversion, definition of rate expression, conservation equations
4	The problem of heterogeneous reactor design—the pseudohomogeneous rate
5	Langmuir-Hinshelwood kinetics
6	Quasi-steady state methods
7	Thiele-Zeldovich problem
8	Falsification of kinetics by transport phenomena
9	Generalized treatment
10	Heat effects, complex reactions, criteria
11	Parameters of model: BET area, metal area,
12	diffusivity
13	Single pellet diffusion reactor
14	Models of poisoning
15	External mass transfer
16	Reactor design, residence time distribution
17	Residence time distribution
18	Application of RTD to reactor modeling
19	Reactor-regenerator; fouling
20	Examination
21	Chlorination of benzene: example
22	Stability: Van Heerden,
23	Bilous and Amundson
24	One-dimensional reactors
25	Stability: NH_3 synthesis, Grens problem
26	Two-dimensional reactors
27	Boundary conditions, hot spot example (phthalic anhydride)
28	Fluidized reactors
29	Slurry reactors
30	Trickle-bed reactors

If this single example possesses any generality, it would tend to indicate that a degree of consensus exists concerning the lower level graduate course similar to undergraduate courses. Beyond this level, however, offerings become quite varied depending on the interests and resources of individual departments. Normally, one finds some course dealing with various aspects of detailed reactor design, such as two dimensional, two phase fixed beds, fluidized beds, slurry, or trickle bed reactors.

A final note concerning graduate education in

... a degree of consensus exists concerning the lower level graduate course similar to undergraduate courses.

this field is the high potential value of individualized seminar courses or research seminars. These can be organized about special topics and made complimentary to material presented in more formal courses. At Northwestern, for example, there is a rather sizeable group of individuals in ChE, Chemistry, and Materials Science who are involved in catalysis research. Faculty, students, and visitors participate in a "Catalysis and Surface Science" seminar approximately every other week amid the munching of potato chips at Friday noon. A typical schedule of speakers, affiliations, and topics is given in Table 6. This seminar series is a nice supplement to courses in advanced reaction kinetics and catalysis which are generally offered in the winter and spring quarters.

In summary, we see a large measure of agreement on the content of undergraduate and entering level graduate courses in chemical reactor engineering, as illustrated here. What of the future? Assuming that current research interests are

TABLE 6.
Catalysis and Surface Science Seminars
Spring Quarter, 1977, Northwestern University

1. Professor J. J. Fripiat, C.N.R.S., Orleans, France (visitor), "Aspects of Zeolite Catalysts: Evidence for Hydrogen Spillover"
2. Dr. R. Bjorklund, Dept. of Chemistry, Northwestern (post-doctoral fellow), "Properties of $\text{Ni}/\text{Al}_2\text{O}_3$ Catalysts Prepared by Reaction of $\text{Ni}(\text{CO})_4$ with Alumina"
3. Dr. M. Jarjoui, University of Lyons, France (post-doctoral fellow), "Partial Oxidation of Ethylene over Silver Catalysts"
4. Dr. Y. Inoue, Department of Chemistry, University of Tokyo (post-doctoral fellow), "The Reactivity of Supported Pt with O_2 "
5. Professor J. B. Cohen, Department of Materials Science, Northwestern, "EXAFS and Its Applications in Surface Science"
6. Mr. D. M. Downing, Dept. of Chemical Engineering, Northwestern (graduate student), "Modeling Thermal and Mass Transport Interactions in Deactivated Catalyst Particles"
7. Mr. P. Otero-Schipper, Dept. of Chemical Engineering, Northwestern (graduate student), "Hydrogenation and Hydrogenolysis on Supported Pt"

going to show up in higher level graduate courses and thence diffuse downwards, we would expect to see increasing emphasis on unsteady state models, polyfunctional catalysis, catalyst deactivation, stability and sensitivity problems of various types, and lumping schemes for analysis of complex reaction networks. Can we be blamed if this sounds like a listing of our own research interests? □

A Kinetics Course*

INFLUENTIAL PAPERS IN CHEMICAL REACTION ENGINEERING

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THIS PAPER DESCRIBES the genesis, development, implementation, and evaluation of a graduate level kinetics course based upon selected influential papers in chemical reaction engineering. The starting point was the following letter of January 1976.

This spring I will be teaching a graduate course in Chemical Reaction Engineering. My thought is to select ten to fifteen of the most influential research papers in this area and to build the course around them. Just to pick a couple of examples, consider "Hougen, O. A., and Watson, K. M., "Solid Catalysts and Reaction Rates," *Ind. Eng. Chem.* 35, 529-541 (1943) and Danckwerts, P. V., "Continuous Flow Systems, Distribution of Residence Times," *Chem. Eng. Sci.* 2, 1-13 (1953).

No doubt you have your own favorites. So I am asking you along with a number of our colleagues to send me the references to a few papers that you consider to be of special importance.

One should not conduct a survey without sharing the results with the respondents. Also you may be interested in the cumulative opinion of your peers. So I will send a tabulation of the responses to everyone who contributes. Thank you for your help.

Twenty-two such letters were sent to individuals prominent in chemical reaction engineering. Sixteen responses were received including four from the researchers surveyed outside of the United States. All responses came from academic researchers although one industrial person was solicited. The list, shown in Table I, comprises the suggestions of fourteen of the respondents. Two respondents referred only to chapter bibliographies in their books. These responses, while useful, would produce an even longer list. Papers are listed first by frequency of mention and second by date of publication.

*Presented at the Summer School for Chemical Engineering Faculty held at Snowmass, Colorado, 1977.

TABLE I
List of Suggested Influential Papers

5 MENTIONS

Thiele, E. W., "Relation Between Catalytic Activity and Size of Particle," *Ind. Eng. Chem.* 31, 916-920 (1939).

3 MENTIONS

Denbigh, K. G., "Velocity and Yield in Continuous Reaction Systems," *Trans. Faraday Soc.* 40, 352-373 (1944).

Wheeler, A., "Reaction Rates and Selectivity in Catalyst Pores," *Advances in Catalysis* 3, 249-327 (1951).

Aris, R., and Amundson, N. R., "An Analysis of Chemical Reactor Stability and Control I," *Chem. Eng. Sci.* 7, 121-131 (1958). See also parts II and III, pp. 132-155.

Weisz, P. B., and Hicks, J. S., "The Behaviour of Porous Catalyst Particles in View of Internal Mass and Heat Diffusion Effects," *Chem. Eng. Sci.* 17, 265-275 (1962).

2 MENTIONS

Hougen, O. A., and Watson, K. M., "Solid Catalysts and Reaction Rates," *Ind. Eng. Chem.* 35, 529-541 (1943).

Van Krevelen, D. W., and Hoftijzer, P. J., "Kinetics of Gas-Liquid Reactions Part I. General Theory," *Rec. Trav. Chim. Pays-Bas* 67, 563-586 (1948). See also Part II pp. 587-599.

Yang, K. H., and Hougen, O. A., "Determination of Mechanism of Catalyzed Gaseous Reactions," *Chem. Eng. Progr.* 46, 146-157 (1950).

Danckwerts, P. V., "Continuous Flow Systems—Distribution of Residence Times," *Chem. Eng. Sci.* 2, 1-13 (1953).

Weisz, P. B., and Prater, C. D., "Interpretation of Measurements in Experimental Catalysis," *Advances in Catalysis* 6, 143-196 (1954).

Wheeler, A., "Reaction Rates and Selectivity in Catalyst Pores," in *Catalysis*, Vol. II, Emmett (ed.), 105-165 (1955).

Van Heerden, C., "The Character of the Stationary State of Exothermic Processes," *Chem. Eng. Sci.* 8, 133-145 (1958).

Uppal, A., Ray, W. H., and Poore, A. B., "On the Dynamic Behavior of Continuous Stirred Tank Reactors," *Chem. Eng. Sci.* 29, 967-985 (1974). Also "The Classification of the Dynamic Behavior of Continuous Stirred Tank Reactors—Influence of Reactor Residence Time," *Chem. Eng. Sci.* 31, 205-214 (1976).

1 MENTION

1900-1949

- Bodenstein, M., and Wolgast, K., "Reaktionsgeschwindigkeit in Strömenden Gasen," *Z. Physik. Chem.* 61, 422-436 (1903).
- Liljenroth, F. G., "Starting and Stability Phenomena of Ammonia-Oxidation and Similar Reactions," *Chem. Metal. Eng.* 19, 287-293 (1922).
- Hatta, S., *Techn. Repts. Tohōku Imperial Univ.* 8, 1 (1928); 10, 119 (1932).*
- Damkoehler, G., *Chem. Eng.* 46, 430 (1937).*
- Frank-Kamenetskii, D. A., *Zhur. Fiz. Khim.* 13, 756 (1939).*
- Voorhies, A., "Carbon Formation in Catalytic Cracking," *Ind. Eng. Chem.* 37, 318-322 (1945).
- Denbigh, K. G., "Continuous Reactions Part II. The Kinetics of Steady State Polymerization," *Trans. Faraday Soc.* 43, 648-660 (1947).

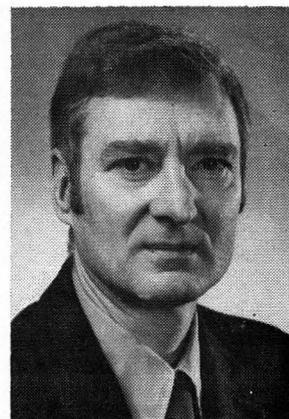
1950-1959

- Bernard, R. A., and Wilhelm, R. H., "Turbulent Diffusion in Fixed Beds of Packed Solids," *Chem. Eng. Progr.* 46, 233-244, (1950).
- Eldridge, J. W., and Piret, E. L., "Continuous Flow Stirred-Tank Reactor Systems," *Chem. Eng. Progr.* 46, 290-299 (1950).
- Singer, E., and Wilhelm, R. H., "Heat Transfer in Packed Beds," *Chem. Eng. Progr.* 46, 343-357 (1950).
- Danckwerts, P. V., "Gas Absorption Accompanied by Chemical Reaction," *AIChE Journal* 1, 456-463 (1955).
- Weller, S., "Analysis of Kinetic Data for Heterogeneous Reactions," *AIChE Journal* 2, 59-62 (1956).
- Boudart, M., "Kinetics on Ideal and Real Surfaces," *AIChE Journal* 2, 62-64 (1956).
- Bilous, O., and Amundson, N. R., "Chemical Reactor Stability and Sensitivity," *AIChE Journal* 2, 117-126 (1956).
- Yagi, S., and Kunii, D., "Studies on Effective Thermal Conductivities in Packed Beds," *AIChE Journal* 3, 373-381 (1957).
- Danckwerts, P. V., "The Effect of Incomplete Mixing on Homogeneous Reactions," *Chem. Eng. Sci.* 8, 93-102 (1958).
- Zwietering, T. N., "The Degree of Mixing in Continuous Flow Systems," *Chem. Eng. Sci.* 11, 1-15 (1959).
- Barkelew, C. H., "Stability of Chemical Reactors," *Chem. Eng. Progr. Symposium Series* 55, 37-46 (1959).

1960-1969

- Van Deemter, J. J., "Mixing and Contacting in Gas-Solid Fluidized Beds," *Chem. Eng. Sci.* 13, 143-154 (1961).
- Chu, C., and Hougen, O. A., "Optimum Design of a Catalytic Nitric Oxide Reactor," *Chem. Eng. Progr.* 57, 51-58 (1961).
- Bischoff, K. B., "A Note on Boundary Conditions for Flow Reactors," *Chem. Eng. Sci.* 16, 131-133 (1961).

This paper describes the genesis, implementation, and evaluation of a graduate level kinetics course based upon selected influential papers in chemical reaction engineering.



Robert L. Kabel received his B.S. degree from The University of Illinois in 1955 and his Ph.D. from The University of Washington in 1961. From 1961-1963 he served in the U.S. Air Force Space Systems Division receiving the Commendation Medal for Meritorious Achievement. Since 1963 he has been at The Pennsylvania State University where he is Professor of ChE. He was at The Technical University of Norway (1971-72) and Pahlavi University in Iran (1978) as visiting professor and lecturer, respectively. He has served recently as Chairman of the AIChE's Chemical Engineering Education Projects Committee (1976-77) and the Central Pennsylvania section of the American Chemical Society (1970). His research centers around catalytic kinetics and air pollution meteorology. He is active in industrial consulting, flying, and squash.

- Hougen, O. A., "Engineering Aspects of Solid Catalysts," *Ind. Eng. Chem.* 53, 509-528 (1961).
- Yagi, S., and Kunii, D., "Fluidized-Solids Reactors with Continuous Solids Feed—I. Residence Time of Particles in Fluidized Beds; II. Conversion for Overflow and Carryover Particles; III. Conversion in Experimental Fluidized-Solids Reactors," *Chem. Eng. Sci.* 16, 364-371, 372-379, 380-391 (1961).
- Yoshida, F., Ramaswami, D., and Hougen, O. A., "Temperatures and Partial Pressures at the Surfaces of Catalyst Particles," *AIChE Journal* 8, 5-11 (1962).
- Wakao, N., and Smith, J. M., "Diffusion in Catalyst Pellets," *Chem. Eng. Sci.* 17, 825-834 (1962).
- Wei, J., and Prater, C. D., "The Structure and Analysis of Complex Reaction Systems," *Advances in Catalysis* 13, 203-392 (1962).
- Liu, S-L., Aris, R., and Amundson, N. R., "Stability of Nonadiabatic Packed Bed Reactors," *IEC Fundam.* 2, 12-20 (1963).
- Liu, S-L., and Amundson, N. R., "Stability of Adiabatic Packed-Bed Reactors," *IEC Fundam.* 2, 183-189 (1963).
- Weisz, P. B., and Goodwin, R. B., "Combustion of Carbonaceous Deposits within Porous Catalyst Particles I. Diffusion-Controlled Kinetics," *J. Catal.* 2, 397-404 (1963).
- Levenspiel, O., and Bischoff, K. B., "Patterns of Flow in Chemical Process Vessels," *Advances in Chem. Eng.* 4, 95-198 (1963).
- Johnson, M. F. L., and Stewart, W. E., "Pore Structure and Gaseous Diffusion in Solid Catalysts," *J. Catal.* 4, 248-252 (1965).
- Karplus, M., Porter, R. N., and Sharma, R. D., "Exchange Reactions with Activation Energy," *J. Chem. Phys.* 43, 3259-3287 (1965).

- Weisz, P. B., and Goodwin, R. B., "Combustion of Carbonaceous Deposits within Porous Catalyst Particles II. Intrinsic Burning Rate," *J. Catal.* 6, 227-236 (1966).
- Weisz, P. B., "Combustion of Carbonaceous Deposits within Porous Catalyst Particles III. The CO₂/CO Product Ratio," *J. Catal.* 6, 425-430 (1966).
- Masamune, S., and Smith, J. M., "Performance of Fouled Catalyst Pellets," *AIChE Journal* 12, 384-394 (1966).
- Carberry, J. J., "Yield in Chemical Reactor Engineering," *Ind. Eng. Chem.* 58, 40-53 (1966).
- Thiele, E. W., "The Effect of Grain Size on Catalyst Performance," *Amer. Scientist* 55, 176-184 (1967).
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1970-1975

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*These references were not located.

SELECTION OF PAPERS

THE RESULTS OF THE survey led to a very nice course structure with very little artificial juggling. The papers selected for the course included all multiply mentioned ones except those which overlapped other selected papers. For practical reasons, extremely long papers were omitted. With one exception [Flory, P. J., "The Mechanism of Vinyl Polymerization," *J. Am. Chem. Soc.* 59, 241-253 (1937)] all papers selected came from the list of Table I. Table II presents the selected topics

The students were asked to "Choose a chemical reaction of commercial importance and, utilizing the decision process suggested by Weekman, discuss the type of reactor best suited to study the reaction." Toward the end of the course, commercial reactors were considered.

and source papers in the order in which they were taken up in the course. It can be seen that the selected papers yield a reasonably coherent and comprehensive course according to subject matter. The most obvious omission is in the area of fluidized beds where none of the papers appeared to be quite suitable. Thermodynamics also is not mentioned in Table II, but it does play a role in a number of papers. Comments follow on the individual papers selected and their roles in the course.

Hougen and Watson (1943) was treated first for several reasons. Its emphasis on catalytic kinetics was a good starting point. As a very comprehensive paper, it gave a good introduction to

TABLE II
Course Organization by Subject

TOPIC	REFERENCE
Catalytic Kinetics and Reactors	Hougen and Watson (1943)
Laboratory Reactors	Weekman (1974)
Flow Reactors (esp. CSTR's)	Denbigh (1944)
Residence Time Distribution	Dankwerts (1953)
Mass Transfere with Chemical Reaction	van Krevelen and Hoftijzer (1948)
Polymerization	Flory (1937)
Multiple Steady States and Stability	van Heerden (1958)
Stability and Control	Aris and Amundson (1958)
Pore Diffusion	Thiele (1939)
Effectiveness Factors	Weisz and Hicks (1962)
Heat Transfer in Packed Beds	Singer and Wilhelm (1950)
Coke Formation on Catalysts	Voorhies (1945)
Selectivity and Yield	Carberry (1966)
Commercial Reactors	—
Optimization	Chu and Hougen (1961)

much of what was to follow. Their original derivation of the plug flow reactor mass balance could well have appeared later in the course sequence. Nevertheless, it was desirable for me to present this paper first to set an example for the students and to allow them time to prepare their material (see Class Organization).

Weekman (1974) discussed selection of laboratory reactors. This paper is perhaps not a classic but it served well to introduce the various kinds of reactors. The students were asked to "Choose a chemical reaction of commercial importance and, utilizing the decision process suggested by Weekman, discuss the type of reactor best suited to study the reaction." Toward the end of the course commercial reactors were considered.

Denbigh (1944) is surely a landmark paper in the quantitative treatment of flow reactors. We used it especially in relation to continuous flow stirred tank reactors; however, its treatment of plug flow was compared to Hougen and Watson's. Denbigh also analyzed by-passing effects, selectivity and yield, and temperature programming of reactors. These subjects all arose again in subsequent papers.

Danckwerts' (1953) paper on residence time distribution followed naturally after Denbigh's. An important and unique class of heterogeneous reactions, gas-liquid, was powerfully influenced by van Krevelen and Hoftijzer (1948). To bring in more kinetics and the important subject of polymerization, we selected the 1937 paper by Flory on the mechanism of vinyl polymerization. Van Heerden's work on multiple steady states is so well known that no further comment is required to demonstrate its influence. No one in the class discovered that 35-40 years earlier Liljenroth, F. G., "Starting and Stability Phenomena of Ammonia-Oxidation and Similar Reactions," *Chem. Met. Eng.* 19, 287-293 (1918) had made many of the same points. Aris and Amundson (1958) provided a culmination of the treatment of homogeneous reaction systems with a seminal paper in the area of reactor control.

The most mentioned paper was Thiele (1939) on pore diffusion. This served as a basis for much

TABLE III
Some General Characteristics of
Chemical Reaction Engineering

I. Types of Technical Activity	
A. Determination of Effect of Process Variables on Reactor Performance	
1. Variables	2. Performance
Temperature	Conversion
Pressure	Yield
Composition	3. Analysis
Reactor Type	Input + Process → ?
B. Characterization of Reactions and Reactor Specifications	
1. Synthesis (Design)	
Input + ? → Output	
C. Experimentation and Data Interpretation	
1. Data Interpretation	
?? + Process → Output	
II. Some Related Subject Areas	III. Other Important Aspects
A. Thermodynamics	A. Uniqueness
B. Thermostatics	B. Quality Specifications
C. Stoichiometry	C. Optimization
D. Chemical Kinetics	D. Scale Up
E. Economics	E. Communication
F. Statistics and Distribution	F. Integration

of the work on the ubiquitous effectiveness factor and its ramifications, of which the paper of Weisz and Hicks (1962) is a foremost example. Way ahead of their time were Singer and Wilhelm (1950) on heat transfer in packed beds. This paper was chosen for the course but a sister paper [Bernard, R. A., and Wilhelm, R. H., "Turbulent Diffusion in Fixed Beds of Packed Solids," *Chem. Eng. Progr.* 46, 233-244 (1950)] should be acknowledged. Voorhies (1945) was so successful in correlating coke formation on catalysts that very few papers appeared on this subject for twenty years. You might call its influence adverse.

Carberry's (1966) article induced a good look back over our earlier papers in addressing the important and complex topic of selectivity and yield. This moved the class closer to the consideration of the details of commercial reactors. Finally the paper of Chu and Hougen (1961), though not very influential, served as a comprehensive example of design and intuitive optimization.

In addition to the source material, another uncommon aspect to this course was the designation of each student as a specialist with regard to one of the central papers. The student was responsible for advance study of the assigned article including references to earlier work.

TABLE IV
Quantitative Structure of
Chemical Reaction Engineering

- I. Some preliminary considerations
 - A. Reaction stoichiometry
 - B. Determine thermodynamic feasibility
 - C. Heat effects
 - D. Physical and chemical properties
 - E. Analytical techniques
 - F. Mass balances
 - G. Energy balance
- II. Kinetics
 - A. Reaction mechanism
 - B. Find rate equation
 - C. Effect of temperature and pressure
 - D. Experimentation
 - E. Data handling and error analysis
 - F. Flow ramifications
 - G. Selectivity
- III. Engineering aspects
 - A. Catalyst selection
 - B. Select reactor(s) type (simple or combination)
 - C. Heat and mass transfer in heterogeneous and homogeneous systems
 - D. Effectiveness factors
 - E. Residence time distribution
 - F. Process dynamics
 - G. Optimization
- IV. Other aspects
 - A. Safety
 - B. Pollution control
 - C. Preprocessing and subsequent operations
 - D. Further recommendations
 - E. Admission of inadequacies

For each article there was an introductory lecture of about 15 minutes and assignment of homework. At the next class, the specialist gave his main lecture, discussed the homework, and made new assignments.

CLASS ORGANIZATION

THE EARLY CLASSES were spent organizing the course and discussing the nature of chemical reaction engineering. Two results of these discussions are shown in Tables III and IV. It can be seen that most of these aspects could be expected to come up in the study of the central papers and their literary kin.

In addition to the source material, another uncommon aspect to this course was the designation of each student as a specialist with regard to one of the central papers. The student was responsible for advance study of the assigned article including references to earlier work. In this way he would

The most mentioned paper was Thiele (1939) on pore diffusion. This served as a basis for much of the work on the ubiquitous effectiveness factor and its ramifications . . .

understand the circumstances in which the article appeared. Further by checking the citation index and recent textbooks he could discover the influence of the assigned article on subsequent work. With consultation with the instructor, the specialist prepared lectures and homework assignments for the class.

For each article there was an introductory lecture of about 15 minutes and assignment of homework. At the next class, the specialist gave his main lecture, discussed the homework, and made new assignments. In the following class period about 30 minutes were devoted to wrapping up all aspects of a given topic. The student also reviewed (as did the instructor) the homework, providing constructive criticism. Sometimes the specialist would assign required or optional supplementary reading. In this course structure each student served as a specialist in one area, studied all of the primary source papers and occasional supplements, worked homework assignments, lectured and reviewed homework papers, and took two written exams prepared and graded by the instructor.

One final activity of the specialist was the preparation of a summary of his area with special attention to the documentation of key references. These summaries were reviewed by the instructor, typed, and distributed to the class. To give a more concrete picture of the course; the assignments, exam question, and summary relating to Hougen and Watson (1943) are given as an appendix to this article.

EVALUATION

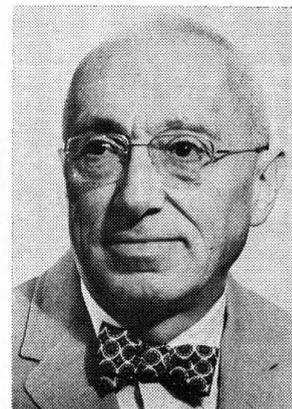
At the end of the term, class members were asked to evaluate the course. Of the twelve respondents, eight were enthusiastic about the course structure (i.e. the use of student specialists), two preferred that the instructor handle it in a conventional manner, and two were neutral. Several students suggested that early in the term (but after the specialty topics have been assigned) instruction should be given in effective teaching.

The students were asked to indicate which two

Continued on page 200

In Memorium

Giuseppe Parravano



Giuseppe Parravano, Professor of Chemical Engineering and of Materials & Metallurgical Engineering at the University of Michigan since 1958, died suddenly April 1, 1978 in his Ann Arbor home. He was born in Florence, Italy, Dec. 17, 1917, received doctorates in both electrical engineering and chemistry from the University of Rome. He held appointments at Milan Polytechnic Institute, Princeton University, University of Rome, Franklin Institute and the University of Notre Dame, before joining the U-M faculty in 1958. He was recognized for his research in the field of catalysis of chemical reactions.

Paul J. Flory, Nobel Prize winner in chemistry, said of Parravano: "His work combines a freshness of viewpoint and breadth of knowledge in the fields of surface catalysis and electrochemistry that is unique. He has introduced important elements of novelty and originality, both in systems investigated and methods applied."

Professor Parravano was pursuing some new theories of catalytic behavior which have application in energy conversion processes and in the design of anti-pollution devices in automobiles.

"With his broad knowledge of several disciplines he was instrumental in initiating and teaching ten courses at the undergraduate and graduate levels," said Prof. Jerome S. Schultz, chairman of the U-M department of chemical engineering.

His high standards of scholarship, creativity, and intensity with which he approached his research attracted students and researchers from all over the world to visit and work in his laboratory. The collaborations have resulted in more than 100 technical publications.

Prof. Parravano's interest was not limited to science as he was intensely concerned with ethical values in present society and served on the Catholic Commission on International and Cultural Affairs.

Always there to help others, his untimely death will be a loss to his many friends in the Ann Arbor community.

He was a Fulbright Scholar at the University of Innsbruck in 1976 and had held visiting appointments at the University of California at Berkeley, Stanford University and the University of Rome. In recent years he had periodically directed a research group on surface catalysis at the Donegani Institute in Novara, Italy.

Prof. Parravano is survived by his wife Ernestina, four sons—Nicola, Carlo, Pietro and Paul—and three grandchildren.

ChE book reviews

THERMODYNAMICS: FUNDAMENTALS, APPLICATIONS

O. Redlich, Elsevier, 1976

Reviewed by Kraemer D. Luks, University of Notre Dame

Redlich's "Thermodynamics: Fundamentals, Applications," on one hand, provides the reader with insights and viewpoints that reflect the author's experience in thermodynamics. These

Continued on page 187

DEPARTMENT OF CHEMICAL AND BIOCHEMICAL ENGINEERING RUTGERS UNIVERSITY THE STATE UNIVERSITY OF NEW JERSEY

Rutgers U. seeks applicants for a tenure-track position of Asst. Prof. effective July 1, 1979. Applicants must have a recent Ph.D. in ChE. Expertise in any of the mainstream areas of classical chemical (not biochemical) engineering fundamentals, including experimental research experience, is most desirable. Send resume, names of at least three references, and statement of research and teaching objectives, to Prof. Burton Davidson, Chrm., Dept. of Chemical and Biochemical Engr., Rutgers U., New Brunswick, N.J. 08903. Rutgers is an equal opportunity/affirmative action employer who encourages applications from minorities and women.

A GRADUATE COURSE IN POLYMER PROCESSING

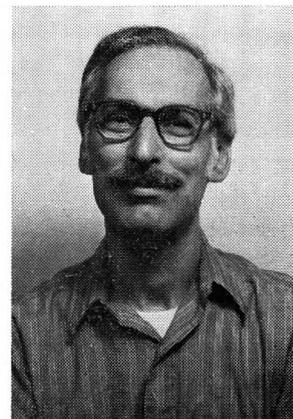
STANLEY MIDDLEMAN
*University of Massachusetts
Amherst, MA 01003*

WHILE THE polymer-related industries hold a most significant position among chemical industries today, and while a large fraction of both B.S. and advanced degree holders in Chemical Engineering today find employment in some area of polymer production or fabrication, a relatively small number of ChE departments provide an opportunity for substantial course and research work in this field. Through its association with the Polymer Science and Engineering (PSE) Department of the University of Massachusetts, graduate students in ChE at U. Mass can elect from a large selection of polymer-related courses which make up the Ph.D. curriculum of the PSE Depart-

TABLE 1
Major Course Offerings of the
Polymer Science and Engineering Department

501	Introduction to Polymer Science
502	Polymer Science Lab
503	Polymer Synthesis Lab
589	Chemistry of Macromolecules
670	Applied Polymer Science
720	Viscoelasticity
721	Polymer Microscopy and Morphology Lab
731	Polymer Properties
733	Polymer Reactions Induced by Stress
734	Degradation and Stability of Polymers
735	Interaction of Radiation with Matter
736	Applied Spectroscopy of Polymers
737	Polymer Reactor Engineering
740	Magnetic Resonance of Polymers
742	Biopolymers
790	Organic Polymerization Reactions
792	Polymer Rheology
793	Polymer Processing
798	Physical Chemistry of High Polymers
799	Physical Chemistry of High Polymers II

ment. Many of these courses cover engineering aspects of the polymer field, and are taught by members of the ChE faculty who hold joint appointments with PSE. This article focuses on one



Stanley Middleman is a Professor of Chemical Engineering at the University of Massachusetts, Amherst, where he holds joint appointments in Chemical Engineering, and in Polymer Science and Engineering. His major research interests are in the areas of fluid dynamics, especially rheology and polymer processing. He is the author of three books: "The Flow of High Polymers," "Transport Phenomena in the Cardiovascular System," and "Fundamentals of Polymer Processing." His baccalaureate and doctoral degrees were both earned at The Johns Hopkins University.

such course: Polymer Processing.

To put the course in the perspective of a broader program, Table 1 shows the total course offerings of the PSE Department. The Polymer Processing course is required of all PSE students, who normally take it in their second year of graduate study. ChE graduate students may elect the course at any time. Indeed, the nature of the course is such that senior ChE majors can and do take Polymer Processing as a technical elective. A typical class "mix" is 20-25 PSE graduate students, 6-10 ChE graduate students, and several

The student must learn that while there can be clearly incorrect models, most engineering processes allow for many levels of modeling which, while not incorrect, do differ in sophistication, ease of application, and detail of correspondence to reality.

Paramount to developing a facility with modeling is examining the correspondence of a model to reality. Thus, the models are compared to industrial or laboratory data to the maximum extent possible.

seniors in the ChE department. In addition, we often have a few (2-4) industrial employed engineers who take the course.

Table 2 shows the major chapter headings of the text used in this course, a book which I wrote myself in response to needs I felt as a teacher for an appropriate text in this area. The book reflects a certain philosophy of education in this field which I have developed from my experiences in teaching, directing research, and consulting in the field of polymer fluid dynamics.

In many ways I regard this course to be one in applied fluid dynamics, with an emphasis on flow processes dominated by viscous effects. As such, it provides a useful follow-up to the usual undergraduate course in fluid dynamics, which offers a broad coverage of fluid flow analysis with, usually, minimal depth of study of problems involving highly viscous and non-newtonian fluids. In addition, the chapter on Heat and Mass Transfer (itself one hundred pages in length) provides an opportunity for reinforcement of the elements of convective transport phenomena usually touched on briefly in an undergraduate course.

Another goal of this course is the development of the student's skill in formulating engineering

models of a process. Much of undergraduate education is occupied with learning to solve problems which have correct solutions. Thus it is clear that the derivative of $\sin x$ is $\cos x$, and there is no room for debate about this. In this Polymer Processing course I try to emphasize the concept of modeling physical phenomena. The student must learn that while there can be clearly incorrect models, most engineering processes allow for many levels of modeling which, while not incorrect, do differ in sophistication, ease of application, and detail of correspondence to reality. The task in this course is to provide sufficient experience, through discussion and problem solving, that the student develops some facility and confidence in formulating a model that is appropriate to the goal at hand. It is very difficult to convince students that in some cases the best model to use is one that is so simple and sloppy that it appears, at first thought, that one might be ridiculed for even entertaining its use.

Another feature of this course arises from the unusual "mix" of student backgrounds that I must deal with. The bulk of the students are in the PSE program, and two-thirds of them are graduates of Chemistry programs. Thus, these students have seen no fluid dynamics, no transport phenomena,

In many ways I regard this course to be one in applied fluid dynamics, with an emphasis on flow pressures dominated by viscous effects. As such, it provides a useful follow-up to the usual undergraduate course in fluid dynamics, which offers a broad coverage of fluid flow analysis with, usually, minimal depth of study of problems involving highly viscous and non-newtonian fluids.

TABLE 2

Contents of "Fundamentals of Polymer Processing," by Stanley Middleman (Published by McGraw-Hill, 1977)

1. Polymer Processing
2. Modeling Philosophy
3. Continuum Mechanics
4. Dimensional Analysis in Design and Interpretation of Experiments
5. Simple Model Flows
6. Extrusion
7. Calendering
8. Coating
9. Fiber Spinning
10. Tubular Film Blowing
11. Injection Molding
12. Mixing
13. Heat and Mass Transfer
14. Elastic Phenomena
15. Stability of Flows

in many cases no mechanics at all. They have had a science education, they believe in science, and for them the concept of crude, approximate, models is often an alien, disturbing, and offensive concept. Thus, the course begins with discussion of the philosophy of modeling and then turns to development of the principles of mechanics as applied to the dynamics of viscous flow. A brief discussion of rheology is included here, since some of the students will not have done the full semester course we offer in that area.

Following this introduction of fundamental concepts and tools, we turn to examining models for a wide range of idealized flow situations and then spend the bulk of the semester on applying

these models to a variety of polymer flow processes. Paramount to developing a facility with modeling is examining the correspondence of a model to reality. Thus, the models are compared to industrial or laboratory data to the maximum extent possible. Below is a typical example from Chapter 13 of the text, in which several models are examined in the light of existing experimental data. The assumptions inherent in the models are reviewed, and then models which relax these assumptions are developed.

Example: Comparison of measured and predicted Nusselt numbers—Griskey and Wiehe present data for heat transfer to molten polyethylene pumped through a 3/8-in heated pipe. They present the data in terms of an “arithmetic average Nusselt number,” shown plotted in Figure 1. Compare the data with theory.

We begin by constructing the theoretical curve in terms of the average Nusselt number Nu_a . For very small values of $U\pi R^2/\alpha_T L = wC_p/kL$ the Leveque solution holds, and since the extent of heat transfer is not great, we expect that $Nu_a = \overline{Nu}$. If the Leveque equation is used for the local Nusselt number, and if integration is carried out to obtain the average, the result is found to be

$$Nu_a = \overline{Nu} = 1.61 \left(\frac{3n + 1}{4n} \right)^{1/3} \left(\frac{4UR^2}{\alpha_T L} \right)^{1/3} \quad (1)$$

$$= 1.75 \left(\frac{3n + 1}{4n} \right)^{1/3} \left(\frac{wC_p}{kL} \right)^{1/3}$$

It is much more tedious to carry out the same procedure using the Graetz infinite series solution, and instead we examine the limiting behavior at the extreme where the fluid is almost completely heated to the wall temperature. Under those conditions we find

$$q = -wC_p(\langle T \rangle - T_o) = -wC_p(T_w - T_o)$$

and, it follows that

$$Nu_a = \frac{2wC_p}{\pi kL} \quad (2)$$

Figure 1 shows this asymptotic relation, as well as the Leveque limit [Eq. 1] for $n = 0.7$ (the value noted by Griskey and Wiehe). It is not very difficult to interpolate a smooth curve between the two asymptotic limits.

The data of this example are seen to be in reasonably good agreement with the theory. Other sets of experimental data, obtained with polymer solutions, also bear out the general validity of the models presented above. We must recall,

A second goal, and an important one, is development of a coherent set of principles of transport phenomena (fluid dynamics, heat and mass transfer) as applied to the design and analysis of highly viscous, often non-newtonian, systems.

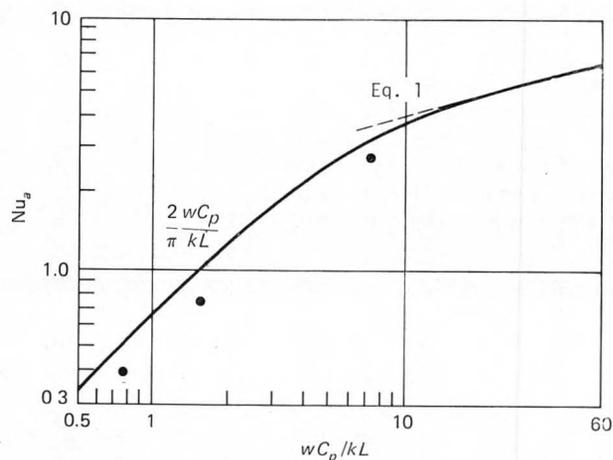


FIGURE 1. Data of Griskey and Weihe compared to theory (Eq. 1, using $n = 0.7$).*

however, that the models are subject to certain assumptions which are not always met. In particular we have assumed:

1. The viscosity is independent of temperature.
2. The pipe wall is isothermal.
3. No viscous heat generation occurs.*

The example continues with an examination of several additional models.

At present there is no laboratory experience associated with this course. However, we are presently building a Polymer Process Fundamentals Laboratory, and expect to integrate this facility into the graduate teaching program.

In summary, then, while this course is nominally one in the area of polymer transport phenomena, it serves several more general roles as well. Of greatest importance, I think, is the development of the capacity to examine a process, think about it in simple physical terms, and then produce a mathematical model of the process that represents the best compromise between simplicity of solution and application, on the one hand, and correspondence to reality, on the other. A second goal, and an important one, is development of a coherent set of principles of transport phenomena (fluid dynamics, heat and mass transfer) as applied to the design and analysis of highly viscous, often non-newtonian, systems. Finally, of course, the major polymer processes are discussed and illustrated, thereby providing an introduction to an area of engineering practice that is already of major importance, and that continues to grow. □

*Reproduced by permission from Middleman, S., “Fundamentals of Polymer Processing”, McGraw-Hill—1977.



Individuals are alike. Aren't they?

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REACTOR DESIGN

FROM A STABILITY VIEWPOINT

D. D. PERLMUTTER
University of Pennsylvania
Philadelphia, PA 19104

IT MIGHT, IN ALL fairness, be asked what it is in the subject of Chemical Reactor Design that provides the central themes. On what basis, for example, does one decide to include one topic and exclude another? Are the subjects of mixing and residence time distributions pertinent and important? They are in essence physical effects rather than chemical, and could as well be presented in a context of transport processes. If utilitarian needs are to provide the distinctions, one might move to include selective material on multiphase reactions, but such models are rather complicated and still distant from practical use. The decisions are often a reflection of the textbook and expertise that happen to be available. Under the circumstances, with a vast range of topics to choose from, the dependence on an available expert may in fact be a fine basis for choice, even if



Daniel D. Perlmutter is Professor of ChE at the University of Pennsylvania since 1967. He served as Department Chairman from 1972 to 1977 and as Chairman of the Graduate Group in ChE from 1969 to 1972. Before that he was on the faculty at the University of Illinois, and a visitor at Harvard, at the University of Manchester (England) and at the University of Zagreb (Yugoslavia). He was twice a Fulbright Fellow (1968, 1972) and received a Guggenheim award in 1964. He has authored two textbooks and over 50 journal articles.

a bit arbitrary in nature.

One might focus on the same question from another viewpoint. Should one not expect growth and development from the subject matter in a course? If the material of later weeks is interchangeable in sequence with that of the early weeks in the series and does not build upon it as a requisite, if there is no unifying theme, then is there a legitimate basis for claiming that the series of lectures form a single course? A similar point could be made in categorizing a textbook (or for that matter, any book). It is often an excellent idea to publish an anthology or a collection of short stories, but no one would call such a book a novel.

The graduate reactor design course at the University of Pennsylvania uses stability as a central theme around which to organize a wide range of reactor concerns. This approach brings together the subject matter of catalyst particles with that on well-stirred vessels and tubular reactor geometry. It emphasized the similarities among the diverse models rather than their differences. It does, however, make distinctions between lumped and distributed models, between algebraic and differential equation models, and among the assumptions that are commonly made in arriving at numerical solutions from each starting point. The course is built around the author's textbook called "Stability of Chemical Reactors" (Prentice-Hall, 1972).

Of the term stability, Richard Bellman has said that it has an unstable definition. In the ChE literature, for example, it has been used to mean steady state multiplicity, as well as parametric sensitivity. Even in its closer-to-mathematical sense, the term has been used to refer to local behavior (in the "neighborhood") about a steady state, and to trajectory motion in a large region of state space. The clarification of such ambiguity is an early objective of this course. It is handled by means of a variety of examples that illustrate the need for rigorous definitions. A detailed course outline is presented as Table 1.

The graduate reactor design course . . . uses stability as a central theme around which to organize a wide range of reactor concerns. This approach brings together the subject matter of catalyst particles with that on well-stirred vessels and tubular reactor geometry. . . . It does, however, make distinctions between lumped and distributed models, between algebraic and differential equation models, and among the assumptions that are commonly made in arriving at numerical solutions from each starting point.

TABLE 1
Chemical Reactor Design
Course Outline

- I. INTRODUCTION
 - A. What is reactor design: objectives and justification
 - B. Stability approach as a unifying theme
- II. REVIEW OF BASICS
 - A. Nomenclature, CSTR equations, special cases
 - B. Volume and density changes
 - C. Unsteady state behavior
 - D. Batch reactor quadratures
 - E. Kinetics review: mechanisms and rate equations
- III. MULTIPLICITY AND STABILITY
 - A. Various definitions of stability
 - B. Uniqueness in an isothermal CSTR
 - C. Local stability criteria
 - D. Two-equation models
 - E. Is uniqueness good? Design questions.
 - F. Temperature variation
 - G. Techniques for simultaneous equations
- IV. PHASE-PLANE ANALYSIS OF THE CSTR
 - A. Trajectories, isoclines, eigenvectors
 - B. Feedback control
 - C. Regions of stability
 - D. Liapunov stability
 - E. Gerschgorin's theorem
 - F. Practical stability
 - G. Tracking function graphical technique
- V. TUBULAR REACTORS
 - A. Plug flow model, isothermal
 - B. Volume comparisons to CSTR
 - C. Simultaneous and sequential reaction
 - D. Staged reaction and cold-shot cooling
 - E. Maintenance and cooling considerations
 - F. Parametric sensitivity: Barkelew's correlation
 - G. Steady state operating curves
 - H. Adiabatic reactors
 - I. Harriot's and Wilson's Rules for cooling capacity
 - J. Effect on recycle on PFTR: multiplicity and stability criteria
- VI. DISPERSION EFFECTS
 - A. Characterization of dispersion in a tube
 - B. Danckwartz boundary conditions
 - C. Special cases of axial or radial dispersion
- VII. CATALYST PARTICLES
 - A. Effectiveness factors
 - B. Experimental tests
 - C. Multiple profiles and stability
 - D. Collocation technique

LUMPED MODELS

A STRAIGHTFORWARD ANALYSIS of the isothermal CSTR provides a vehicle for the development of new ideas in the context of an already familiar model. It is a surprise to some students to learn that multiple steady states can arise at all in an isothermal system. They explore this idea as an outgrowth of kinetic forms and carry the arguments to apply to free radical initiations and to chemostat biochemical models. The subject matter turns to temperature dependent energy considerations, but by this time the students have already handled the essential concepts arising from multiplicity. They learn to draw van Heerden diagrams and ignition and extinction hysteresis loops as particular cases of phenomena previously encountered in the isothermal systems.

In an analogous way, the techniques of linearization and eigenvalue analysis are introduced together with the simplest one-equation models. Local stability and regions of stability are first demonstrated for single-variable equations; they are then developed for multidimensional models,

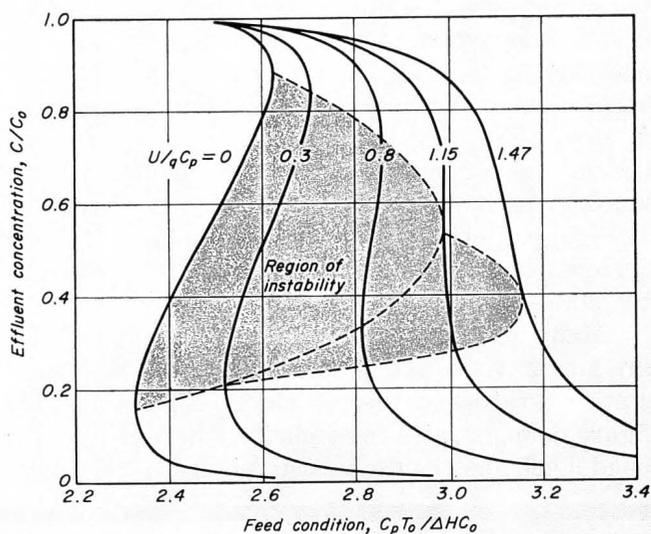


FIGURE 1. Steady-state operating curves for the temperature-dependent CSTR with region of instability.

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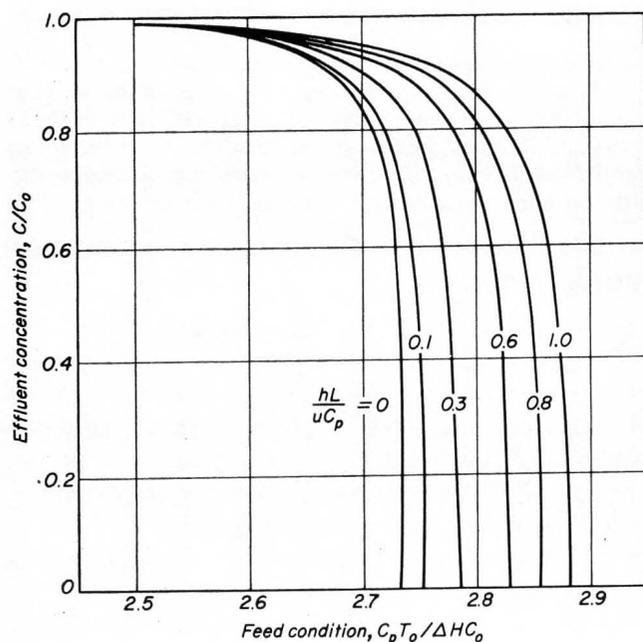


FIGURE 2. Steady-State operating curves for the PFTR.

Reprinted by permission from Daniel D. Perlmutter, "Stability of Chemical Reactors", Prentice-Hall, Inc., 1972.

some including thermal effects, some with feedback control loops. This leads naturally into a review of linear algebra and phase-plane analysis. The results are used to consider trajectories during start-up, physical interpretation and eigenvectors, and direct methods for establishing stability.

Some time is devoted to Liapunov analysis in part because of its applicability to nonlinear systems, but also because it provides an excellent point of departure for questions of practicality in engineering as well as numerical analysis. This subject leads one to question the fundamental objectives of reactor design: Is multiplicity good or bad in design? Should the designer prefer a large stability region or a small one? What is a practical stability criterion? When is a Liapunov-unstable system acceptable for practical use, and when is the stable system unacceptable?

Many of the numerical results of the CSTR are summarized and presented as a set of steady state operating curves, such as Figure 1. This figure demonstrates multiplicity where the curves bend back on themselves, it shows a relatively

large region in the parameter space where steady states are unstable, and it includes a range of parameter values for which a single, but unstable steady state is found (a limit cycle).

DISTRIBUTED MODELS

THE POINT OF DEPARTURE for the realm of distributed models is the observation that a plug-flow (PFTR) geometry can produce steady state profiles with great parametric sensitivity, but it does not exhibit any multiplicity or instability for a given choice of design parameters. This argument is developed in considerable detail by discussion of the well-known work of Barkelew, Harriot, and Amundson. It is shown pictorially by Figure 2, where the lack of any sigmoid-shaped curves corresponds to a lack of multiple intersections for a given feed condition.

A second major milestone in this part of the course is the connection with feedback by recycle. The technique is based on the simultaneous solution of a recycle equation of the form:

$$C_o = (1-f) C_F + f C_E \quad (1)$$

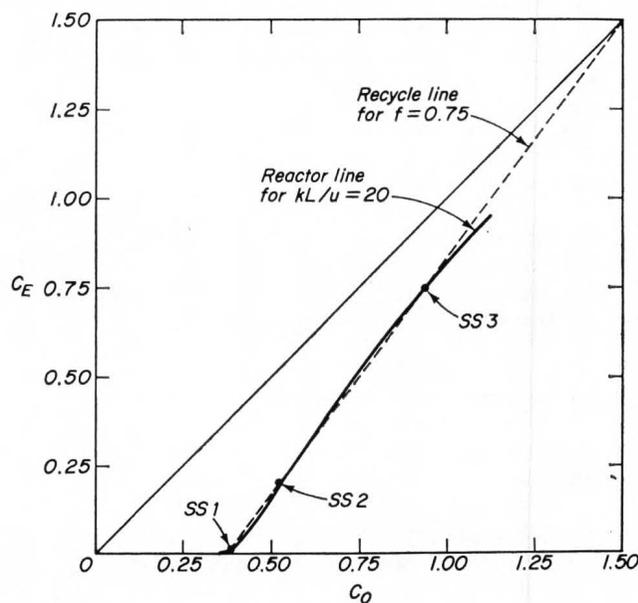


FIGURE 3. Multiple steady states for an isothermal PFTR-recycle system.

Reprinted by permission from Daniel D. Perlmutter, "Stability of Chemical Reactors", Prentice-Hall, Inc., 1972.

Of the term stability, Richard Bellman has said that it has an unstable definition. In the ChE literature, for example, it has been used to mean steady state multiplicity, as well as parametric sensitivity. Even in its closer-to-mathematical sense, the term has been used to refer to local behavior (in the "neighborhood") about a steady state, and to trajectory motion in a large region of state space.

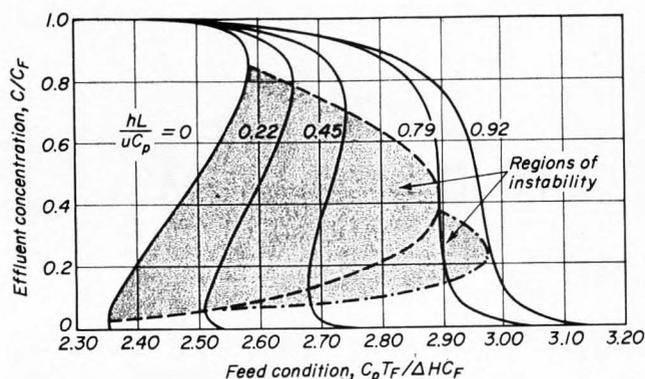


FIGURE 4. Steady-state operating curves for PFTR-recycle system with $f = 0.5$ (Reilly and Schmitz, 1966).

Reprinted by permission from Daniel D. Perlmutter, "Stability of Chemical Reactors", Prentice-Hall, Inc., 1972, with the PFTR isothermal mass conservation statement.

$$\frac{L}{u} = \int_{C_0}^{C_E} \frac{dC}{R} \quad (2)$$

When the latter equation is integrated to produce an algebraic relation, the simultaneous solution is most readily obtained from intersection points on a C_E vs C_0 graph.

An illustration is given in Figure 3, obtained by postulating a rate equation of the form

$$R = \frac{kC}{(1 + KC)^2} \quad (3)$$

and choosing selected values of f , K , C_F , and the group (kL/u) . The solution shows three steady

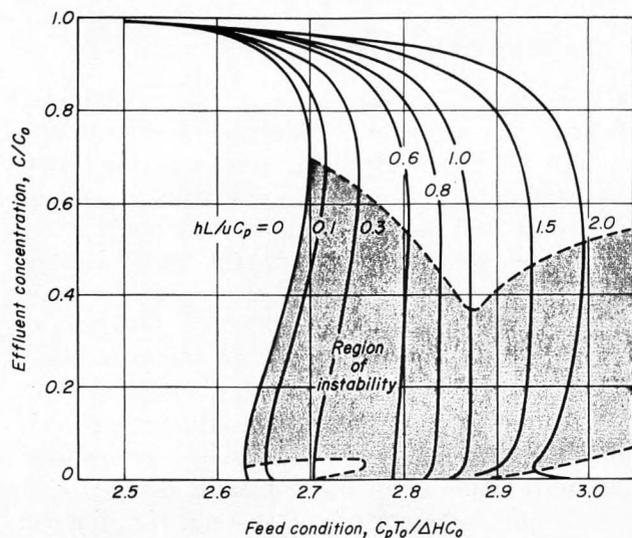


FIGURE 5. Steady-state operating curves for the TRAM [$\alpha = D$, $(uL/D = 10)$] showing a region of instability.

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state solutions (profiles in the PFTR) and very marked sensitivity to the choice of recycle rate. From a presentation of results such as Figure 3, it becomes apparent that multiplicity in these systems must be associated with recycle (or mixing), since even the isothermal PFTR reactor can show multiple steady state profiles when some of the product is appropriately recycled.

When this problem is extended to include adiabatic and then temperature-dependent changes, the recycle behavior can be described in terms of sets of finite-difference equations. The similarity to ordinary differential equations is noted as is also the major point of difference in terms of eigenvalue criteria. The results of a numerical

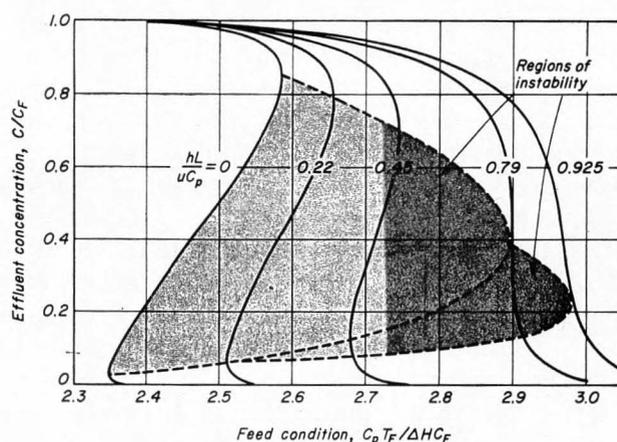


FIGURE 6. Steady-state operating curves for TRAM-recycle system with $f = 0.5$, $uL/D = uL/\alpha = 100$.

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study by Reilly and Schmitz are presented to illustrate the essential features of this system (see Figure 4).

The consideration of tubular reactor geometry takes a more ambitious direction as dispersion effects are introduced in terms of a Peclet number and second derivative term. The need is established for new boundary conditions, and it is demonstrated that this mode of backmixing can also lead to multiplicity and instability of solutions. From this perspective the catalyst particle problem is viewed as merely a special case for which no macroscopic flow term exists.

When it is appropriate to call for numerical solutions to the distributed parameter models, they serve as a natural bridge to a presentation of the methods of weighted residuals. In particular, both

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A Course in

THE DYNAMICS OF HYDROCOLLOIDAL SYSTEMS

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THE TECHNOLOGICAL importance of the study of colloidal dispersions and macromolecular solutions needs no special emphasis, as even a casual glance at the flow charts and process diagrams of numerous chemical, biochemical and food processing operations will demonstrate. Aside from their industrial importance, hydrocolloidal suspensions (of even the simplest structure) can serve as sufficiently reasonable models of rheologically complex fluids and deserve careful scrutiny. Given this, one would readily agree to the addition of a course in this general area to the ChE curriculum. But what should it address? The topics are numerous, their nuances different, and the difficulties staggering; yet, one can easily identify a few general areas that certainly deserve a place in such a course, viz, the transport properties of the suspensions, which include the thermal and rheological behavior, the physicochemical properties, which include the stability and associated problems, and certainly, processes where sols and macromolecular solutions display unique behavior, as for instance in membrane phenomena.

But the question of emphasis still remains. ChE students rarely have the opportunity or the encouragement to pursue a structured program in this area, which has appropriately been called "the world of neglected dimensions". Without doubt, a general treatment of even one of the above topics is perhaps too specialized and probably even too broad to form the subject of an undergraduate course, but an expository introduction to colloidal interactions certainly belongs in an undergraduate program in ChE. However, at the graduate level the emphasis and contents rest on one's philosophy and needs. If problems of immediate industrial relevance dictate the emphasis, a practical concoction along the lines of Soo's monograph [7] will be probably satisfying in a certain sense, but if one allows that a prime duty



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of a strong graduate program is to foster a taste for fundamental analyses, a rethinking seems to be in order.

SCOPE AND OBJECTIVE

THIS SOMEWHAT LENGTHY preamble is meant to provide a glimpse of the line of thought that led to the course described here. Designated as a "special topics" course and addressed to advanced graduate students (preferably, second year and beyond), the course is based on the premise that a sound base in the mechanics and electrokinetics of the dispersed phase is essential for an understanding of the macroscopically apparent behavior of such disperse systems. In handling or processing colloidal or macromolecular systems, one observes, through appropriate instrumentation or by other means, primarily the macroscopic behavior of the system, viz., the concentration gradients, velocity gradients, stress, and the like. These are observed on a scale over which changes in these variables are resolvable, spatially or temporally. This macrostructure, how-

ever, emerges from microscopic interactions among the particles or macromolecules, at a scale over which macroscopic properties such as concentration have no meaning. The deductive theories of such phenomena proceed on the premise that one can, in principle, start with the description of the system at the microscale and build a general theory step by step through the application of well-established physical and chemical principles. The philosophical basis of this approach is of course hardly new, although this route is seldom emphasized in engineering curricula despite the fact that in many cases it is the only means of obtaining correct (qualitative, if not quantitative) description at the macroscale. The objective of the course, then, is to expose the student to the microstructure of the dispersion*, its electrokinetics, dynamics at the microscale and how these combine to project the general features that manifest at the macroscale.

What follows is a description of a course under development along these lines at the Rensselaer Polytechnic Institute, approximately in the form in which it was presented last year.

STRUCTURE AND CONTENTS

A BRIEF ORGANIZATIONAL structure of the course and a fairly detailed list of contents follow in Figure 1 and Table 1, respectively.

Introduction

The course begins with a brief outline of the underlying philosophy and clear definitions of the relevant length scales and time scales, since subsequent developments depend critically on these concepts. A few simple, but representative, examples can be presented to provide an intuitive appreciation for these concepts and to motivate more rigorous materials that will follow subsequently. These could be the dumbbell models of polymeric liquids, adsorption/desorption phenomena at interfaces or membrane phenomena, but sufficient care is needed in this outline and it pays to break down these examples according

*Contrary to normal convention I have used the terms 'dispersion' and 'colloid' in a loose sense, permitting them to denote not only what they usually stand for but also solutions of macromolecules.

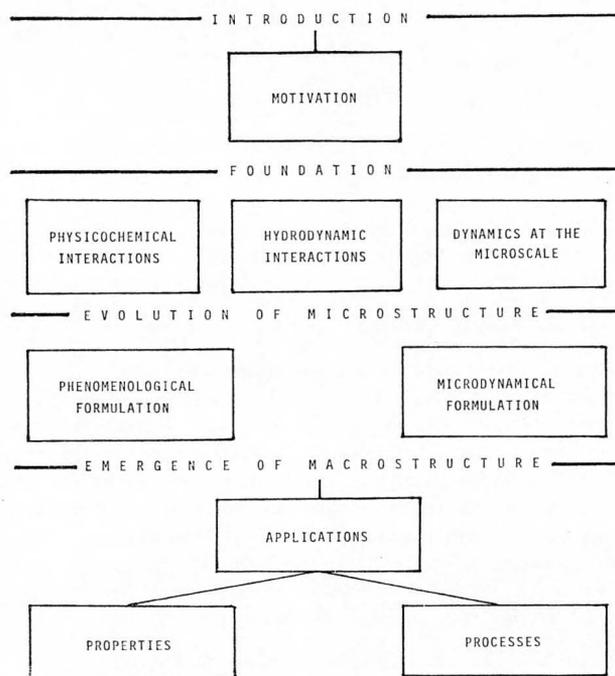


FIGURE 1. Course Structure

to the structural format and details presented in Figure 1 and identify the individual segments and their logical interaction. Pedagogically, this overview forms a crucial introduction to a course that rests essentially on an axiomatic base, a relatively unfamiliar territory for most engineering students.

Foundation

The above bird's-eye view of what is ahead prepares the students for appreciating the lengthy introductions to the background materials on physicochemical and hydrodynamic interactions and stochastic dynamic systems that follow. Despite the fact that usually few students have had any prior exposure to electrokinetic phenomena and related subjects, these and the hydrodynamics present little problem as the physical and mathematical concepts relevant here are fundamental to the general structure of chemical engineering programs currently in vogue. On the other hand, the background material on random processes and the attendant mathematical operations require some care. While the information gained in previous sections (such as electrokinetic interaction potentials and hydrodynamic

... the course is based on the premise that a sound base in the mechanics and electrokinetics of the dispersed phase is essential for an understanding of the macroscopically apparent behavior of such disperse systems. In handling or processing colloidal or macromolecular systems, one observes, through appropriate instrumentation or by other means, primarily the macroscopic behavior of the system, viz., the concentration gradients, velocity gradients, stress, and the like

TABLE 1
Contents

PART 1. INTRODUCTION

Section 1. The World of Neglected Dimensions

Definitions and examples of colloidal and macromolecular dispersions;

Definition of length scales and time scales;

Definitions of the terminology and brief overview of course structure.

PART II. FOUNDATION

Section 2. Physicochemical Interactions

London-van der Waals Forces Between Disperse Particles: Forces between atoms and molecules; Forces between macroscopic particles; London-Hamaker theory; Effect of suspending medium on the dispersion energy; Effect of a homogeneous adsorption layer on the dispersion energy; Effect of electromagnetic retardation; Measurement of the London-van der Waals force and the Hamaker constant; Lipshitz theory and microscopic theory for Hamaker constants; Tables of Hamaker constants.

Electrostatic Forces Between Disperse Particles:

Origin and nature of surface charges; Electrical double layer and its historical development; Capacitor model of the double layer; Debye-Huckel approximation; Gouy-Chapman theory; Corrections for specific adsorption—the Stern theory; Overlapping double layers and interparticle repulsion; Deryaguin-Landau-Verwey-Overbeek theory—for sphere-plane systems and for spherical particles.

Electrophoresis and Other Electrokinetic Phenomena:

Electrophoresis, electro-osmosis, streaming potential; Experimental aspects and applications.

Section 3. Hydrodynamic Interactions

Basic Equations for Creeping Flow and Some General Solutions:

Axisymmetric flow; Stream function; Properties of stream functions; Boundary conditions satisfied by the stream function; Flow past spheres, cylinders, oblate spheroids, prolate spheroids, circular disks, and elongated rods.

Motion of a Rigid Particle in an Unbounded Liquid:

Translation; Rotation; Combined translation and rotation; Resistance to motion; Forces and torques; Settling of spherically isotropic and orthotropic bodies.

Interaction Between Particles:

Between spheres falling along their line of centers; Multiple spheres; Spheroids.

Motion of Single Particles in Confined Regions:

Sphere moving in a cylinder; Sphere moving in the presence of a planar wall; Spheroid in a cylinder and in the presence of a plane wall; Unsteady motion of a sphere near a plane wall.

Particle Clusters:

Flow relative to dilute systems—with and without first order interaction; Viscosity of such systems; Concentrated suspensions; Packed beds and porous media models.

Section 4. Dynamic at the Microscale

Physical Nature of Motion at the Microscale:

Introduction to origin and nature of random fluctuations and the tools necessary for examining them.

Fundamentals of Probability Theory:

Events, random variables, density functions, distribution functions; Integrating theory, expectation, convergence concepts; Products of probability spaces, independence, limit theorems; Conditional expectations and conditional probabilities; Random processes.

Fundamentals of Stochastic Processes:

Markov processes; Transition probabilities, the Chapman-Kolmogorov equation; White noise, Wiener process, derivatives and transformations of stochastic processes; Diffusion processes, Kolmogorov backward and forward equations.

Stochastic Differential and Integral Systems:

Stochastic differentials and integrals; Convergence; Ito differential and integral; Solutions as Markov processes and as diffusion processes.

Conceptual Difficulties in Stochastic Modeling and Approximation:

Convergence of a non-Markovian noise to a Markov process; Stratonovich integral and differential, their relation to the Ito systems; Wong-Zakai processes.

PART III. EVOLUTION OF MICROSTRUCTURE

Section 5. Phenomenological or Direct Continuum Formulation

Evolution of Probability Distribution for unsteady-state one-dimensional case:

Einstein's derivation; Mobility; Thermodynamic force; Smoluchowski's extension.

General Treatment and Liouville Equation:

Introduction to μ -space and Γ -space; Hamiltonian; Ensembles; Derivation of Liouville equation; Poisson bracket.

Section 6. Microdynamical Formulation

One-Dimensional Linear Processes:

One-dimensional Langevin equation and its solution; Definitions of drift and diffusion coefficients; Ensemble averages and transformation to Fokker-Planck equation; Generalization by Uhlenbeck and Ornstein; Definition of time scales; Brownian motion with inertia; Phase-space Fokker-Planck Equation.

General Non-Linear Processes:

Non-linear white-noise-driven processes; Ito differential systems; Ito and Stratonovich calculus; Transformation to Fokker-Planck-Kolmogorov equation; Drift coefficients and diffusion coefficients; Extension to Phase-space Fokker-Planck-Kolmogorov equation; Relation to Liouville Equation.

PART IV. EMERGENCE OF MACROSTRUCTURE

Section 7. Applications

Definition and Examples of Macrostructure.

Specific Applications:

Stability of colloidal systems; derivation of rate constants; general population balances; Concentration-dependent diffusion coefficient; possible models; Models of Polymeric

Liquids; Ultrafiltration and Membrane Phenomena; Chromatographic Separations; Adsorption/Desorption in Colloidal Systems; Surface Diffusion.

drags and torques) is required primarily for setting up the equations of motion, the procedures presented in Section 4 are needed for both formulation and analysis of the equations. Consequently, simple examples (such as random walk problems or simpler versions of Langevin equations) from the general treatment that will follow in Part III are often helpful and serve to maintain the continuity of the subject matter.

Graduate education extends far beyond the confines of the classroom, and that is particularly true in a course of this type. Firstly, there are no standard textbooks although a substantial portion of the material can be found in related books, monographs, and technical articles.

Microstructure

Having established the required fundamentals, one is now ready to develop the framework for describing the evolution of microstructure, viz., temporal changes in the distributions of the configurations and momenta of the particles. Two approaches are possible, each with its own advantages and disadvantages, but both are necessary. The first of these, which I shall call "the phenomenological formulation" (over the objections of MacDonald [4])* , relies on certain assumptions regarding the form of the constitutive equations, such as the Fickian form of the diffusive flux, and leads to the traditional derivation of the Liouville equation of statistical mechanics. This is introduced first despite its weaknesses, since this development is merely a generalization of the familiar "continuity" and "diffusion" equations. Moreover, when the more appropriate dynamical systems are introduced later and resources for in-depth analyses are at hand one can go back and resolve the questions regarding the accuracy of the assumed forms of constitutive equations and demonstrate the distinct advantage of the latter formulation. Einstein's [2] or Smoluchowski's [6] derivation of the familiar diffusion equation (along with the associated concept of "thermodynamic force") serves as a good starting point here before the more general phase-space Liouville equation is introduced.

The second of the two approaches, which I shall call "the microdynamical formulation", is the more funda-

*Phenomenological in the sense that the formulation rests on perceived rules, whether such perception answers to reality or not. MacDonald prefers phenomenal, whose other (and more common) usage, in the sense of remarkable, extraordinary, or prodigious, 'is a sin against the English language', according to Fowler (3), although as he reluctantly concedes 'the consequences seem to be irremediable'!

mental of the two and is based on a generalized Langevin equation for the macromolecular motions. Since the previous section began with the simpler diffusion equation, it is probably advisable to start this section with its microdynamical analogue due to Langevin and Uhlenbeck and Ornstein [8]. Aside from providing a logical transition, this choice is particularly helpful in defining the relevant time scales. One can now proceed to show the difficulties associated with the formulation of the constitutive equation for the diffusion of probability using the one-dimensional Stratonovich equation (see Rajagopalan [6]). These also show, through simple and familiar examples, how the exact forms of drift and diffusion coefficients follow in a straightforward manner from the underlying equations of motion. The generalization of the above results to the phase-space formulation of the Fokker-Planck-Kolmogorov equation now follows simply, and its relation to the Liouville equation is evident.

Macrostructure

The final part, on the structure resolvable at the usual temporal and spatial scales, forms the heart of the course. General and specific examples are discussed here, and the students are encouraged to do further work on some specific problems. For convenience, I have divided the applications discussed here into two rough categories, under properties and processes. The applications concerned with deriving macroscopically observed properties of the system through an examination of the microstructural details are grouped under "properties". These may include the colloidal stability problems, where the macroscopically observed kinetics and the required kinetic rate expressions for population balances depend on microdynamical formulations, or problems concerned with the derivation of the constitutive relations for transport processes in dispersions and macromolecular solutions. The latter group of applications includes the important class of bulk rheological phenomena—a source of many good problems and examples [1]. The second group of applications, under "processes", forms a somewhat artificial classification and is motivated by pedagogical reasons. The primary goal here is to emphasize those examples where the behavior of the sols or solutions in the presence of some extraneous "objects" is of interest. For instance, these may include ultrafiltration or membrane phenomena, adsorption/desorption problems,

The objective of the course, then, is to expose the student to the microstructure of the dispersion, its electrokinetics, dynamics at the microscale and how these combine to project the general features that manifest at the microscale.

some of the newer chromatographic separations, or surface rheological problems. The difference between the former group of applications (properties) and the latter is that in the former one is essentially interested in phenomena intrinsic to the liquid (e.g., suspension rheology), whereas

in the latter the behavior is dependent on the nature of the extraneous object or is induced by it (e.g., diffusion through a membrane).

OTHER REMARKS

GRADUATE EDUCATION EXTENDS far beyond the confines of the classroom, and that is particularly true in a course of this type. Firstly, there are no standard textbooks although a substantial portion of the material can be found in related books, monographs, and technical articles. (A list of some useful references can be obtained from me.) In addition, considerable amount of independent work and self-study is essential to keep abreast of the lecture material, and this can be encouraged through appropriate exercises and term-paper assignments (usually critiques of recent technical articles)—a not-uncommon practice in graduate-level courses. A few prerequisites, such as first-level courses in real analysis and probability theory, are desirable especially since a student unfamiliar with the mathematical notions and terminology is usually overwhelmed by the analytical techniques. Needless to say, while techniques should be available at command, they should never take precedence over the concepts.

REACTOR DESIGN: Perlmutter

Continued from page 171

Galerkin's method and collocation techniques are introduced as a means of reducing partial differential equations to sets of simultaneous ordinary differential equations. The latter lead smoothly to the earlier lumped stability techniques, and make available the wide range of prior methods in the treatment of distributed systems.

It is pointed out that this approach can also be used to compute complete numerical solutions to the same equations, if they are needed in addition to the stability finding.

Yet another demonstration of the use of stability analysis as a unifying theme may be found in Figure 5, where results are presented for a tubular reactor with axial dispersion (TRAM). Here again, one can detect regions of multiplicity and instability introduced by the backmixing effect. If the specific parameter values are chosen differently, this pattern of behavior can be modified to approach either the CSTR or PFTR results as the dispersive effect grows or diminishes with respect to the other parameters. When a recycle stream is added to the TRAM system, it serves to reinforce

Finally, it is not the intention of the course to create, in the words of Bertrand Russell, an ordered cosmos where pure thought can dwell remote from human passions and remote from the pitiful facts of nature. The intention certainly is not the latter, and in fact I feel that the "pitiful facts of nature" demand approaches of this type. And, more importantly, a prime objective of the course is to emphasize not the special nature of the subject matter but the synthesis of a set of diversified, yet structurally similar, classes of problems and the need and the benefits of such a synthesis.

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the backmixing that arises from the action of dispersive flow, and the overall effect shows a great resemblance to the CSTR result. Such operating curves are presented in Figure 6 for a typical set of parameters. □

NOMENCLATURE

C	= reactant concentration
C _o	= reactant concentration in reactor feed
C _E	= reactant concentration in reactor effluent
C _F	= reactant concentration in make-up feed
C _p	= heat capacity
D	= dispersion coefficient
f	= fraction recycled
h	= heat transfer coefficient for PFTR
ΔH	= heat of reaction
k	= kinetic rate constant
K	= kinetic rate constant
L	= reactor length
q	= volumetric flow rate
R	= reaction rate
T _F	= temperature of make-up feed
T _o	= temperature of reactor feed
u	= linear flow rate
U	= overall heat transfer coefficient for CSTR
α	= thermal dispersion coefficient

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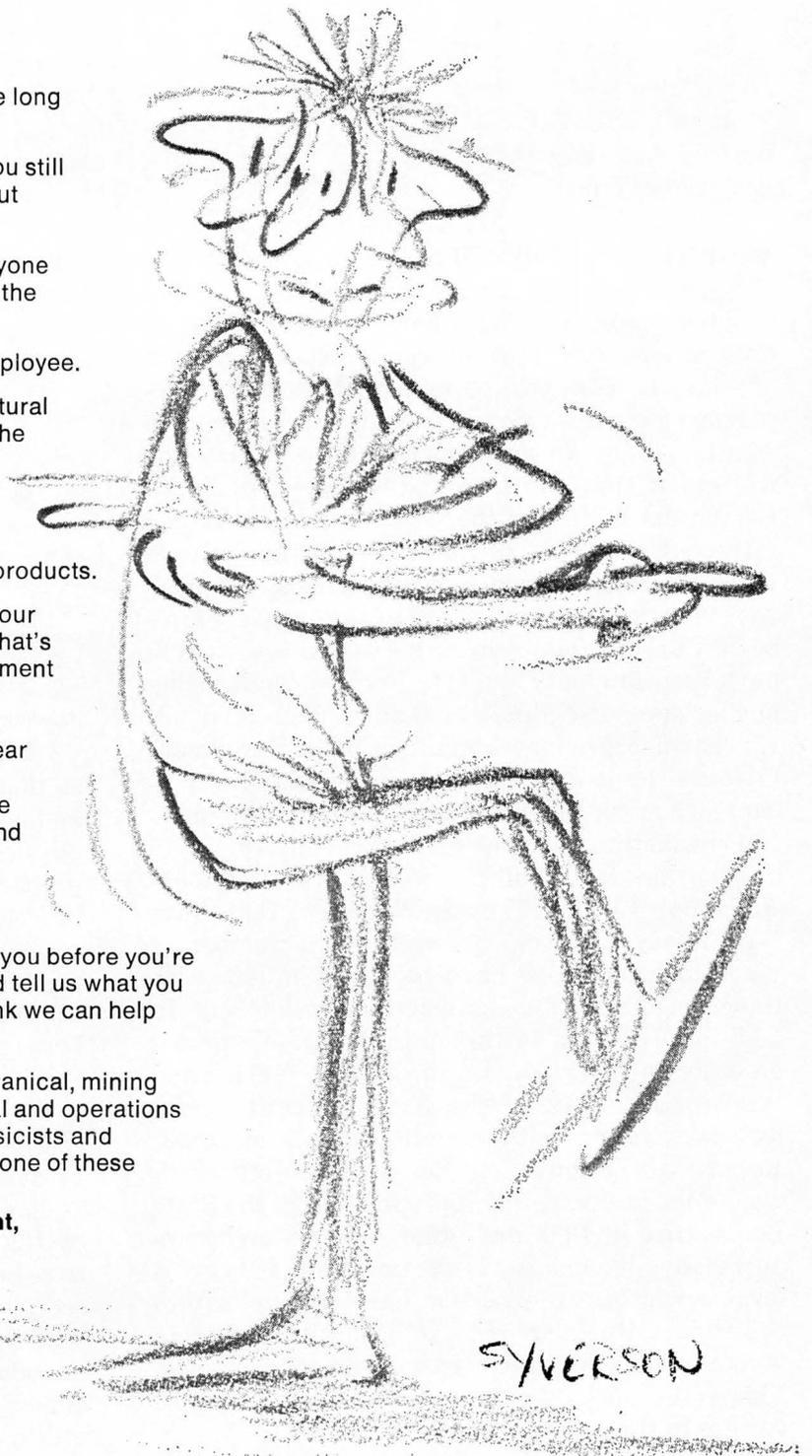
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FALL 1978

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A Course in

COAL SCIENCE AND TECHNOLOGY

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WITH AN INCREASING public awareness of the important role coal will play in our future, it is not surprising that a new graduate course in Coal Science and Technology attracted a number of students when offered recently by the ChE Department of Iowa State University. The course was taught on an experimental basis during the winters of 1974 and 1976 and was presented on a regular basis during the winter of 1978. It has attracted from 8 to 22 students each time offered with the largest number enrolling most recently. Although on the average 40% of the enrollees have been ChE graduate students, about one-fourth have been graduate students in other engineering and science disciplines and about one-third advanced undergraduates, mainly ChE's. Enrollment has been limited to science and engineering students who have taken courses in organic and physical chemistry as well as general chemistry.

The developers of the course are Professors Allen Pulsifer and Thomas Wheelock. Both have been involved in coal research for a number of years and therefore have become familiar with the general field of coal science and technology. In addition, they are fortunate in being able to call on other members of the Iowa State faculty and the technical staff of the Ames Laboratory for lectures dealing with certain specialized areas. Because of the Iowa Coal Research Project which was funded by a special appropriation of the State Legislature in 1974 and other coal research supported by the federal Department of Energy, a large reservoir of expertise has built up within the University community to deal with the problems of producing, transporting, and utilizing coal. This reservoir of knowledge is readily available for use in the course.

The purpose of the new course is to introduce graduate students and advanced undergraduates to the general field of coal science and technology



T. D. Wheelock is a Professor of ChE at Iowa State University. He received his BS and Ph.D. from Iowa State. His principal research interests are the investigation of fluidized bed reactors, the application of these reactors to various chemical treatment processes such as coal gasification and mineral reduction, and the study of various processes for removing sulfur from coal. He has had wide professional and consulting experience, and is the author of over 20 publications dealing with the development of fluidized bed reactors and processes based on these reactors.

so that they will become familiar with the nature and occurrence of coal, its principal chemical and physical characteristics, methods of cleaning and preparing coal, and processes for converting it into clean solid, liquid and gaseous fuels as well as coke. To achieve this purpose the one term course is presented as a series of seventeen 90 minute lectures (Table 1) and a tour of the Iowa State University coal preparation plant (Figure 1). Collateral reading is assigned as well as a term paper. Since a suitable textbook is not available, specific sections of certain reference books (Table 2) and a number of current technical papers are assigned. Many of the papers have been authored by the course lecturers. In addition, two movies have been shown. One of these, "An American Asset", is available from the National Coal Association in Washington, D.C., and provides a good introduction to the subject because it touches on almost every aspect of modern coal mining and utilization. The other film, "The Last Pony Mine", is available from the Iowa State University Film Production Unit and provides a historical perspective since it shows how coal was once mined

by hand and transported by pony cart. Although it does not describe current technology, it is a masterpiece which creates great interest among its viewers whether experienced with coal mining or not.

LECTURE TOPICS

THE SERIES OF LECTURE topics is flexible and has varied somewhat each time the course has been offered. The most recent series (Table 1) included several lectures at the beginning of the course which dealt with the basic properties and characteristics of different types of coal and the genesis, nature, and extent of major coal deposits so that the student would gain an appreciation of the properties of the material and its availability. These lectures were followed by a lecture on mining, not only to acquaint the student with how coal is produced but also to show how the methods of production affect the properties of the material such as size distribution and degree of contamination with foreign matter. Two lectures on coal preparation were presented next to show how coal is presently prepared and cleaned for use in combustion and coking. The operating principles, characteristics and limitations of various particle separation methods used for cleaning coal were discussed and current research and development in this area of technology was reviewed. Following these lectures, the class was given a tour of the coal preparation plant which is located on the campus of Iowa State University (Figure 1).

TABLE 1.
Winter 1978 lecture topics in Coal Science and Technology.

TOPIC & PERIODS	LECTURER & DEPARTMENT
Introduction	Wheelock, Chem. Engr.
Geology of coal	Lemish, Earth Sci.
Microstructure	Greer, Engr. Sci.
Petrography	Biggs, Earth Sci.
Analytical Chemistry	Bachman, Ames Lab
Surface mining	Anderson, Ag. Engr.
Preparation and cleaning	Wheelock, Chem. Engr.
Plant tour	Grieve & Birlingmair, Ames Lab
Chem. desulfurization	Wheelock, Chem. Engr.
Chem. and phys. structure	Markuszewski, Ames Lab
Carbonization and coking	Pulsifer, Chem. Engr.
Gasification	Pulsifer, Chem. Engr.
Chem. of liquefaction	Markuszewski, Ames Lab
Liquefaction technology	Wheelock, Chem. Engr.

The purpose of the new course is to introduce graduate students and advanced undergraduates to the general field of coal science and technology so that they will become familiar with the nature and occurrence of coal, its principal chemical and physical characteristics, methods of cleaning and preparing coal, and processes for converting it into clean solid, liquid and gaseous fuels as well as coke.

Subsequent lectures dealt with the chemical structure of coal, important chemical reactions of coal, and industrial processes for desulfurizing, coking, gasifying and liquefying coal. In addition to reviewing state of the art technology, attention was given to new processes under development as well as the chemical reaction kinetics and thermodynamic principles underlying these processes. In a course of this type other topics could also be covered, such as coal combustion or coal storage and transportation or environmental regulations.

The University's coal preparation plant provides a unique backdrop for the course. The preparation plant can process up to 70 ton/hr. of coal and is equipped for crushing, sizing, and heavy media separation. It is also equipped with a Deister table for cleaning smaller-size coal. Equipment is being installed for demonstrating the cleaning of fine-size and ultra-fine size coal by hydroclones, froth flotation and selective oil agglomeration. Since the latter will demonstrate new technical features developed at the University, it will be possible to show future classes how a process is scaled up from lab bench to pilot plant.

TERM PAPERS

THE TERM PAPER, which is an important part of the course, is designed to familiarize the student with some aspect of coal research and its associated literature. Although a number of topics are suggested to the class, each student is free to choose his own topic and students are encouraged not to select identical topics. Each topic should deal with an important question or problem in the area of coal science, utilization, or conversion. Ideally, the paper should define the problem, present a careful analysis of it, describe and evaluate alternate ways of solving it, indicate how others may be trying to solve the problem, and make recommendations. The following is an example of a topic which might be the subject of a term paper:

TABLE 2.
**Book list for the course in Coal Science
and Technology.**

- Casidy, S. M., (ed.), "Elements of Practical Coal Mining," Coal Division of SME-AIME, New York, 1973.
- Leonard, J. W., and D. R. Mitchell, (eds.), "Coal Preparation," AIME, New York, 1968.
- Lowry, H. H., (ed.), "Chemistry of Coal Utilization," Supplementary Vol., Wiley, New York, 1963.
- Meyers, R. A., "Coal Desulfurization," Dekker, New York, 1977.
- Van Krevelen, D. W., "Coal," Elsevier, New York, 1961.
- Wheelock, T. D., (ed.), "Coal Desulfurization, Chemical and Physical Methods," ACS Symp. Series 64, Washington, D.C., 1977.

- Determine the suitability of Iowa bituminous coal for various types of industrial gasification processes.
- What are the properties of Iowa coal and its occurrence which may either limit or promote its utilization for gasification?
- Considering the different characteristics of various gasification processes, which process may utilize Iowa coal most effectively?

Needless to say, a topic such as this requires a student to become quite familiar with the nature of Iowa coal and the character and size of the Iowa coal deposits. He should consider whether there is enough coal to support a major gasification plant or only a few, small, scattered plants and whether the coal can be gasified efficiently and economically. He should also become familiar with the various types of gasification processes to see which can best match the characteristics of Iowa coal and other local or regional conditions. Information has to be gleaned from technical journals, government reports, and other sources. But most importantly the student has to analyze the situation, make judgements and synthesize a solution on the basis of incomplete technical information.

For the overall course the students are graded on the basis of two written exams and the term paper. The exams are given at midterm and at the end of the course. They consist mainly of essay questions and some objective type questions.

STUDENT POLL

SEVERAL WEEKS AFTER the last offering of the course, the students were polled to determine their reaction to the course and to see what suggestions they might have for improvement. A formal questionnaire was sent to each student who responded voluntarily and anonymously. Among the 22 students who were polled,

15 or 68% returned the completed questionnaire. All of the respondents considered the material presented in the course to be relevant; 93% considered the information presented to be valuable and the time spent beneficial. Only three indicated that they would not have taken the course if they had known what they were getting into. On a scale of poor to excellent, 47% rated the course as

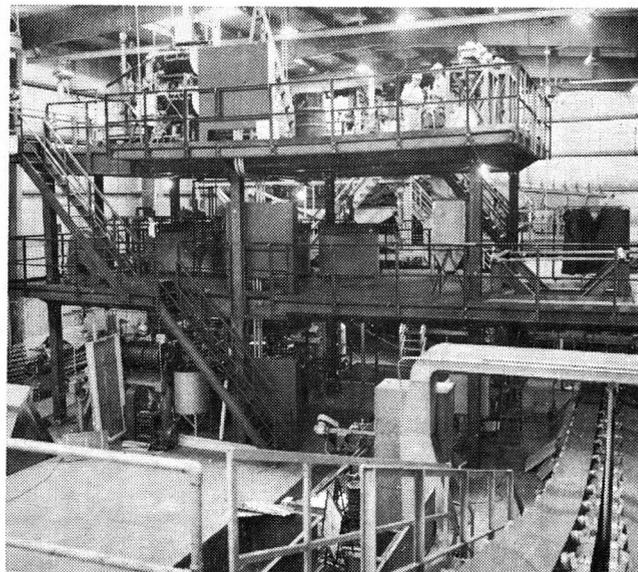


FIGURE 1. The Iowa State University coal preparation plant provides an interesting backdrop for the course in Coal Science and Technology.

average, 40% as good, and 13% as excellent. All but one of the respondents regarded the tour of the University coal preparation plant as worthwhile and most thought that the two motion picture films made a valuable contribution. Some 70% of the respondents thought the reading assignments were "dull but informative", but about right in length. Somewhat more than half thought the course would have been better with fewer outside lecturers. About a fifth of the respondents indicated learning a lot about coal through working on their term paper while the rest indicated learning a moderate amount and none reported learning very little.

In the future the course will probably be offered every other year unless increasing demand causes it to be offered more frequently. Since the field of coal science and technology is developing and changing rapidly, the course must also evolve and change. But keeping up with these changes and new technical developments provides challenge and inspiration to the student and teacher alike. □

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A Course in

TRANSPORT PHENOMENA IN MULTICOMPONENT, MULTIPHASE, REACTING SYSTEMS

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MOST OF THE SYSTEMS that are of interest to chemical engineers involve two or more phases, several chemical components, and a strong coupling between heat, mass and momentum transport. A cursory examination of the classical reactor design and mass transfer operations encountered in ChE suggests that the course title listed above would encompass a major segment of all ChE processes. A quick survey of the currently available texts designed for the training of graduate students in ChE reveals the need for a rigorous treatment of multicomponent, multiphase systems.

With the exception of the excellent text by Slattery (1972), the method of volume averaging as a rational route to the transport equations for multiphase systems is generally ignored. Although the method is little more than a decade old [Whitaker (1967), Slattery (1967)], we are rapidly approaching the point where the formalism is sufficiently well understood so that it is suitable for incorporation into our graduate courses. Under the circumstances, we believe that the general knowledge now available under the heading of "transport phenomena" is ready to be extended to include a rational treatment of multiphase systems.

One of the major strengths of the graduate program in ChE at U.C. Davis is a series of core courses available to the graduate students in fluid mechanics, heat transfer, mass transfer and chemical reactor design. These courses are taught at a level consistent with texts by Aris (1962), Whitaker (1968, 1977a), Bird, Stewart and Lightfoot (1960) and Smith (1970). These courses provide a sound introduction to the laws of continuum physics for single component systems and deal with a variety of multiphase systems via simplified models. To supplement and consolidate this material, a course was instituted that would

concentrate on a rigorous development of the multicomponent transport equations, boundary conditions at phase interfaces, and volume-averaged transport equations for multiphase reacting systems. The lecture notes represent the origins of a graduate level text in chemical reactor design.

Reactor design texts uniformly assume a level of sophistication below that of Bird, Stewart and Lightfoot (1960) and have paid no heed to the method of volume averaging given by Slattery (1972). While these developments are perhaps recent by engineering time scales, the subject of fluid mechanics is ancient by comparison (Truesdell, 1968) and its incorporation into our studies of reactor design is long overdue.

Reactor design is the one area that is purely the province of the ChE, and it is the most appropriate vehicle for describing the intricacies of the coupling of momentum, heat and mass transport for multicomponent multiphase systems. It is not unusual to find reactor design texts (Smith, 1970; Carberry, 1976; Aris, 1969) that do not mention the governing differential equations for conservation of a given species, or the momentum and thermal energy equation for multicomponent systems, even though these equations govern all transport processes in chemical reactors. The development of appropriate governing differential equations (via volume averaging) for transport in multiphase systems (chemical reactors) is not included. This is probably the major failure of such texts. The normal procedure is to assume in an ad-hoc fashion that the form of the transport equations and fluxes in multiphase systems are the

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same as those for a homogeneous fluid but with appropriate empirical parameters. The dependence of these parameters on the structure of the porous media and the physical properties of the components and the chemical reaction rate is left unexplored.

A good example of this approach is the governing equation usually proposed to describe diffusion and chemical reaction within a catalyst pellet. The catalyst pellet is treated as a homogeneous medium, and diffusion in such pellets is assumed to be governed by means of flux expression analogous to Fick's Law of Diffusion with an effective intraparticle diffusivity. However, using volume-averaging techniques, it is possible to obtain differential equations for diffusion in a porous media and a mathematical description of the dependence of the intraparticle diffusivity on system parameters. One advantage of such an approach is that it allows for a more thorough investigation of the assumptions normally made regarding the magnitude of terms in the governing differential equation. Furthermore, an accurate mathematical description of transport parameters in multiphase systems allows for the development of a more rational experimental program aimed at unraveling the magnitude of different contributions to the transport parameters. Finally, this type of analysis provides the student with a more rigorous framework to carry on further studies and helps to place in perspective within the student's mind the interrelations between transport processes in a homogeneous fluid and in a porous media.

In the paragraphs that follow, we outline the content of this course and the way in which the material is presented. We feel this provides a more rational approach to the training of graduate students in chemical engineering.

AXIOMS FOR SPECIES BODIES

THE FIRST THIRD OF the course is always devoted to the essential theoretical elements of transport in multiphase systems. The presentation is based on the continuum point of view, thus the laws of physics for multicomponent systems are the first order of business. Here we follow the approach of Truesdell and Toupin (1960) and introduce the concept of a *species body*. The kinematics, i.e., time derivatives of point functions and volume integrals, of species bodies are carried over from previous studies of single component systems. The general balance equation for single component systems

$$\frac{D}{Dt} \int_{V_m(t)} \psi dV = \int_{A_m(t)} \omega dA + \int_{V_m(t)} \sigma dV \quad (1)$$

is easily extended to the species body and the axioms for mass are stated as

I. The mass postulate for the A^{th} species

$$\frac{D}{Dt} \int_{V_A(t)} \rho_A dV = \int_{V_A(t)} r_A dV \quad (2)$$

II. Conservation of total mass owing to chemical reaction

$$\sum_{A=1}^{A=N} r_A = 0 \quad (3)$$

Equation 2 quickly leads us to the species contin-



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uity equation in terms of the species density and mass average velocity,

$$\frac{\partial \rho_A}{\partial t} + \nabla \cdot (\rho_A \mathbf{v}) = -\nabla \cdot \mathbf{j}_A + r_A \quad (4)$$

or in terms of the concentration and the molar average velocity

$$\frac{\partial c_A}{\partial t} + \nabla \cdot (c_A \mathbf{v}^*) = -\nabla \cdot \mathbf{J}_A + R_A \quad (5)$$

The latter form is, of course, preferred by chemical engineers because kinetic constitutive equations and phase equilibrium relations are most conveniently stated in terms of molar quantities.

The presence of the mass average velocity in Eq. 4 and the molar average velocity in Eq. 5 naturally raises questions about the determination of these velocities by means of the laws of mechanics. At this point the revised linear and angular momentum postulates are introduced and the derived species equations are summed to obtain

$$\rho \frac{D\mathbf{v}}{Dt} = \rho \mathbf{b} + \nabla \cdot \underline{\underline{\mathbf{T}}} \quad (6)$$

$$\underline{\underline{\mathbf{T}}} = \underline{\underline{\mathbf{T}}}^t \quad (7)$$

Here the stress tensor consists of the sum of partial stresses and species diffusive stresses. It is consistent with the kinetic theory of dilute gases to represent $\underline{\underline{\mathbf{T}}}$ in terms of the rate of strain tensor; however, the idea of equipresence (Truesdell and Noll, 1965) is invoked in order to keep the door open for more general constitutive equations.

The pattern of analysis is now established and the revised energy axioms are presented for a species body. The development is restricted to what Bataille and Kestin (1977) refer to as "strongly interacting mixtures", and the thermal energy equation for the mixture is obtained by summing the individual species equations leading to

$$\rho \frac{De}{Dt} = -\nabla \cdot \mathbf{q} - \nabla \cdot \sum_{A=1}^{A=N} h_A \mathbf{j}_A - p \nabla \cdot \mathbf{v} + \nabla \mathbf{v} : \underline{\underline{\tau}} + \Phi + \left\{ \begin{array}{l} \text{diffusive terms of} \\ \text{negligible importance} \end{array} \right\} \quad (8)$$

where e is the internal energy of the mixture defined in the usual manner. The result is also presented in terms of the enthalpy for later use in constructing boundary conditions at phase interfaces, and in terms of the temperature. The latter form is, of course, useful for solving energy trans-

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port problems and gives rise to the source term owing to chemical reaction. The diffusive terms in Eq. 8 consist of the diffusive kinetic energy, diffusive rates of working, etc., and order of magnitude analysis (Whitaker, 1977) can be used to establish that these terms are negligible for practical cases.

BOUNDARY CONDITIONS AT PHASE INTERFACES

WITH THE TRANSPORT equations for multi-component systems at our disposal, we are naturally led to consider the matter of boundary conditions at phase interfaces. Following a route similar to that proposed by Slattery (1972), we develop a general surface transport equation. In integral form this transport equation is represented as

$$\frac{D}{Dt} \int_{A_{\alpha\beta}(t)} \psi dA + \int_C \Omega ds - \int_{A_{\alpha\beta}(t)} \Sigma dA = \int_{A_{\alpha\beta}(t)} [\psi^\alpha (\mathbf{v}^\alpha - \mathbf{w}) - \psi^\beta (\mathbf{v}^\beta - \mathbf{w})] \cdot \underline{\underline{\xi}}_{\alpha\beta} dA + \int_{A_{\alpha\beta}(t)} (\omega^\alpha - \omega^\beta) dA \quad (9)$$

Here the upper case Greek letters denote the intrinsic surface quantities associated with the lower case Greek letters in Eq. 1, the area $A_{\alpha\beta}(t)$ represents a material surface element, $\underline{\underline{\xi}}_{\alpha\beta}$ represents the unit normal vector pointing from the α -phase into the β -phase, and \mathbf{w} represents the velocity of the interface.

At this point in the course, special forms of Eq. 9 are considered, i.e., the surface element $A_{\alpha\beta}(t)$ is fixed in space, or the surface is flat, or all the terms on the left hand side are zero. These severe restrictions are necessary because the rigorous analysis leading to the surface transport equation (Aris, 1962), makes use of the surface divergence theorem and a general understanding of differential geometry (McConnell, 1957). The subject is of considerable interest to chemical engineers (Rosner, 1976; Berg, 1970), but, as yet, a

simple route to the desired result has not yet been found. Both Professor Rosner at Yale and Professor Slattery at Northwestern are preparing monographs on this subject, and their works will certainly help us with the treatment of this aspect of multiphase transport phenomena.

We avoid the vector form of Eq. 9 altogether, and consider only special cases associated with heat and mass transfer along with chemical reaction at the interface. While the attack here is obviously something less than what we would desire, it does allow us to point out just how it is that we go about constructing boundary conditions at phase interfaces, i.e., we make specific statements about the left hand side of Eq. 9 based on experimental observations. For example, if we use the *species form* of Eq. 9 associated with the mass postulate given by Eq. 2 and make the statements

$$\psi_A = \text{constant (surface concentration is constant)}$$

$$\Omega_A = 0 \text{ (follows from Eq. 2)}$$

$$\Sigma_A = 0 \text{ (there is no surface reaction)}$$

$$A_{\alpha\beta}^{(A)} = A_{\alpha\beta}^{(A)} \text{ (the } A^{\text{th}} \text{ species surface element is fixed in space)}$$

we find that Eq. 9 leads us to *continuity of mass flux* expressed as

$$\rho_A^\alpha (\mathbf{v}_A^\alpha - \mathbf{w}) \cdot \underline{\xi}_{\alpha\beta} = \rho_A^\beta (\mathbf{v}_A^\beta - \mathbf{w}) \cdot \underline{\xi}_{\alpha\beta} \quad (10)$$

This approach forces one to specifically identify the characteristics of the surface en route to Eq. 10, as opposed to specifying continuity of mass flux with either vague or non-existent references to the properties of the surfaces.

THE VOLUME AVERAGING THEOREM

With the multicomponent transport equations and multiphase boundary conditions at our disposal, we can proceed to the study of transport phenomena in multiphase systems. Our prime mathematical tool here is the spatial averaging theorem [Slattery, 1967; Whitaker, 1967; Gray and Lee, 1977; Bachmat, 1972] which can be stated as

$$\langle \nabla \psi_\alpha \rangle = \nabla \langle \psi_\alpha \rangle + \frac{1}{V} \int_{A_{\alpha\beta}(t)} \psi_\alpha \mathbf{n}_{\alpha\beta} dA \quad (11)$$

for a two phase system. Here the angular brackets are used to denote the volume average which is given by

$$\langle \psi_\alpha \rangle = \frac{1}{V} \int_V \psi_\alpha dV = \frac{1}{V} \int_{V_\alpha(t)} \psi_\alpha dV \quad (12)$$

where V represents the averaging volume

$$V = V_\alpha(t) + V_\beta(t) \quad (13)$$

The second of Eqs. 12 is obtained because ψ_α is zero in the β -phase.

AREAS OF APPLICATION

Armed with the governing differential equations, a scheme for constructing boundary conditions and the volume averaging theorem, we are ready to explore a variety of phenomena. The choice here depends on the students and instructor. On the Davis campus there is a large Water Science and Engineering group, and students from that discipline are interested in the theoretical underpinnings of d'Arcy's law (Gray and O'Neill, 1976), dispersion in porous media (Whitaker, 1967), and multiphase flow in porous media (Slattery, 1970). Chemical engineering students show an interest in these subjects provided one mentions oil reservoir calculations, tertiary oil recovery processes and the moderate Reynolds number flows that occur in packed bed reactors. Recent studies of trickle bed reactors (Herskowitz, Carbonell and Smith, 1978) indicate the importance of the hydrodynamics of two-phase flow in packed bed reactors and this subject can be attacked in a rational manner using the method of volume averaging, although the contact line phenomena escapes our understanding at the moment. The hydraulics of distillation trays and the mechanics of sediment transport are other subjects that can be profitably analyzed using the volume averaging method.

For chemical engineering students, the problems of heat and mass transfer in porous media hold the most interest. In particular, the unravelling of previous ad hoc developments of transport processes in catalyst pellets has considerable appeal and represents a challenging theoretical problem. If one avoids the problem of Knudsen and transition region diffusion and restricts one-

Chemical engineering students show an interest in these subjects provided one mentions oil reservoir calculations, tertiary oil recovery processes and the moderate Reynolds number flows that occur in packed bed reactors.

self to linear adsorption isotherms and linear, irreversible kinetics, one can volume average Eq. 5 to obtain

$$\epsilon_\alpha \left(1 + \frac{K a_v}{\epsilon_\alpha} \right) \frac{\partial \langle c_A \rangle^\alpha}{\partial t} + \nabla \cdot [\langle c_A \rangle^\alpha \langle \mathbf{v}^* \rangle] + \nabla \cdot \langle \tilde{c}_A \tilde{\mathbf{v}}^* \rangle = \nabla \cdot \left\{ \epsilon_\alpha D_A \nabla \langle c_A \rangle^\alpha - \frac{D_A}{V} \int_{A_{\alpha\beta}} \tilde{c}_A \mathbf{n}_{\alpha\beta} dA \right\} - a_v k K \langle c_A \rangle^\alpha \quad (14)$$

Here we are confronted with two unknown parameters $\tilde{c}_A \tilde{\mathbf{v}}^*$ and \tilde{c}_A for which we need constitutive equations. The route to be followed here has been hinted at in prior publications (Whitaker, 1967, 1971, 1977b) but never fully exploited. Essentially, it represents the closure problem of turbulence (Launder, 1976) and requires that the transport equations for \tilde{c}_A and $\tilde{c}_A \tilde{\mathbf{v}}^*$ be derived. In the study of turbulence the closure is obtained by proposing constitutive equations for the higher order correlations in the Reynolds stress transport equations; however, this is impossible for the \tilde{c}_A and $\tilde{c}_A \tilde{\mathbf{v}}^*$ transport equations because the geometric details of the porous media are unknown. Nevertheless, the transport equations for \tilde{c}_A and $\tilde{c}_A \tilde{\mathbf{v}}^*$ can be used as a guide for the direct construction of constitutive equations required in Eq. 14. This type of approach leads to a transport equation for $\langle c_A \rangle^\alpha$ of the form

$$\epsilon_\alpha \left(1 + \frac{K a_v}{\epsilon_\alpha} \right) \frac{\partial \langle c_A \rangle^\alpha}{\partial t} + (\langle \mathbf{v} \rangle + \mathbf{A}) \cdot \nabla \langle c_A \rangle^\alpha = \nabla \cdot \left\{ \underline{\underline{\mathbf{D}}} : \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle \nabla \langle c_A \rangle^\alpha + \underline{\underline{\mathbf{K}}} : \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle \nabla \langle c_A \rangle^\alpha (a_v k K \langle c_A \rangle^\alpha) \right\} + \nabla \cdot \left\{ \epsilon_\alpha D_A \nabla \langle c_A \rangle^\alpha - \epsilon_\alpha D_A \underline{\underline{\mathbf{B}}} \cdot \nabla \langle c_A \rangle^\alpha \right\} - a_v k K \langle c_A \rangle^\alpha \quad (15)$$

Here the vector \mathbf{A} and the second order tensor $\underline{\underline{\mathbf{B}}}$ are functions of the reaction rate parameter $a_v k K$ thus suggesting that the effective diffusivity may depend on the reaction rate and that the portion of the dispersive term which appears in the convective transport term also depends on $a_v k K$.

Equation 15 can be simplified for a variety of special cases and compared to transport equations in current use. Use of this method allows us to clearly identify the origin of dispersion coefficients and effective diffusivities and to say something

about the dependence of these quantities on system parameters. It is important to notice that all the terms in Eq. 14 are precisely defined and thus susceptible to determination by the solution of boundary value problems for model porous media. Here we are thinking in terms of the work of Snyder and Stewart (1966), Sorensen and Stewart (1974), Payatakes et al, 1973, and forthcoming works by Brenner (1978) on both flow and mass transfer in spatially periodic porous media.

Other topics of interest in the reactor design area that can be handled using the volume-averaging approach include:

1. An analysis of flow distributions and flow instabilities in chemical reactors, in particular, trickle bed and fluidized bed reactors.
2. Determination of effective thermal conductivities for catalyst pellets and chemical reactors.
3. Determination of dispersion coefficients for chemical reactors. These topics and many others can be handled at the discretion of the instructor.

What we find most attractive about the approach followed in this course is that it provides the student with a rigorous framework with which to carry on further studies, and puts in perspective the interrelation between transport processes in a single phase and the analogous processes in multiphase systems.

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BOOK REVIEW: Thermodynamics

Continued from page 163

features made the book a treat to review. On the other hand, the book has an unevenness about its presentation, in its continuity and its definition of some concepts. These shortcomings would make its use as an undergraduate text quite difficult; at the graduate level, a competent teacher would be required to aid the student in "reading between the lines" and filling in what this reviewer feels are gaps in the unified presentation of thermodynamics. There are very few problems to solve in the text except for the later chapters. The price of this book will probably discourage widespread course adoption as well.

In all fairness, however, the book is constructed from the viewpoint of an eminent thermodynamicist and, in that context, will satisfy the scientist or engineer who has had some experience or is presently working in the area of applied thermodynamics. Such an individual would find this book an enlightening refresher course on the fundamentals, with a broad enough selection of applications (presented in the form of examples) to satisfy most readers' particular interests. Those seriously interested in thermodynamics per se or the instruction of thermodynamics owe themselves more than a casual perusal of this book.

Chapter 3 on pure phases is a strong chapter particularly in its discussion of equations-of-state. Unfortunately, such an area is constantly undergoing change, and current workers will find the content somewhat outdated, a risk that every writer in this area runs. This chapter is preceded by thoughtful and challenging chapters on physics and the two laws of thermodynamics. This reviewer was impressed by Chapters 5-7 on phase equilibria and solutions; the author employs a kind of "case method" in the sense of using examples prior to the complete statement of what concept he has in mind demonstrating. The examples are quite interesting and often probe deeper into certain well-known thermodynamic phenomena than one is accustomed in a text (e.g., the inflection in the vapor pressure curve of a pure substance; the discussion of azeotropy; vapor-liquid criticality, although this topic is preceded by only a shallow attempt at explaining phase stability). Chapter 8 on electrolytes and Chapter 10 on work modes other than those of compression or expansion (entitled "various phenomena") are unique in comparison with existing texts and quite well done. Chapter 9 on chemical reactions is basically a collection of examples of the author's choosing.

This reviewer, although finding more than an occasional "gem" of insight in this book, had the feeling that the text was for the most part composed of material which significantly predates its publication date. The author appears influenced by the text of Lewis and Randall. The book lacks the "freshness" one finds in, e.g., the book by Modell and Reid, who are more successful in unifying the field of thermodynamics. Despite the shortcomings mentioned above, Redlich's book can reward the diligent reader with a sound perspective of thermodynamics and its practice. □

ALL A CHEMICAL ENGINEER DOES IS WRITE

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WE HAVE JUST STARTED teaching a course called "ChE 302: Introduction to Engineering" in which we teach freshman ChE's something of what engineering is and try to instill in them the pride that engineers feel in carrying out their profession. In addition, we teach them to write FORTRAN and to appreciate the use of the computer as yet one more useful engineering tool. We also teach them to communicate, the subject of this article, by setting homework assignments on engineering topics discussed in class. For essay titles we choose such subjects as "The Role of Engineers in Society" and "The Scope of Chemical Engineering." We also discuss their curriculum and then assign essays on each future class we discuss, such as "Unit Operations" or "Thermodynamics." Eight essays and three computer programs are the only set work; there are no tests and no final examination. Thus, their final grades depend solely on their developing skills in written communication and their acquired computer skills.

The essays are graded by experts in composition and technical writing from the English Department. Because of the guidance they receive from the engineering faculty in class, the feedback in their homework from the English Department graders, and the threat of reduction of their final grades, the students take more time with their written work and, hopefully, learn that it is just as easy to write well as it is to write poorly after a few fundamentals and a respect for the language have been learned. They leave the class able to produce work they are proud of and, ideally, with the ambition to continue to practise what they have learned. This is the story of how it came about.

THE NEED TO WRITE WELL

THE CHE FACULTY HAD NOTICED a general worsening of their students' written work and a lowering of standards. About two years ago, the point was reached when some corrective action

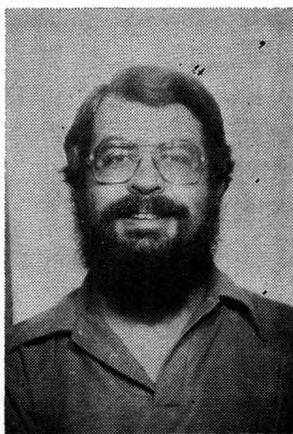
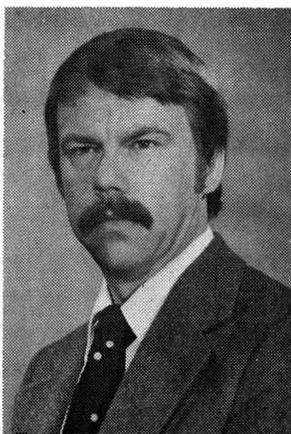
was necessary to improve performance and standards. It was decided to modify the freshman engineering class (ChE 302) to improve communication as an engineering skill. This should not have been necessary, and the faculty knew it. The students had already taken English in high school and had had some composition training at the University, but they were not writing good English in technical reports in upper-division classes. Grammar, spelling, and style varied from mediocre to abysmal with few exceptions. Sentences were constructed weakly and mechanically, without force, clarity, or variety, and in many cases, paragraphs were composed almost entirely of buzz words, jargon, and clichés. There was no individualism and little evidence of sincere interest in the language.

And yet, any of the students, when asked, would reply that they were aware of the pride that exists among engineers. We would then point out the contradiction: "How can you speak of pride in engineering and yet put your names on such poor written work?" "That's different," they would answer, "writing is not engineering."

We remind them of the old joke about how God was designing Man and the professions. Aware that future squabbles would exist between chemists and ChE's, He said to His typist, "All a chemical engineer does is *right*." Unfortunately, the typist mis-spelled the last word. It certainly is like that in ChE. In fact, we get quite good at writing. And when we do, we find that we enjoy it.

In class, we tell the freshman that in their first few months of work they will spend about 30% of their time doing their engineering and 70% of their time writing about it. Soon the ratio will be 20% to 80% and, thereafter, will slowly dwindle to 0% to 100%, except in exceptional circum-

We discovered that around half the class resisted the idea that clarity of communication was any more than a minor talent compared to the skills of engineering.



Dr. Leesley graduated from the Department of Fuel Technology and Chemical Engineering in Sheffield, England with B.Sc.Tech. and Ph.D. He has worked in the steel and mining industries. He headed the ChE Group at the Computer-Aided Design Centre, Cambridge, England, where he developed a number of software systems including CONCEPT and PDMS. In 1974 he immigrated to U.S.A. and joined the faculty at the University of Texas at Austin. He is a member of the AIChE, the Institution of Chemical Engineers (UK) and the Institute of Fuel (UK). He holds a Royal Charter to practice engineering in Great Britain. (C.Eng.). (L)

Marvin L. Williams, Jr., a resident of Texas for over 25 years, received his B.A., M.A. and Ph.D. in English from the University of Texas at Austin. Besides technical and literary editorial work, Dr. Williams has published articles in both literary and bibliographical journals. He is a member of the Bibliographical Society and the Modern Language Association. (R)

stances. They don't believe us of course; not at first anyway.

One of them told of how he went home and, incredulously, repeated this story to his father. His father, a nationally-known ChE, said, reflectively, that it was true; furthermore, he said that the engineering content of what he wrote had also dwindled. It was perhaps when the class was startled into knowing that they are going to have to write often and well and that they might as well get used to it and make the best of it, that they settled down and began to take pride in their writing.

We tell them that the people who read their written work in the future will either want to or have to. In the first case, it is as well to keep the reader interested. In the second case, an *interesting* message will be brought home far more strongly to those who are forced by whatever circumstances to read the letter, report, or article. We tell them that they have to give their reader staying power. They must quickly establish a certain ethical appeal that causes the reader to take both the author and his message seriously. They will accomplish this by logical thinking, careful

planning, and the avoidance, by proofreading and revision, of careless errors in punctuation, grammar, and spelling which, if left in, may irritate the reader and take his attention away from the message.

The students often ask for suggestions on how to capture and sustain the interest of the reader. We suggest that they read as much material as they possibly can and criticize as they read. It is unlikely that graceful and effective style will be recognized, if it has never been noticed or even read.

We discovered that around half the class resisted the idea that clarity of communication was any more than a minor talent compared to the skills of engineering. They preferred to believe that the engineering aspects of a project far outweighed its comprehensive documentation. Their stubbornness, at least in part, is because of their non-engineering viewpoint of what engineering is. Perhaps they imagine that engineering is making money out of applying to community problems the laws of nature and the laws of man, i.e., the codes of practice. Although this is not a complete definition of engineering, let us look at it for a start.

We remind them of the old joke about how God was designing Man and the professions. Aware that future squabbles would exist between ChE's, He said to His typist, "All a chemical engineer does is right." Unfortunately the typist misspelled the last word.

In order for them to know all of these laws, they have to read about them, which means that someone has had to write them down with sufficient clarity and accuracy that they can be understood by others. Some of these laws are quite difficult to understand. In ChE, there are concepts of incredible complexity. Therefore, the engineers that prepare our reference books and texts have to bestow upon their readers ample staying power or the desire and the ability to follow and to understand what is written.

We suggest to the students, as another learning device, that every time they encounter a difficult concept, it would improve their own writing and communication if they, after having finally grasped the concept, go back to the difficult passage and decide how they would have written it in order to lead the reader more quickly to comprehension.

Of course, the application of laws is not the

We began to ask teachers at all levels what they felt about this problem. Every group of teachers wanted to blame the group of teachers immediately before them in the student's academic careers. The few kindergarten teachers with whom we spoke were convinced that television was the major problem.

whole of an engineer's job. Also, of great importance are self-satisfaction, creativity and the ability to interact with others of varied talents and backgrounds. For every engineering problem there are an infinite number of situations. Hopefully, the engineer's training and experience will lead him by instinct to pick out the best few for examination by himself and the other members of his team. Some of his ideas will be simple, some complex. In any event, he has to transplant these ideas into the heads of his colleagues using, to a large degree, reports and drawings. There is hardly an engineer alive who doesn't succumb at least occasionally to the spell of the drawing board. The fact that most engineers are fair draftsmen ensures their enjoyment and satisfaction when drawing and gives them pride in the finished drawing.

On the other hand, most engineers are, at best, average writers. Perhaps this is why, often, the engineer feels little enjoyment, satisfaction, or pride in the finished pages. We wondered why this seemed, in the experience of one of the authors, to be worse in America than in Britain. We began to ask teachers at all levels what they felt about this problem. It was odd. Every group of teachers wanted to blame the group of teachers immediately before them in the students' academic careers. It seemed that upstream teachers do not do their jobs properly. The few kindergarten teachers with whom we spoke were convinced that television was the major problem.

A colleague on a year's sabbatical leave from Scotland, horrified at the low intellectual level of most American television, spent his visit without television. When he was about to go back to Scotland, he remarked that he had decided not to buy one upon their return. Both his children had become avid readers and, consequently, their spelling, grammar, and general writing ability had improved immeasurably. The significance of television on educational development can be debated elsewhere, but what needs to be noted here is that everyone agreed that a problem exists.

Most professors have their own horror story. Mine concerns a student who, having struggled

from spelling mistake, to misplaced comma, to verbless sentence for over four pages, managed, on the last page, to make a spelling mistake in every single line and in some more than one. I am certain that most students do not read their essays through after writing them. I deduced this once when a student laboriously printed out, capital letter after capital letter, a story in which he told me that "a professional engineer is one whose work comes under the pubic (sic) eye."

Such writing just won't do. We have a need to express our ideas to each other as engineers and the better we can make our message understood, the quicker we can interact, cooperate, and finish the job. Bad grammar leads to incomprehensible sentences, misleading statements and, finally, to a reader sufficiently confused and irritated to lose the flow of the argument. Thus, no communication takes place. We must learn to improve our writing in order to, first, give our readers the staying power that is necessary if communication is to be possible. Second, we must adhere to principles of brevity and economy, that is, get our message down into as few words as possible without sacrifice of meaning. Hopefully, a third benefit will be that we become good at doing this and, then, we will enjoy writing, be satisfied by it, and take pride in it, as we do our other engineering skills. Our initial task with ChE 302 was to determine how we could transfer this philosophy to the students and yet still meet the conventional objectives of the course.

THE NEW COURSE FORMAT

TRADITIONALLY, ENGINEERING departments at this University have a course called "Introduction to Engineering" which is used to teach freshmen the nature of their academic career in their chosen engineering discipline and, in some cases, to teach FORTRAN and familiarity with the university computer system. In ChE, it was decided to upgrade the course and, keeping the same general objectives, to include an emphasis on good written communication also. The course was first taught in this revised form in Fall 1976.

The objectives of the expanded course are: to

introduce freshmen to the idea that ChE is a profession and to explain to them exactly what the profession involves; to give a brief description of the mainstream courses between ChE 302 and graduation in order that freshmen will have a basis upon which to affirm or reject ChE as their major at an early stage; to encourage the freshmen to take an early pride in their written work; and to teach FORTRAN as a programming language and give them familiarity with the computer by setting meaningful FORTRAN programming exercises.

There is insufficient time to meet all of the above objectives singly, and in the level of detail required, unless some considerable overlap procedure is employed. This was in fact the case, and students were asked to carry out written work assignments on subjects related to ChE which were discussed in class. Each topic to be discussed was considered to be a distinct help to their academic career. Essay titles were chosen to enable the professor to discuss ChE as a profession and follow with non-technical lectures on various industries and the main-stream topics the students need in this major.

The class discussions which preceded each essay were just as important as the essays themselves. The class was encouraged to discuss the problem and make suggestions which could be incorporated into their essays. In some cases, for example during discussion of the heat exchanger, we started off with a basic problem definition. The students were asked to consider the problem of recovering heat from the output stream of a reactor and transferring it to the input stream. By involving all the class, it was possible to let the principle of a heat exchanger evolve in the class period. It was astonishing that the students evolved the heat exchanger principle to an incredibly high degree. It was *they* who decided that a multi-tubular device would be needed, that multi-pass heat exchangers would be preferable, that baffling would be required, that a floating head was desirable, and that horizontal heat exchangers were preferable to vertical ones. They decided that straight tubes were better than tortuous-path tubes because of cleaning and that space must be

I deduced this once when a student laboriously printed out . . . a story in which he told me that a "professional engineer is one whose work comes under the pubic (sic) eye."

allowed beside the heat exchanger for tube-bundle removal. In fact, the class conceived the principle of the heat exchanger when most of them had never seen or heard of a heat exchanger before. They then wrote an essay on the subject. During the semester, they wrote eight essays on engineering topics, each essay carrying a maximum of ten points.

Thus, the essays served three purposes. First, they were a means of introducing a discussion in class about the scope of ChE and its implications as a profession. Second, and also in class, topics related to their academic future were discussed. Finally, there was feedback on writing strengths and weaknesses from the English department grader.

The students were given specific instructions about their audience for these writing assign-

Perhaps they imagine that engineering is making money out of applying to community problems the laws of nature and the laws of man, i.e., the codes of practice.

ments. They were told to write to a generally educated audience with no knowledge of the heat exchanger or whatever else the specific topic happened to be. The instruction to the grader was "if you fail to understand the topic by the end of an individual's essay, then the individual has failed to communicate." Of course, spelling, grammar, sentence construction and style were also evaluated.

The teaching of FORTRAN in ChE 302 can be approached in two ways. Either the self-paced approach could be used or the students could be taught the syntax of FORTRAN formally and be left to learn the "tricks of usage" by practice. Having had to learn many different computer languages in his career, the first author chose the latter method since he knew that, like tennis, the rules are easy to learn, but it is the actual use that makes the learner proficient. FORTRAN sections were given in six one-hour lectures and two problems were set.

The first problem was a solution of 'n' simultaneous equations with test data for four unknowns, and the second was a curve-fitting program in which they were encouraged to try a hyperbolic, a logarithmic, and an exponential curve, to a set of 36 data points (which, in fact, were the burning away data for carbon in a flame). Both problems were difficult, and gave

some students trouble at first. But with an occasional FORTRAN clinic in class and a FORTRAN grader available five hours a week, all students reached the point where they were proficient in FORTRAN. There were no exceptions to this; all students finished the course with their programs written.

The final essay the students wrote was entitled "How to Approach the Teaching of ChE 302." This was set (at some considerable risk!) in order to obtain far more feedback than the usual teacher evaluation system would provide. In the discussion period which preceded this assignment, the students were advised that they should take whatever view they felt appropriate, whether it be highly constructive, highly destructive or somewhere in between. They were assured of a fair grade as long as they were able to defend their views. As it turned out, all of the students had to say that even though the work had been hard, they were deeply aware that their writing had improved. They could hardly say, in a well-written essay, that it hadn't! However, there were one or two minor criticisms, such as that the work load was high, but most of the students recognized that good writing and a crisp individual style will only come with practice and, reluctantly, they admitted that this was the best course. On the subject of teaching FORTRAN, however, their attitude was different. They reported that the class sessions were quite sufficient for the formal syntax of FORTRAN, but they felt that the two set problems were difficult and about 90% of the students said that they wished a simple program had been set first in order that they could learn the protocol of using the university computer system and "get their feet wet" more gradually. We agreed with this criticism and adjusted the schedule for the following semester's class accordingly.

The experience gained in the initial class experiment has been invaluable in redesigning the class. The number of essays has been reduced to eight:

- The Scope of Chemical Engineering
- Transport Phenomena
- Thermodynamics
- Unit Operations
- Reactor Design
- Process Plant Design
- Project Development and Economic Evaluation
- Computer-Aided Design in Chemical Engineering

The FORTRAN classes are now given early in the semester in order to maximize the time allowed

for the students to write the programs. Three computer problems are now set. The first is a simple exercise in reading a list of numbers, summing them and their squares, roots and squared deviations, and printing out the answers. The second and third programs will be more difficult and chosen so that they will be useful to them in their ChE careers. There will also be exercises in computer output manipulation and effective use of the full capabilities of FORTRAN. However, they will be no more difficult than those set in the first semester.

The key to our success was the strong support from the English department grader. During discussions between the ChE and English departments, a way was found to utilize Teaching Assistants with extensive experience in grading all types of essays in English composition courses, and, as a result, two English graders, both final year PhD candidates, have been retained for ChE 302, and two upper division courses. Also, the *Harbrace College Handbook* has been chosen as an additional text for the course in order to introduce the abbreviated Harbrace grading system as a method of increasing communication between grader and student.

THE BENEFITS

WE HOPE THAT OUR graduating engineers will be better than engineers from other universities where this training has not yet been incorporated into the curriculum. We hope that the word will get around and that more companies will seek and employ University of Texas ChE's because, among other things, they communicate more easily and more carefully. We have this hope for many reasons.

First, other universities may copy us when they see our success. This will benefit all of us because the standards in written English in the engineering fields will gradually rise and, therefore, text books, scientific papers, reports, codes of practices, scientific journals, policy statements, and construction details will all be easier to read and understand. Second, we will begin to see the re-appearance of writing that gives its readers the staying power to read and re-read, not only to gain an increased understanding of the topic, but for sheer pleasure. Third, we will show that academic engineers are entitled to as much pride in their finished products, even though they are from the classroom rather than the factory or plant. □

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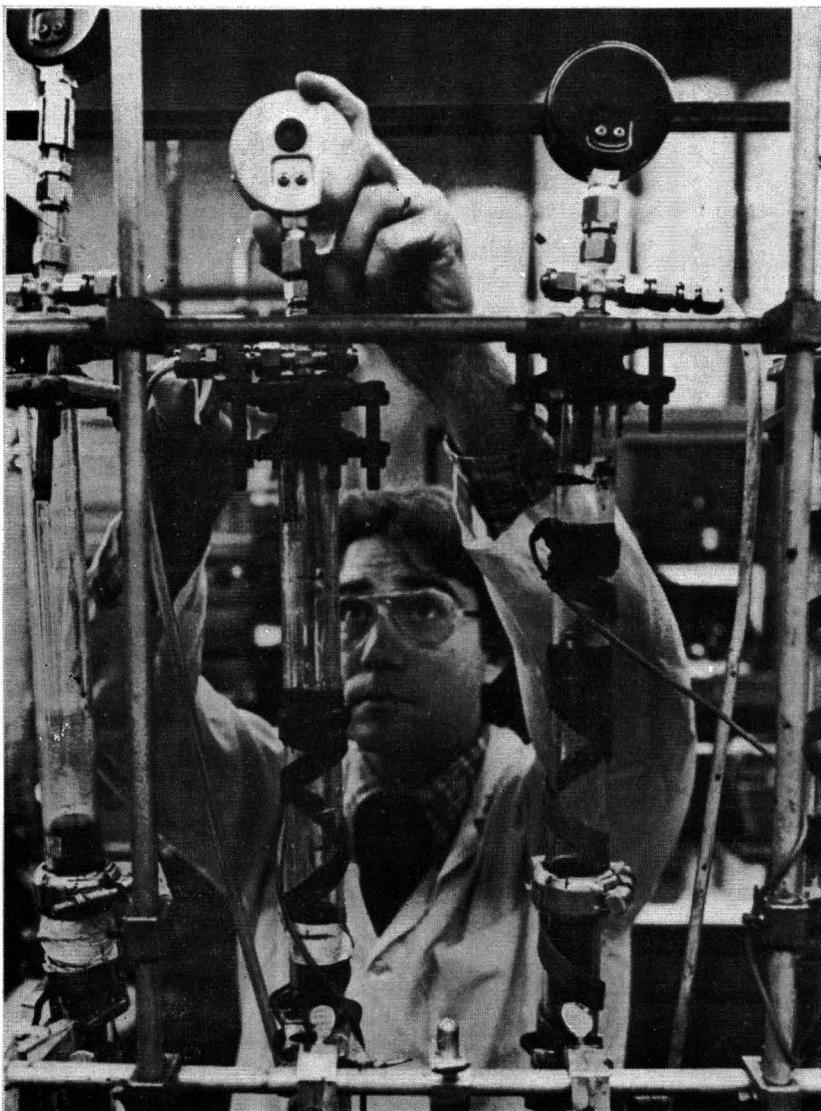
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SUPERHEATED LIQUIDS A LABORATORY CURIOSITY AND, POSSIBLY, AN INDUSTRIAL CURSE

Part 3: Discussion and Conclusions

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MOLTEN SALT-WATER EXPLOSIONS

ANDERSON AND ARMSTRONG (1973) injected water into molten sodium chloride under carefully controlled laboratory conditions (Figure 19). The vertical force resulting from the explosion was monitored with a transducer as shown. High speed motion pictures were also obtained. The key results are:

- explosions could begin in the bulk salt or at points on the crucible wall touched by the water jet,
- the water jet was coherent and separated from the salt by a vapor film until the explosion occurred,
- no freezing of the salt was noted.
- there were delay times of a few ms to a few hundred ms between injection and explosion,
- the explosion step developed very rapidly. Even with the highest framing speed (65 μ s/frame), the explosion occurred between successive frames.

In a later study, to explore larger scale interactions, water columns were allowed to fall upon a molten-salt surface (Anderson et al., 1975). Surprisingly, no coherent explosions were noted. High speed photographs showed, however, that the coherent water column was always preceded by a few drops of water. As the authors noted: "The contact of these leading water droplets with the salt caused minor explosions of sufficient magnitude to either break the apparatus or reverse the motion of the water column and prevent major contact between the molten salt and water."

Throughout, we have continued to suggest vapor explosions may occur when the volatile fluid superheats, nucleates, and fragments both the hot and cold liquids thus sustaining and enhancing the violence of the ultimate explosion. Yet Anderson and Armstrong's careful experiments force us to re-examine this model. Refer to Figure 20 from

their paper. This bar graph indicates the important temperature levels of the NaCl-water system. Water at 20°C contacts salt at 1000°C. At the water-vapor film boundary, the temperature is presumably close to 100°C while in the salt-vapor boundary it is between 800 and 1000°C. The calculated interface temperature using a two-slab, perfect-contact theory* is 691°C—a value exceeding the minimum film boiling temperature of 500°C (Henry, 1972). The critical temperature of water is 373°C, and the homogeneous nucleation temperature is \sim 300°C. These values indicate that liquid-liquid contact should not be possible as the resulting interface temperature would cause immediate film boiling of water and freezing of the salt.

Similar temperature bar-graphs could have been constructed for the titanium-water, smelt-water, and aluminum-water cases described in Part 2. Similar conclusions could also be drawn; how can superheating and homogeneous nucleation processes play a role in such cases?

A valuable observation is provided by Anderson and Armstrong (1973): "Reinspection of the . . . NaCl-H₂O movies show that every explosive case was initiated by an external force which tended to drive the two liquids across the insulating vapor film into near or actual contact with each other." The external force may be due to instabilities in the film, external causes, etc. However, as noted "(if) the fluids actually come into

*Eq. (11), Part 2.

We know superheated liquids exist. In the laboratory they behave as expected from theoretical considerations and distintegrate violently when heated to their superheat limit temperature.

contact, the theory would predict immediate surface vapor production which, in turn, would inhibit further heat transfer between liquids."

Anderson and Armstrong proposed this "dynamic impact heating model" and indicated that, when the hot and cold liquids are in close proximity, the heat transfer rate may be high enough to vaporize water in a short period of time. This

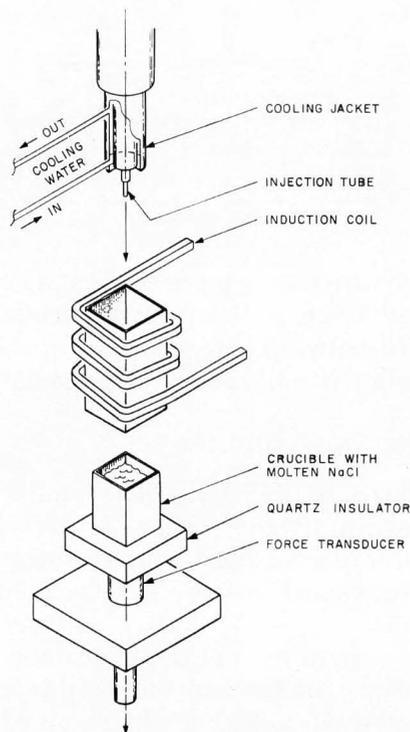


FIGURE 19 INJECTION OF WATER INTO MOLTEN NaCl

vapor production then causes (somehow) other near contacts and the explosion propagates.

Perhaps there is a critical impacting force. If too small, then, as the liquids approach, the increase in vapor generation opposes the force and the gap widens. On the other hand, for impacting forces greater than the critical value, very close contact may be achieved. Evaporation increases rapidly but may there be a limit to this rate? Kinetic theory suggests that the limit would occur when the flux $\sim (1/4) \rho \bar{v}$. ρ is the mass density of the vapor in the film and \bar{v} the average molecular velocity. The maximum evaporating flux is then

$$q_{\text{evap}} = (1/4) \rho \bar{v} \Delta H_v$$

The energy flow into the water is given as

$$q_{\text{in}} = (k/\delta) (\Delta T)$$

with k the average thermal conductivity in the film of thickness δ . Using the NaCl-H₂O system as

an example, when $q_{\text{in}} = q_{\text{evap}}$, $\delta \sim 0.3 \mu\text{m}$. If the film thickness should become less than this value, energy is conducted into the bulk water to raise its temperature above 100°C. Should temperature of $\sim 300^\circ\text{C}$ be attained, homogeneous nucleation would result and intense, local shock waves develop. These, in turn, could provide the force to propagate the microevent to a macroexplosion.

The critical impacting force should vary from system to system and should increase as the temperature of the hot fluid increases. Experiments involving impinging drops of a volatile liquid onto a hot surface (preferably liquid) could be of value in testing this hypothesis. Unfortunately, most such experiments have employed small drops with sufficient drag to limit the impact velocity. However, if the hot fluid is only slightly above the homogeneous nucleation temperature of the cold liquid, then a less drastic model may suffice. Waldram et al. (1976) obtained vapor explosions with drops of many organic liquids on hot silicone oil.

SODIUM-URANIUM DIOXIDE EXPLOSIONS

TO ILLUSTRATE THAT VAPOR explosions are not confined to systems involving water, one need only cite the results obtained at the Argonne National Laboratory where the system molten sodium-molten uranium oxide has been studied. Obviously, these experiments were motivated by concern should a nuclear reactor ac-

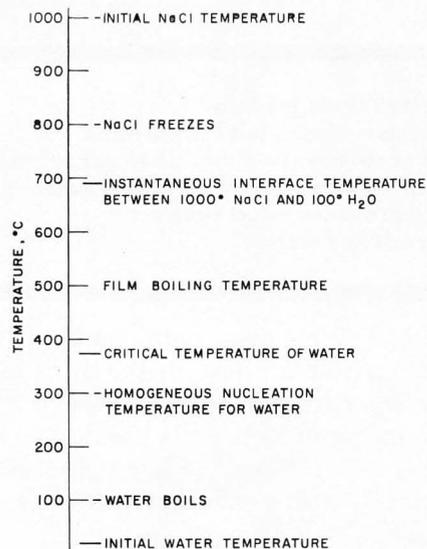


FIGURE 20 TEMPERATURES ASSOCIATED WITH H₂O-NaCl INJECTION EXPERIMENTS

cident in the LMFBR lead to this type of liquid-liquid contact.

The facts indicate that if liquid sodium is injected into molten UO_2 , vapor explosions are consistently produced (Armstrong et al., 1975; Henry et al., 1974). Sodium temperatures have ranged from the melting point to above 600°C with UO_2 temperatures up to 3200°C . Injection velocities varied from 0.35 to 35 m/s.

The important temperatures for this system are shown in Figure 21 (Fauske, 1977) assuming the sodium is initially at 400°C and the UO_2 at 3200°C . There are some significant differences between this case and the $\text{NaCl-H}_2\text{O}$ case discussed earlier.

First, the very high temperature required for film boiling indicates that contact between liquid sodium and liquid UO_2 would result in nucleate boiling—assuming that sufficient nucleation sites are available. Thus, the problem of heat transfer through a thin vapor sodium film is not present. However, if these two liquids do come into contact, and if boiling is suppressed, the theoretical two-slab interface temperature is only 1082°C ; this is below the temperature required for the homogeneous nucleation of sodium, so it would appear unlikely that a vapor explosion could result in a simple contact experiment.

Yet vapor explosions do seem to occur when liquid sodium is injected into molten UO_2 !

The model proposed by Fauske (1973, 1974) assumes that the injected sodium breaks up (at least partially) to form some small liquid sodium drops. A Weber number criterion of about 10^*

"The contact of these leading water droplets with the salt caused minor explosions of sufficient magnitude to either break the apparatus or reverse the motion of the water column and prevent contact between the molten salt and water."

indicates that stable drop radii can be as small as $20\ \mu\text{m}$. With a drop of this size, the theoretical two-slab interfacial temperature in Figure 21 is not relevant and the drop tries to heat up to the bulk UO_2 temperature. When the homogeneous nucleation temperature is reached, it explodes and the

* $N_{we} = \rho r^2 V^2 / \sigma$ with ρ the sodium density, r the stable drop radius, V the relative velocity of the sodium- UO_2 , and σ the interfacial tension.

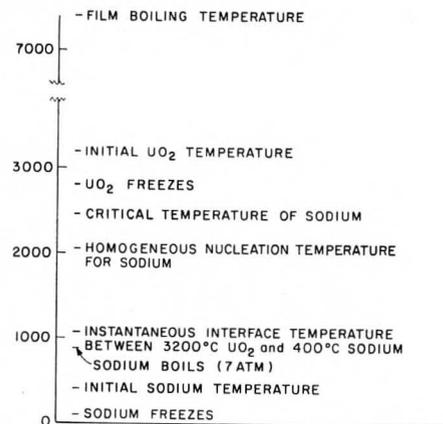


FIGURE 21 TEMPERATURES ASSOCIATED WITH Na-UO_2 EXPERIMENTS

local shock waves propagate the reaction by causing further fragmentation. In this model a delay is predicted between injection and explosion and this prediction is confirmed by experiment.

DISCUSSION AND CONCLUSIONS

WE KNOW SUPERHEATED liquids exist. In the laboratory they behave as expected from theoretical considerations and disintegrate violently when heated to their superheat limit temperature.

We also know of numerous instances where discrete masses of hot and cold liquids have been contacted (on purpose or as the result of an accident) and where this contact has resulted in an explosion. Of course, we must also admit that in a number of other similar cases contact led to no explosion.

In this paper we have taken a biased position in an attempt to link superheated liquids to vapor explosions. This is a minority position and the field is active and in ferment as new theories and experiments appear and demand to be given their due before any general explanation is accepted. There may, in fact, be no single, universal cause for vapor explosions and each particular situation should then be examined separately. We have rejected this hypothesis since there are too many commonalities in the various events reported. It is true, however, that in various vapor explosions there may be different parameters which assume primary importance in determining if a coherent vapor explosion will occur.

In the past decade, numerous theories have been proposed which do not involve superheated

Continued on page 203

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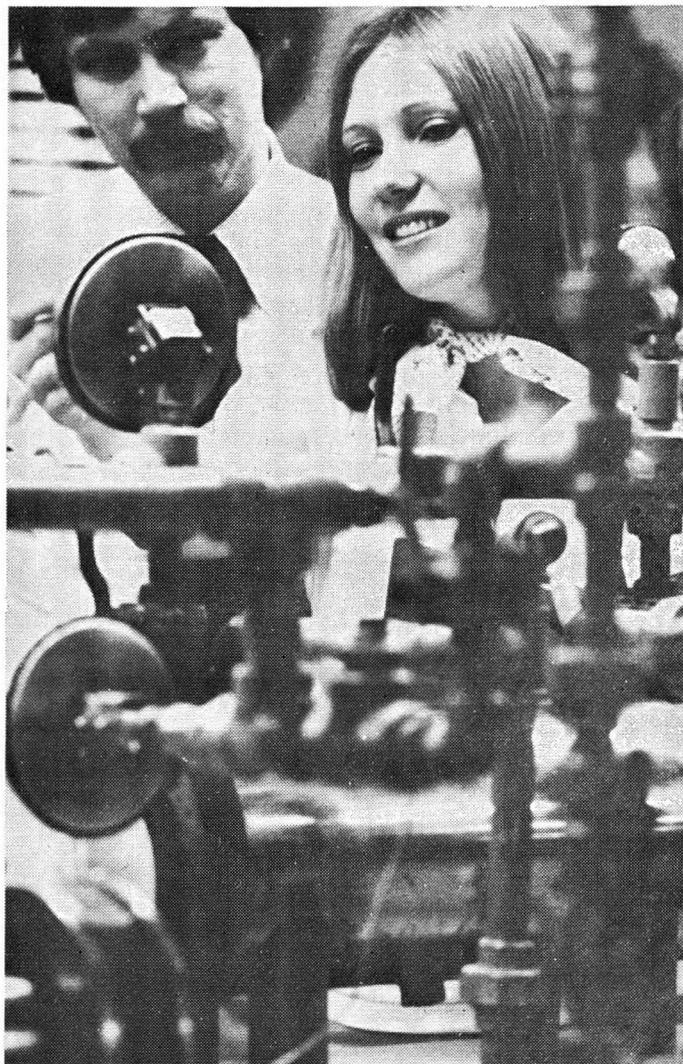
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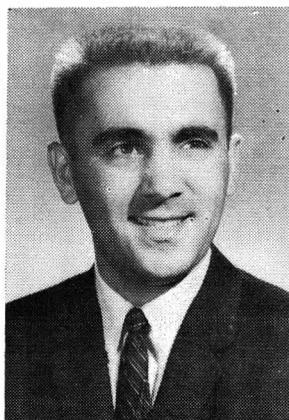
CHEMICAL ENGINEERING EDUCATION REVISITED

LOUIS THEODORE

*Manhattan College
Riverdale, New York 10471*

LAST YEAR, Joe Reynolds—my department chairman and long-time friend—approached me about the possibility of my attending the Summer School Workshop for Chemical Engineering Faculty. He felt the trip would do me good since most of my professional interests and consulting activities in the last six years have been in air pollution. In addition, my wife was excited about the possibility of another trip to the Colorado area. The Workshop, conducted in Snowmass, Colorado, provided the right atmosphere for a conference of this nature. A total of 36 sessions were offered in the program with topics varying from Unified Rate Concepts to Workload Evaluation.

After some manipulation, I had Mike Williams, one of the Workshop Directors, assign me to the following sessions on kinetics:



Louis Theodore received his B.Ch.E. from the Cooper Union in 1955 and his M.Ch.E. (1957) and Eng.Sc.D. (1964) from New York University. He is presently Director of Research for Manhattan College's ChE Department. Dr. Theodore has had wide experience as an industrial consultant and lecturer, and is the author or co-author of numerous publications and texts. Two main areas of interest are in air pollution and computer application.

1. Applied Chemical Kinetics.
2. Catalysts and Physical Chemistry of Catalyst Systems.
3. Chemical Reaction Engineering.

I specifically requested these sessions because I teach Chemical Reactor Design, a required senior-level course in ChE at Manhattan College. I had always felt that the course suffered somewhat in that I did not provide enough practical applications. I hoped that attending these sessions would help alleviate this problem. Unfortunately, this proved not to be the case. The lectures, which primarily centered on program curricula and course content, emphasized the theoretical rather than the design or pragmatic approach to ChE. For example, Session (1): Applied Chemical Kinetics, contained no applications, at least not as I have come to know the meaning of that term as an engineer. As another colleague at the workshop commented: the use of the word "applied" by this professor was an insult to any engineer's intelligence. These sessions served to substantiate the fears of a good number of ChE professors and industrial personnel: education in ChE programs at so many of the "big-name" schools has gone off the deep end. Course content seems to emphasize the professor's research and/or professional interests with little or no regard for the real needs of a ChE student. So much time is apparently spent on material that will serve no use to the practicing engineer. For example, the emphasis on the presentation at Session 1 was on kinetic theory. Yet, I would defy anyone to provide me with a case study where a reactor was designed using kinetic theory. Much of this useless material could be removed from course offerings if the professor would simply ask (and answer) the following question before entering class: Will the student ever use this material?

The same criticisms of the kinetics course offerings can also be leveled at so many other courses. I say this because of the recent prolifera-

tions of texts in ChE that have emphasized the fundamental rather than the engineering approach. Texts seem to be written by professors for their colleagues rather than their students. This has caused several of us at Manhattan to use earlier editions of ChE publications.

I would issue a call to those responsible individuals in ChE education to put an end to this nonsense. Something has to be done, and it *must* be done soon.

REFERENCE

1. CEP, August 1976, pages 13-16.

ChE book reviews

STRATEGY OF POLLUTION CONTROL

By P. Mac Berthouex and Dale F. Rudd,
John Wiley and Sons, 1977.

Reviewed by Noel de Nevers, University of Utah.

This book is very similar in organization, style, and contents to "Process Synthesis" by Rudd, Powers and Siirola, Prentice-Hall, 1973. It has the same basic organization and style and borrows several large sections verbatim from that book. Those who like that book will like this one.

In this book, Professor Rudd has teamed with Professor Berthouex, who is an expert on waste water treatment and water supply, to produce a book which might better be named, "Process Synthesis, Rewritten to Emphasize Water Pollution Control."

In both books, a very brief and sketchy treatment is given of conservation of mass, conservation of energy, equilibrium relationships, and rate equations. The subjects are illustrated by numerous excellent examples.

It is interesting to speculate what the audience for this book will be. The reviewer has personally used "Process Synthesis" as a text for an "Introduction to Chemical Engineering for Freshman" course. The response seems to be that the professor likes the book and the students don't. It is, to some extent, over their heads. However, it does not seem to fit logically into the Chemical Engineering curriculum anywhere else. Similarly, "Strategy of Pollution Control" seems to have no obvious place in the Chemical Engineering curriculum. The emphasis is very heavily upon waste

water treatment. As a Chemical Engineer who does not know a great deal about waste water treatment, the reviewer found the discussions and examples there very interesting. But he scarcely feels competent to teach a course on waste water treatment based on the availability of this textbook (and knowing the obvious jurisdictional conflict with the active water pollution control group in our Civil Engineering Department).

The best part of this book (as is the best part of "Process Synthesis") is the abundance of well-worked out and very interesting examples. In both books, these are truly outstanding, and justify the purchase of the book by many engineers merely to have the opportunity to study these interesting examples.

The reviewer has several minor criticisms; first, the title of the book is misleading. Very little is said about the strategy of pollution control. Mostly, the discussion is about internal optimization of waste water treatment facilities given a set of externally applied constraints which the engineer has relatively little to say about. "Strategy of Pollution Control" implies a global view of what we ought to be doing in the pollution control field, given our limited resources and limited knowledge of the true effects of various pollutants on ourselves and other parts of the ecosystem. Second, although the authors have provided some literature references, they are not as careful in citing sources for their material as they should be. For example, figures 7.5.8 and 7.5.17 are direct copies of figures 5.82 and 20.99 of Perry "Chemical Engineers Handbook," Fifth Edition. This is not mentioned at all in the place where these figures are introduced, and the only clue the reader is given that these might be from that source is a reference in the bibliography at the end of that chapter to Perry's as a general reference source in this area. Third, the three-page, double-spaced index is inadequate.

In summary, chemical engineers who wish to see a chemical engineer's view of the whole waste water treatment problem, with various other pieces of information about other pollution problems appended, will find this a very interesting and useful book. The reviewer sees no place where it will fit in as a textbook in any standard chemical engineering course except if there is a faculty member who is strongly involved in waste water treatment, and who can teach this subject without jurisdictional conflict with the civil engineers. □

INFLUENTIAL PAPERS

Continued from page 162

articles they liked best and which two they liked least. The results are given in Table V. Perhaps there is a message here, perhaps not.

My opinion is that the course was less efficient than a conventional textbook course in teaching facts, concepts, methods, etc. Still it was much more effective in conveying a comprehensive view of chemical reaction engineering than anticipated. The dynamics of history are not so easily and dramatically conveyed via technical texts. Also, with this course format, it was natural to bring each topic right up to date. With one or two exceptions only, these "influential papers" were excellently written. The students enjoyed a realistic teaching experience. Because of the nature of

TABLE V
Article Preference

	(most - least = net)
Hougen & Watson	(6 - 0 = 6)
Thiele	(3 - 0 = 3)
Carberry	(3 - 1 = 2)
Danckwerts	(3 - 1 = 2)
Denbigh	(2 - 0 = 2)
Weisz & Hicks	(2 - 0 = 2)
van Krevelen & Hoftijzer	(2 - 0 = 2)
van Heerden	(1 - 0 = 1)
Weekman	(1 - 1 = 0)
Voorhies	(1 - 2 = -1)
Flory	(1 - 2 = -1)
Singer & Wilhelm	(1 - 4 = -3)
Aris & Amundson	(0 - 6 = -6)
Chu & Hougen	(0 - 9 = -9)

their involvement, they were surely provided with a strong feeling for the flow of research and technology.

There is much more to be said about the central and related papers than can be accommodated by this article. At the suggestion of one respondent, Michel Boudart, it is my intention to prepare an annotated collection of "Influential Papers in Chemical Reaction Engineering." Your suggestions on papers to be included will be appreciated.

ACKNOWLEDGMENTS

I would like to acknowledge the contributions of the respondents to the original survey and the students in the course. Special thanks go to Mr. Deepak Perti for his assistance in the large

amount of library work necessary to develop this course and for his service as a specialist in an area where he had unique expertise. □

APPENDIX

CHEMICAL ENGINEERING 535

Assignments

Monday 28 March 1977

Read Hougen and Watson (1943)

Work #1 and 2 below.

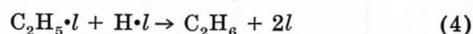
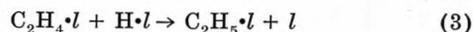
Wednesday 30 March 1977

Read Weller (1956) and Boudart (1956). Photocopies of these two articles are available in the ChE Reading Room and on reserve in the Physical Sciences Library. In addition the *AIChE Journal* is available in both of these locations.

Optional reading—Weller (1975) gives excellent up-to-date perspective on the topic of catalytic kinetics. Copies of this article are also located in the reading room and the library.

Work #3 and 4 below.

- The vapor phase hydrogenation of ethylene ($C_2H_4 + H_2 \rightarrow C_2H_6$) on a well dispersed platinum catalyst (0.05% Pt on SiO_2) is described by Sinfelt, *J. Phys. Chem.*, 68, 856 (1964). The overall reaction is virtually irreversible and is considered to occur according to the following mechanism.



Reaction (4) is very rapid. Reaction (3) is the rate determining step.

- Use the methods of Hougen and Watson (1943) to derive an equation for the rate of reaction of ethylene. The equation should contain only rate and equilibrium constants and partial pressures of the reaction components.
 - It is known that hydrogen adsorption, although significant (K_H is finite) and necessary, is slight. Use this information to simplify your rate equation.
 - At rather low temperatures the rate of reaction at constant ethylene partial pressure will be directly proportional to the square root of the hydrogen partial pressure and at constant hydrogen partial pressure will be inversely proportional to the ethylene partial pressure. Explain why these experimental observations are consistent with your rate equation from part (b).
- Write a three dimensional, unsteady state mass balance on a differential element of a fixed bed catalytic reactor. Show how to reduce this equation to the one dimensional, steady state form for a plug flow reactor, given by equation (56) in Hougen and Watson (1943).
 - Refer back to the system of problem #1. For experiments conducted at constant P_{H_2} but over a wide range of $P_{C_2H_4}$, sketch a graph of $\log r$ vs $\log P_{C_2H_4}$. Indicate quantitative features on the graph where you can.

4. Akers and White, *Chem. Eng. Progr.* 44, 553 (1948) reported the following data for the synthesis of methane from CO and H₂ over a nickel-kieselguhr catalyst at 1 atm and approximately 300°C with a feed gas containing 44.5% CO, 53.9% H₂, 0.4% CO₂ and 1.2% inert.

lb catalyst-hr/mol feed	mol CH ₄ in product/mol feed
7.13	0.187
2.97	0.154
1.68	0.120
0.38	0.045

Determine the specific rate and tabulate as a function of the mol CH₄/mol feed.

Examination #1 (Take home)

1. In Hougen and Watson (1943)* equation (12) gives the rate of a catalytic reaction in terms of adsorbed phase concentrations and the concentration of vacant sites, c_v . In equation (14) the adsorbed phase concentrations are gone and fluid phase concentrations appear. During our study of this paper, one student asserted that there was an error in equation (14). Show in complete detail how equation (14) is obtained from equation (12). If there is an error in equation (14), give the correct result and compare it to equation (14).

SUMMARY OF STUDY ON HOUGEN AND WATSON (1943)

This excellent paper was a remarkably comprehensive, trendsetting, and futuristic paper. It dealt effectively with many of the topics which have proved to be important in the more than thirty years since its appearance. Among these are catalytic kinetics, catalyst deactivation, effectiveness factors, external mass transfer, and fixed bed reactor analysis and design. One can see that many of the topics now considered crucial in research, teaching, and practice of chemical reaction engineering were anticipated by Hougen and Watson. This review chooses those two items in which the impact of this 1943 paper has been greatest: catalytic kinetics and the tubular reactor mass balance,

$$r \rho_B dV = F dx_A.$$

The above equation provided a quantitative basis for rational tubular reactor design. Before its appearance semi-quantitative scale up procedures were used. A rather sophisticated illustration of this earlier mode of thought can be provided by reference to an article by Emmett and Kummer (1943). There they give 9 graphs of % NH₃ in the exit gas versus space velocity for three temperatures, three pressures, and three N₂:H₂ feed ratios. From such graphs (which might come from the laboratory or pilot plant) encompassing the processing conditions of interest, one can find the space velocity to achieve a specified conversion. With the assumed analogy between tubular and batch reactors, the intuitive argument that the space veloc-

*Some errata in Hougen and Watson (1943) are as follows:

Eqn (9), C_A should be C_A'

p. 531, left side, line 1, C_{Ai} should be C_{A'i}

Eqn (14), K_A C_{Ai} C_i should be K_A a_{Ai} C_i

p. 533, left side, line 3, 25 should be 27

p. 533, left side, line 10, unadsorbed should be unadsorbed

p. 538, right side, line 4b, absorption should be adsorption

My opinion is that the course was less effective than a conventional textbook course in teaching facts, concepts, methods, etc. Still it was much more effective in conveying a comprehensive view of chemical reaction engineering than anticipated.

ity is inversely proportional to the contact time (imperfect for reactions like ammonia synthesis in which there is a change in the total moles), and the hypothesis that only contact time determines the conversion, the pilot plant could be scaled up directly by calculating the commercial reactor volume from the space velocity and the specified commercial feed rate. It would remain to determine the reactor shape (usually characterized by the length to diameter ratio) from previous experience with similar systems. Major factors in this determination would be catalyst characteristics and heat transfer. Among other things, it was the physical processes like heat and mass transfer and mechanical characteristics of catalysts and reactors that made scale up from small to large reactors so uncertain.

Apart from its design application, the tubular flow reactor mass balance enabled the isolation of reaction kinetics from reactor characteristics. This in turn allowed much better reaction rate data to be obtained in catalytic reactions and led ultimately to improved characterizations (rate equations) of catalytic kinetics.

Probably the earliest attempts to write rate equations for heterogeneous catalytic reactions followed the equation forms which had proved satisfactory in homogeneous reaction rate studies. Empirical use of such equations continues today with a vigorous endorsement in a prominent textbook (Levenspiel, 1972). At the same time the approach of Hougen and Watson finds wide application among academic and (more significantly) industrial practitioners.

The catalytic rate equations of Hougen and Watson stem directly from a classical paper by Langmuir (1922) in which he proposed a number of catalytic mechanisms based upon his monolayer theory of chemisorption. Hinshelwood (1940) applied Langmuir's treatment to a large number of reactions. This approach has become known as the Langmuir-Hinshelwood model of heterogeneous catalysis. Hougen and Watson (1943) rather independently developed, extended, and popularized this model for chemical engineering use. Yang and Hougen (1950) systematized the previous work bringing together the rate equations for many situations and putting them into a generalized form. So influential were these works that the model became known as "Hougen and Watson rate equations" and its use and abuse exploded. In 1956, back-to-back articles by Weller and Boudart appeared. Weller suggested that the Langmuir-Hinshelwood, Hougen-Watson approach does not have the theoretical validity commonly attributed to it and that, lacking theoretical validity, it is unnecessarily complex for use as an empirical equation when compared for simplicity to the common power function (homogeneous) type of equation. Boudart supported the rational use of the L-H, H-W approach with his discussion of the limitations and strengths of that theory. Kabel and Johanson (1962) made an experimental attempt to reconcile the argument using the ion exchange resin catalyzed dehydration of ethanol. They found that the Langmuir equilibrium adsorption constants de-

rived from a Hougen and Watson kinetic analysis of the rate data agreed quite well with the corresponding constants obtained directly from independent adsorption experiments. Their results generated other papers by Lapidus and Peterson (1965), Kabel (1968), and Mezaki and Kittrell (1968).

Almost 20 years after his original article Weller (1975) has written a very comprehensive analysis of the state of catalytic kinetics. It is recommended reading for those wishing an up-to-date perspective.

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ChE book reviews

SI UNITS IN CHEMICAL ENGINEERING AND TECHNOLOGY

By K. D. Chandrasekaran and D. Venkateswarlu
*Indian Institute of Technology
Madras, India. June 1974.*

Reviewed by G. R. Youngquist
Clarkson College of Technology

This paperbound four-chapter handbook presents a summary of the SI system of units, conversion factors, and tables of numerical data in SI for physical and thermal properties. The first chapter briefly but adequately introduces the SI system along with conventions for its use and

provides an extensive list of derived units which are of interest to chemical engineers. The second chapter is devoted to SI units for quantities commonly used in chemical engineering practice. Fifty-five tables listing the preferred SI unit, recommended multiples, and conversion factors for quantities such as mass transfer coefficients, heat flux, viscosity, thermal conductivity and the like are given. The third chapter consists of 88 tables of physical constants, physical properties of solids, liquids, and gases, and thermochemical and thermodynamic properties of selected substances. These are more extensive than found in a typical textbook, but quite naturally less complete than other handbook sources. The final chapter provides 20 example problems.

The background information presented is concise and should be sufficient for most users of SI. The conversion tables are convenient, and the tables of data serve a useful purpose in the absence of other sources which use SI. The book is suitable for desk reference or as a textbook supplement. An annoying feature of the book was the poor quality of the binding. Even the brief use encountered in the course of this review caused several pages to detach. □

FUEL CELLS

By Angus McDougall, Halstead Press, a division of John Wiley & Sons, New York, N.Y. 1976.

Reviewed by Robert D. Walker, University of Florida

This small book of thirteen chapters presents a reasonably adequate discussion of the major aspects of fuel cells at a quite elementary level. It will be useful, therefore, for introducing new students or casual readers to the subject without confusing them with unnecessary details. In spite of this advantage, however, it appears to this reviewer that the book suffers from a number of shortcomings. In the first place, the author includes no references to sources of the data used; indeed, there are no references to any other publications. The reader is, therefore, left with no suggestions as to more advanced literature. Secondly, the case for fuel cells as energy sources is consistently presented too optimistically; the efficiency and performance described are substantially in excess of those achieved practically. Finally, the usefulness of the book for the American reader is diminished by the author's discussion of British fuel cells alone; no American (or other) fuel cells are described. □

SUPERHEATED LIQUIDS

Continued from page 196

liquids. Most have been rejected as new data accumulate. We discuss the major ideas below and show that few are still viable.

Entrapment/Entrainment Theory. When hot and cold liquids are contacted, fragments of the cold (volatile) liquid are assumed to be entrapped or entrained in the hot liquid (Groenveld, 1972; Brauer et al., 1968). Rapid vaporization results and the hot liquid is dispersed. The resultant large area for heat transfer then leads to an explosion. Variations in this hypothesis consider a crust forming on the hot liquid so that any entrained cold liquid, while vaporizing, develops a high pressure. Rupture, when it occurs, leads to the fragmentation of the hot liquid. Another, similar theory, assumes that the cold liquid is trapped on a wall or bottom by the hot fluid and, as noted above, boils so violently that immediate dispersal of the hot fluid results.

As evidence against the entrapment theory, Anderson and Armstrong (1972b) injected water into molten NaCl and reported that, from high-speed movies, there existed a gas layer "between the two liquids during the injection and remained there until the explosion." The explosion duration was less than 65 μm and no salt crust formed. There is no evidence of any stray water droplets encapsulated in the molten salt. Also, in all the hydrocarbon-water tests where the cryogen was spilled on water, there was no indication that entrapment or entrainment occurred.

One method suggested for entrainment of cold liquid is that it would be drawn through voids in the surface crust as the interior hot liquid cools and contracts. This explanation does not seem viable since explosion-fragmentations have also been observed with hot mercury (which did not solidify) and with molten bismuth (which expands rather than contracts upon freezing). Finally, in some experiments (Witte et al., 1973), where there were several molten metal fragments near each other, a vapor explosion or fragmentation in one would trigger like events in those

nearby. This behavior is not indicative of an entrapment.

Weber Instability Theory. Another theory often mentioned as a partial explanation for vapor explosions is the hydrodynamic instability associated with the jetting of one liquid into another under conditions where inertial forces exceed surface tension forces. In such cases there will be a spontaneous fragmentation of the jetted stream into smaller fragments. The increase in area has been cited as a possible trigger to initiate rapid vapor production, further fragmentation, and finally an explosion.

While this instability is well known and may occur in some experiments, vapor explosions have been observed in many cases where this phenomenon could not play a part. No Weber instability was evident in the high speed movies of Anderson and Armstrong (1972b) when they jetted water into molten NaCl. Also, the spill tests in the cryogen-water studies could have had no such initial fragmentation. Witte et al. (1970, 1973) conclude that, even if the critical Weber number were exceeded, and some break-up has occurred, this process has little or no effect on the probability of a vapor explosion occurring at the same or at a later time. McCracken (1973) discounts any Weber number effect as his experiments with injection of molten metals into water indicated a sharp transition between explosions and no-explosions as the coolant temperature was varied over only a few degrees. Such a variation would have little effect on Weber instabilities.

Henry and Armstrong (1976) studied the reaction of single drops of organic liquids in water when exposed to shock waves generated by an exploding wire. Even though the conditions were such as to greatly exceed the drop's critical Weber number for a few μs , no drop fragmentation was noted. Thus, extreme local interactions would not seem to be important in fragmenting drops via a Weber instability.

It is, therefore, now generally accepted that this hydrodynamic effect, though it may occur in certain experiments, plays no major important role in vapor explosions.

In this paper we have taken a biased position in an attempt to link superheated liquids to vapor explosions. This is a minority position and the field is active and in ferment as new theories and experiments appear and demand to be given their due before any general explanation is accepted. There may, in fact, be no single, universal cause for vapor explosions and each particular situation should then be examined separately.

Another theory . . . is the hydrodynamic instability associated with the jetting of one liquid into another under conditions where inertial forces exceed surface tension forces.

Transition Boiling. In this hypothesis, the cold liquid begins to vaporize in the film boiling regime, but as the temperature difference between the two liquids decreases, the Leidenfrost point is reached and transition boiling begins. In this regime, there is some liquid-liquid contact as the vapor bubbles form and leave; if the cold liquid is sub-cooled, the bubbles may even collapse as the turbulence in the interface region increases. It is further postulated that the violence of boiling in this regime is sufficient to fragment the liquids so as to expose extensive area for heat transfer; if this fragmentation is sufficient, an explosion results.

This explanation was first proposed by Swift (1965) and is discussed in detail by Stevens and Witte (1972) and Witte et al. (1970). But, in later papers (Witte and Cox, 1971; Witte et al., 1973), the transitional boiling hypothesis is rejected since the oscillations associated with this regime are in the ms time scale range, much too long unless the very initial contact between liquids is all that is necessary for rapid fragmentation. Brauer et al. (1968) saw no evidence of violent boiling prior to explosions when high speed photographs were studied, but McCracken (1973) feels that the sensitivity of metal-water explosions to water temperature is in agreement with the transition boiling hypothesis.

A number of analyses have been made to predict the temperature difference between fluids when the minimum flux is attained and transition boiling could begin (Henry, 1972; Berenson, 1961; Spiegler et al. 1963; Baumeister and Simon, 1973; Sciance and Colver, 1970; Bell, 1967). Some are based on hydrodynamic and heat transfer models while others are related to thermodynamic stability. No correlation fits all the data with much accuracy; of course, there is a wide spread in some experimental measurements and this indicates that probably there exists a temperature range over which there is a transition from film to transitional boiling. It is also interesting to note (Baumeister and Simon, 1973) that for organic liquids or low-boiling inorganic cryogenes, a good estimate of the Leidenfrost point is often given by the hot surface temperature, T_s , where T_s is the

expected value where for the cold liquid, $(dP/dV)_T = 0$. This is the same criterion introduced in Part 1 to obtain the superheat-limit temperature for pure components.

Most investigators now reject the transition-boiling hypothesis as the major cause of vapor explosions. It is granted that in this boiling regime, the interactions at the surface are rather violent and chaotic; however, this wetting/vaporization/wetting cycle is believed to operate on too long a time scale to cause the very rapid phenomenon of vapor explosions. Also, no one has noted the onset of transitional boiling before a vapor explosion occurred. Rather, there is sometimes a stable film boiling process which, for some reason, ceases, the film collapses very fast and an explosion follows almost simultaneously.

Chemical Reaction Theory. Basically, this concept envisages a rapid (usually exothermic) chemical reaction occurring at the interface. No evidence is available to suggest this is a viable concept.

Inertial Theory. This model is the most difficult to describe in simple terms. A hot and cold liquid are assumed to contact over a limited surface area. Some vapor is formed in the cold but volatile liquid. This vapor film begins to grow but is restrained by the inertia of the bulk liquid phase. The pressure rises. The expansion, while slow initially, accelerates and the bounding liquid is forced away from the interface. The inertial movement of this liquid continues even as the pressure of the vapor drops—and, in fact, can proceed so far as to produce a very low pressure in the vapor film. The bounding liquid then springs back and at this point there are several different theories, all

Most investigators now reject the transition-boiling hypothesis as the major cause of vapor explosions.

of which predict further oscillations leading eventually to violent gross mixing, fragmentation, and explosive boiling.

It is difficult to find compelling reasons either to reject or accept the inertial theory. It may, in fact, be integrated into the superheat-limit theory by providing the mechanism to bring the hot and cold liquids into contact (or near contact).

Board et al. (1974) suggest a somewhat similar concept but they propose that upon film collapse a

jet of liquid is driven across the thin vapor film; fragmentation that results leads to a repeating chain mechanism that is noted in its entirety as an explosion.

CONCLUDING REMARKS

BOARD AND CALDAROLA (1977) have reviewed the extensive data of importance to fuel-coolant interactions in fast reactors and, in addition, discussed much of the available information concerning molten metal-water explosions. From this detailed study, they conclude that energetic vapor explosions always involve three sequential stages:

- a relatively quiescent mixing phase where there is formed a coarse mixture of the hot and cold liquids. The "dwell" time corresponds to this period. The hot and cold liquid fragments are believed to be separated by a vapor film.
- a trigger of short duration (which may be highly localized) that leads to the collapse of the vapor film.
- a propagation step where the interaction rapidly spreads throughout the mixture.

One may infer that vapor explosions could be prevented by eliminating either or both of the first two steps. As stated by Board and Caldarola, "... it is difficult to determine the true explosive potential of a material pair from experiments in which the initial mixing or triggering conditions are left to chance".

Few careful experiments have been carried out to study each of these steps. The R-22 studies by Anderson and Armstrong (1977) do, however, provide some support.

In our work with light hydrocarbons on water, we have possibly neglected the importance of having an initial coarse mixing step and emphasized only the trigger—which we have associated with the cold cryogen film adjacent to the water attaining the superheat-limit temperature. In our direct pours of light hydrocarbons into water, there may indeed have been significant mixing and fragmentation prior to any trigger. But, we also have contacted LNG by tangentially skimming the cryogen over the surface and, even here, we have noted vapor explosions in the same compositional ranges as those found in direct pour experiments.

Also, we have possibly been in error in neglecting the mixing step as being of prime importance because we have been able to obtain or prevent vapor explosions by relatively small changes in either the composition of the LNG or the initial water temperature. We assumed that such minor

changes would have an insignificant effect on the mixing step and only affect the trigger. An active or inactive trigger could be explained well by superheated liquid theory for either variations in LNG composition or water temperature. As pointed out by Anderson (1977), however, the LNG composition and water temperature effects may also affect the film boiling characteristics of the system and this effect could be more important than that involving homogeneous nucleation of a superheated liquid. This critique is important because if superheating plays no real role in the triggering step, then one must (as Anderson states) "recognize the possibility of an explosion in a system where a gas or vapor film is present even when the interface or hot liquid is below the homogeneous nucleation temperature".

More definitive research is needed to clarify the mechanism(s) for vapor explosions. It is, nevertheless, important that any acceptable theory should consider all the facts and experimental data. We still believe that homogeneous nucleation of superheated liquids plays an important role and may even explain the old Blacksmith's adage as told by Dr. Beall:

"When you spit on a piece of red hot iron, it dances around in a little ball. If you hit the ball with your hammer, the explosion will throw the hammer over the barn and blow a hole in the iron!" □

ACKNOWLEDGMENT

Discussions with R. P. Anderson and D. R. Armstrong were very helpful in preparing this manuscript.

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ChE book reviews

THE PRIMARY BATTERY, VOL. 2

Edited by N. Corey Cahoon and George W. Heise. Published by John Wiley & Sons, Inc., New York (1976). 528 pages, \$37.50.

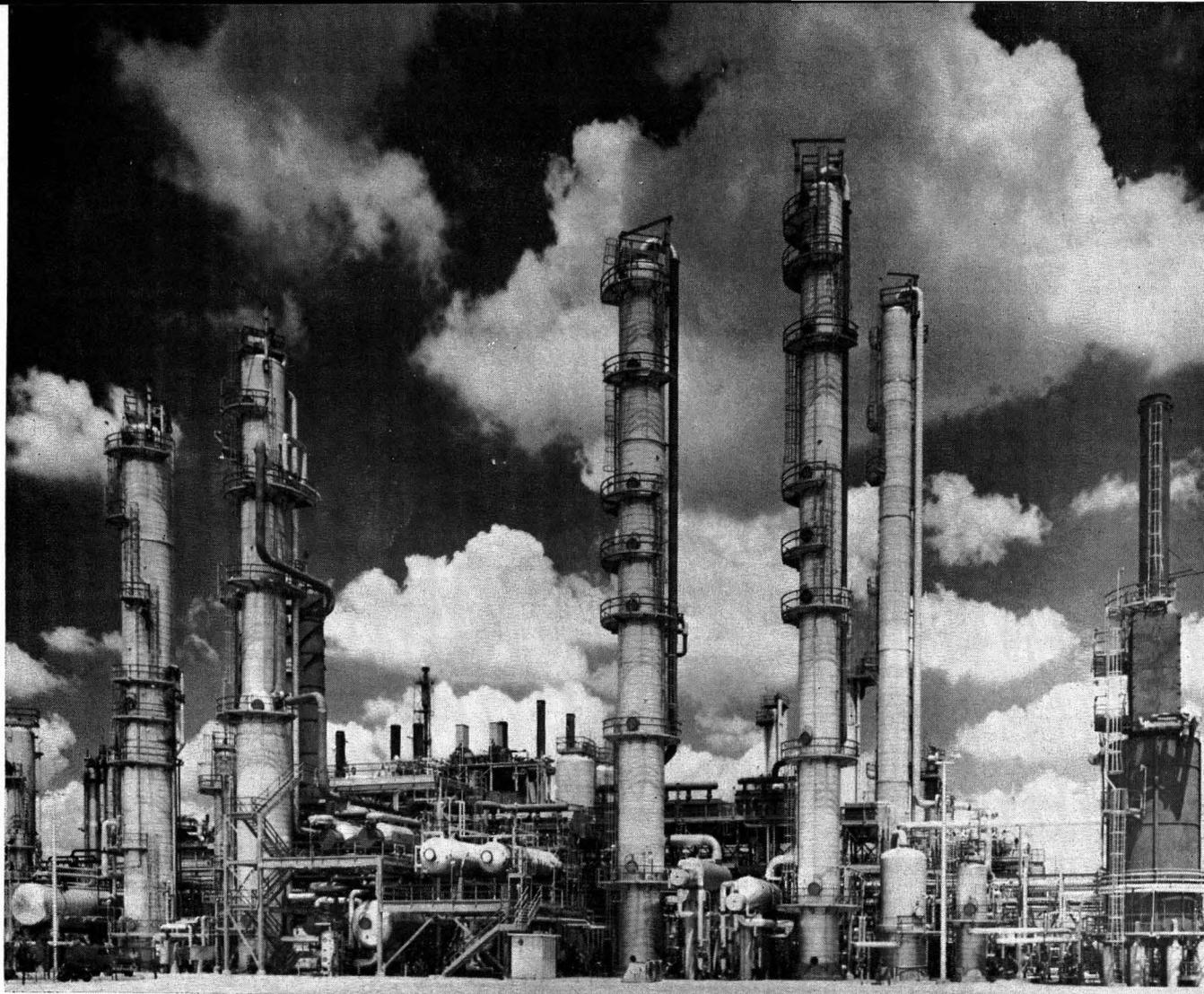
Reviewed by Irwin B. Weinstock
General Electric Company

This is the second in a 2-volume set planned to present a comprehensive view of the primary battery field. It consists of eleven papers covering: Leclanché and zinc chloride cells; magnesium cells; aluminum cells; organic cathodes and anodes; low temperature systems; thermal batteries; water-activated batteries, standard tests for primary batteries; reversability of battery systems; measurement and interpretation of internal resistance; and a survey of energy sources and conversion mechanisms.

The individual chapters are well written, and contain much information which should be of value to serious workers in the field. The large amount of detail, however, makes the book hard to read. Readers with little or no background in the battery field may find it difficult to sort through this large amount of detail in order to discover the general principles governing the operation of the specific battery system being described.

The coverage of the field is, moreover, restricted, with heavy emphasis on the Leclanché cell and its analogs. Not only is the paper describing this system by far the longest in the book (147 pages), but most of the discussion in the chapters on battery testing and measurement of internal resistance is focused on this system. Similarly, the chapter on low temperature systems is almost exclusively devoted to a review of modifications to the Leclanché cell (non-aqueous systems were covered in Volume 1 of the series) and the discussion of organic depolarizers is largely limited to those potentially useful as replacements for manganese dioxide. A further restriction on the comprehensiveness and up-to-dateness of the book is the lack of any discussion of cells with lithium anodes which have been the subject of extensive development over the past 15 years.

Nonetheless, the complete 2-volume set should serve well as an authoritative reference on primary battery technology. The factors listed above, however, will in the opinion of the reviewer, limit the usefulness of this volume as a textbook on the subject. □



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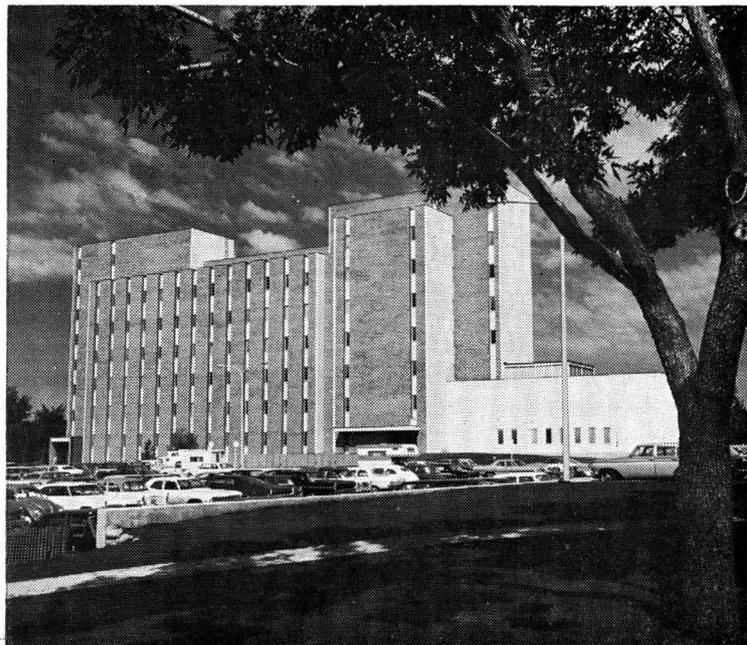
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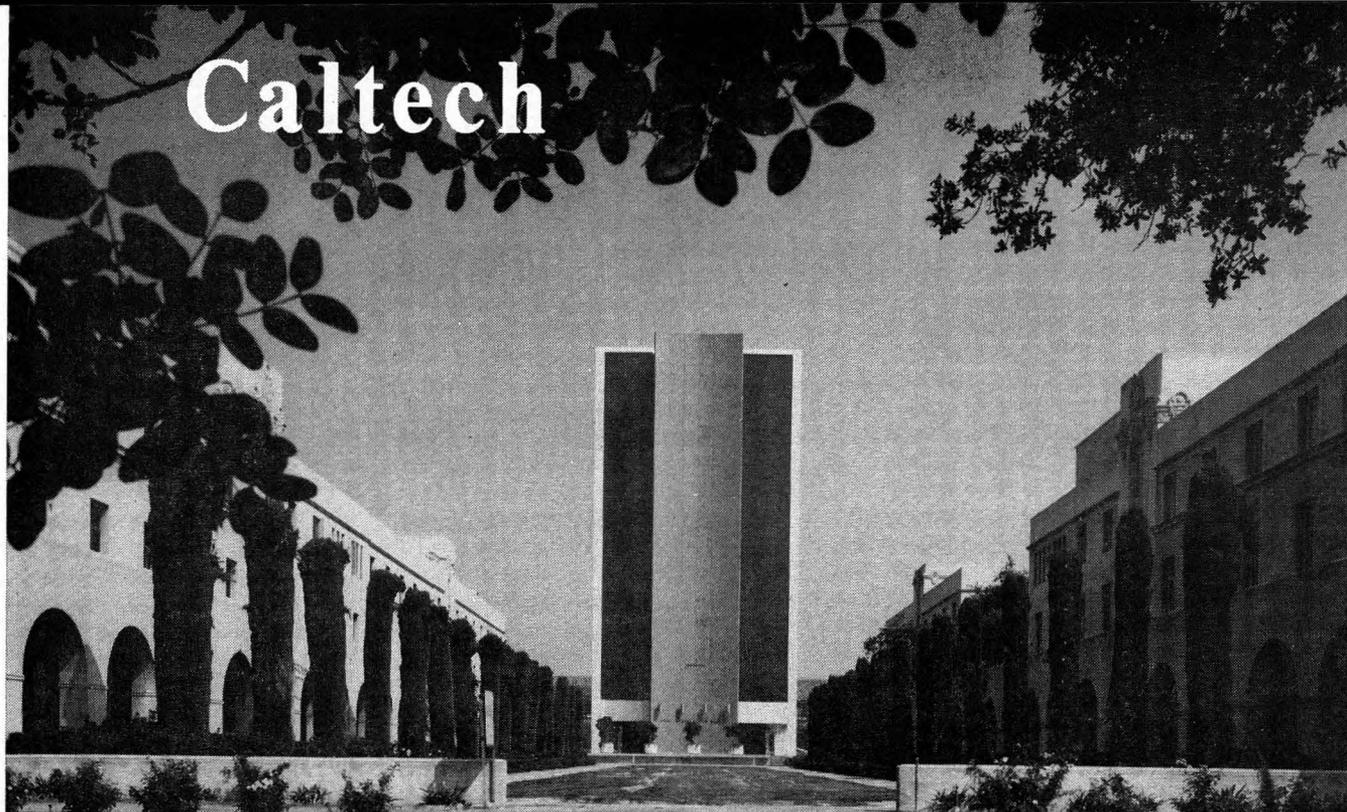
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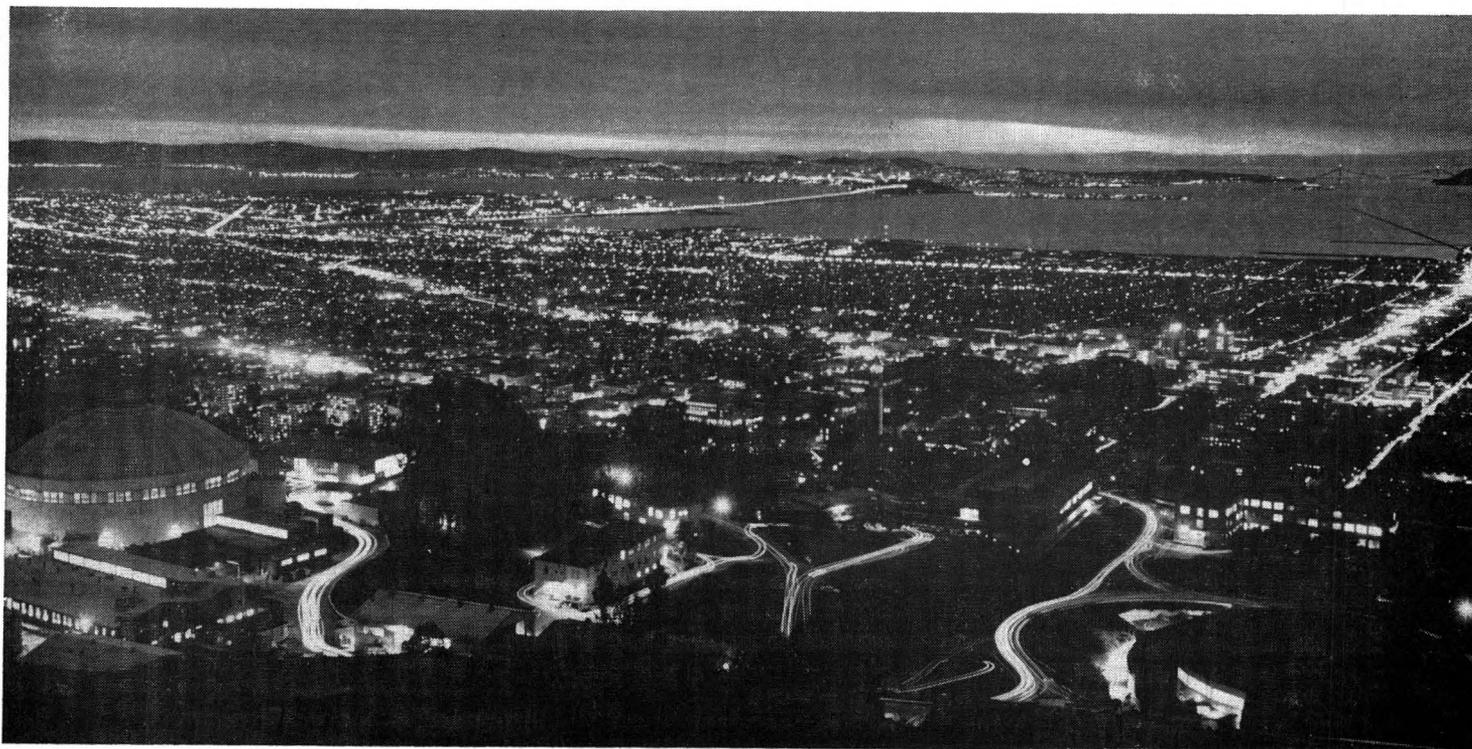
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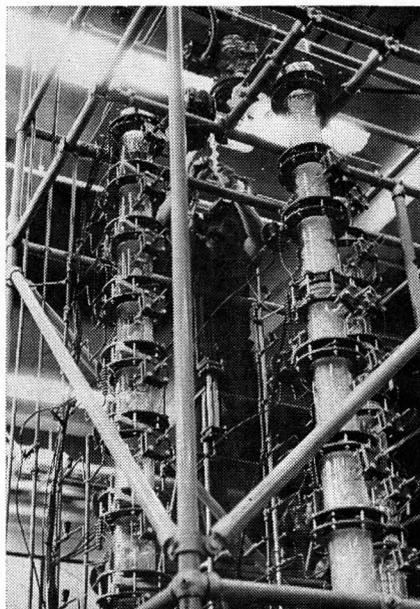
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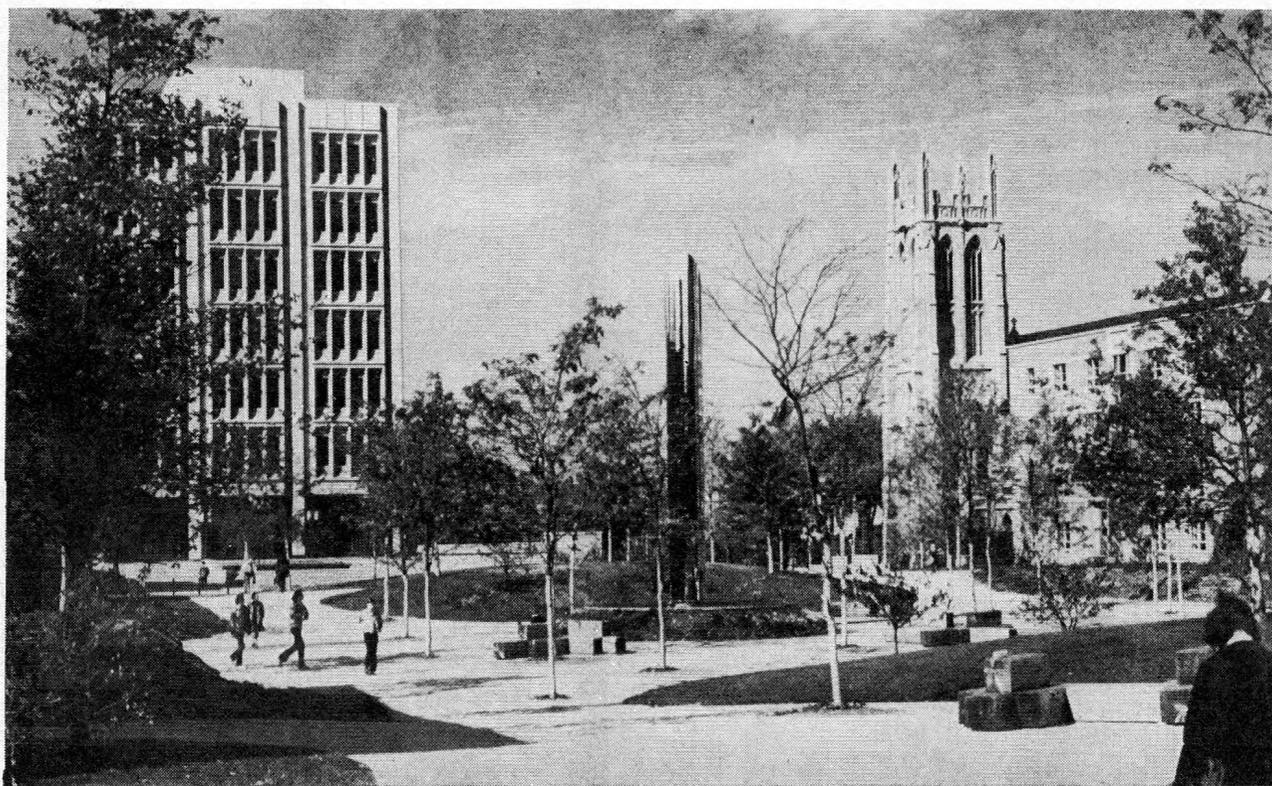
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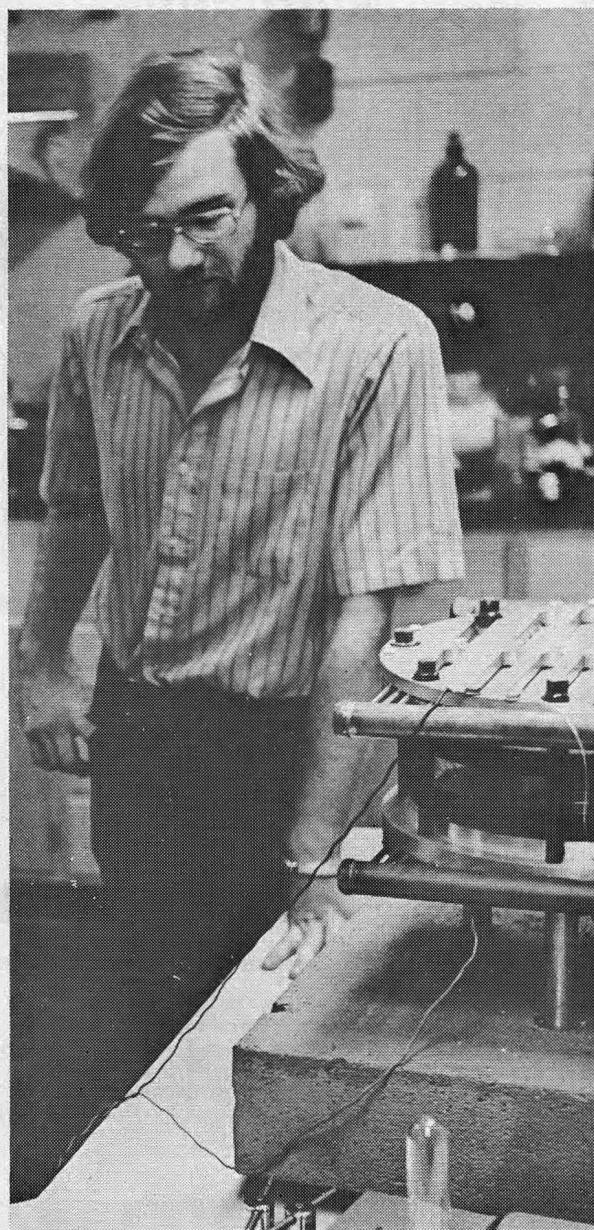
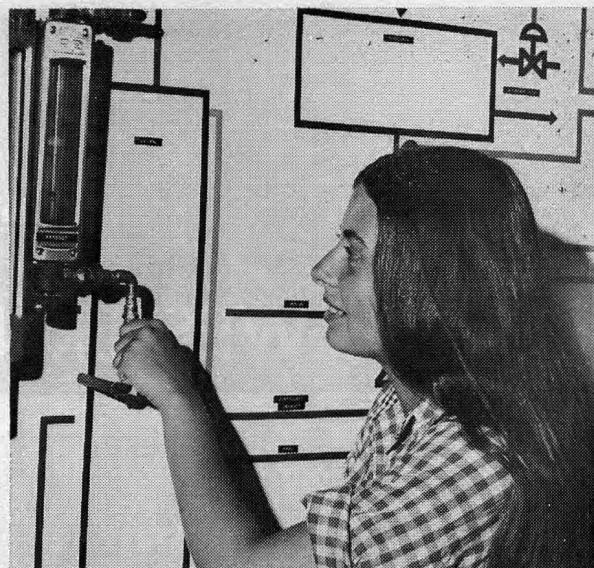
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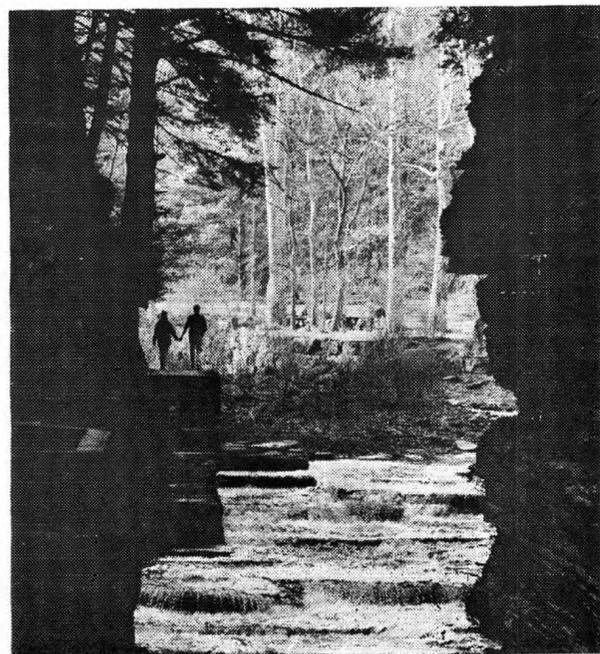
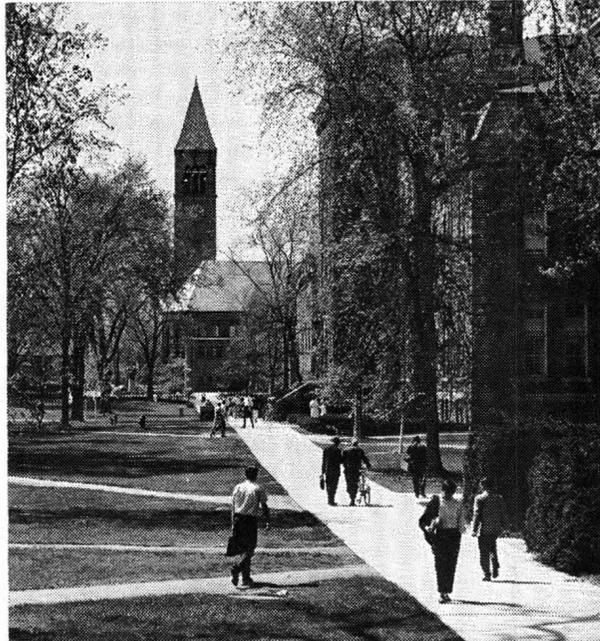
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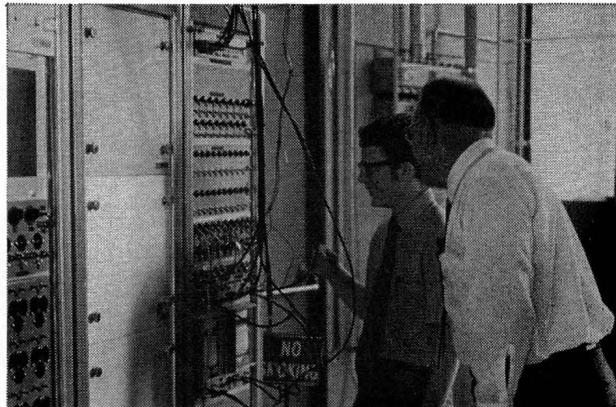
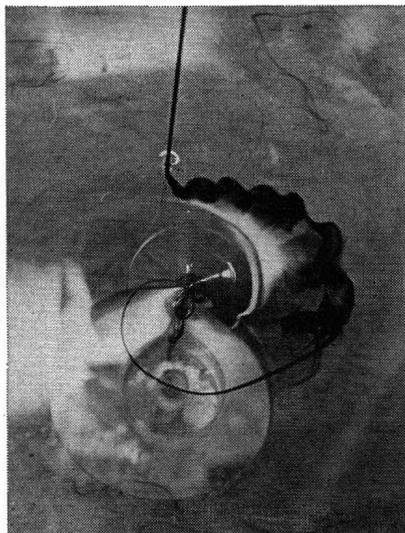
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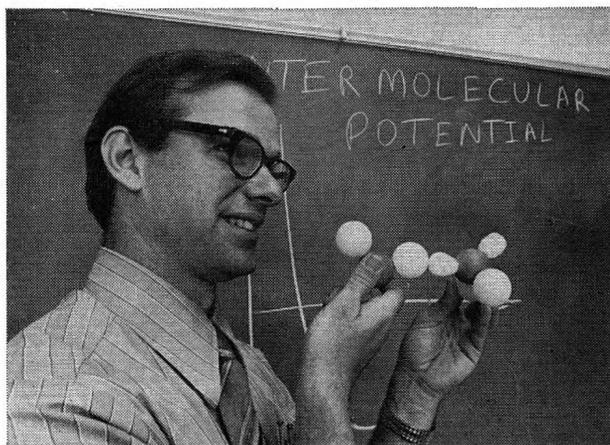
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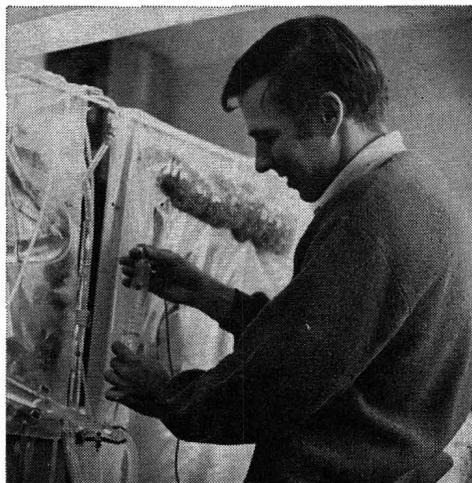
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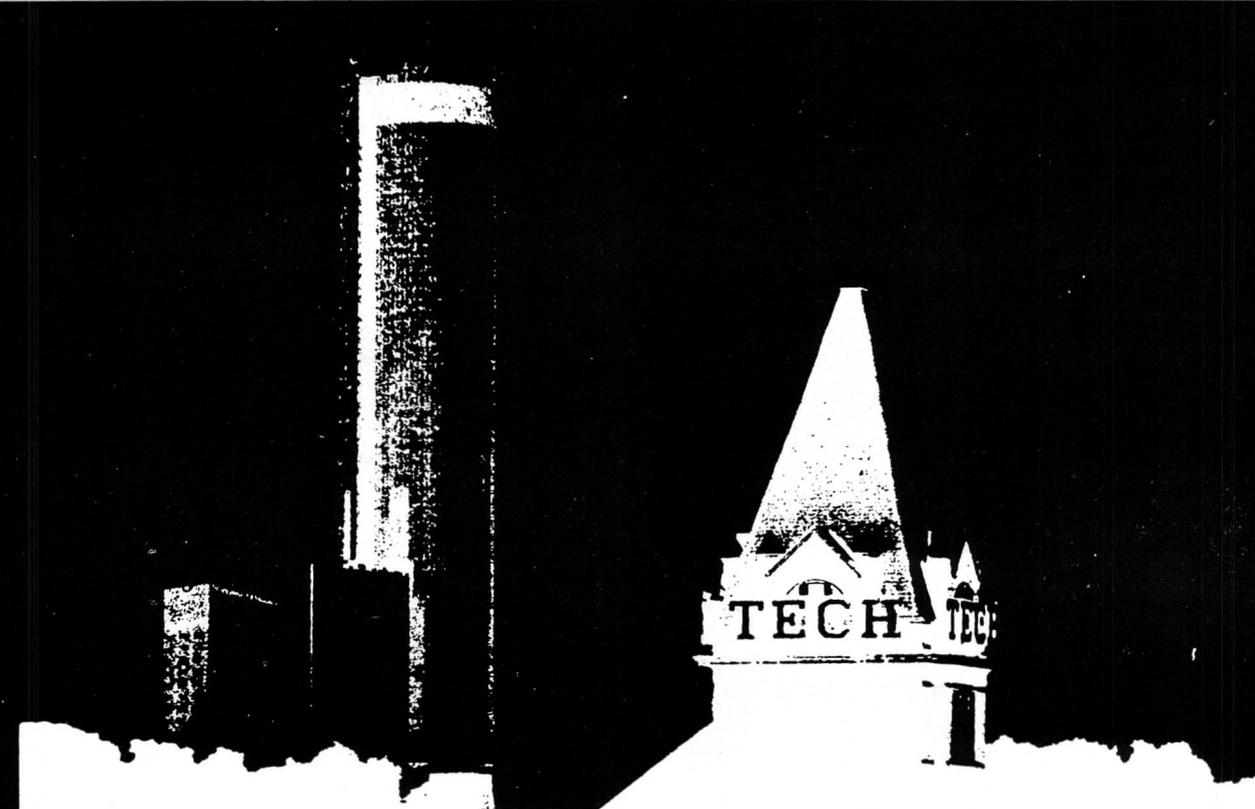
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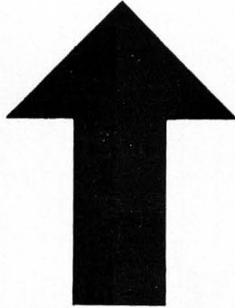
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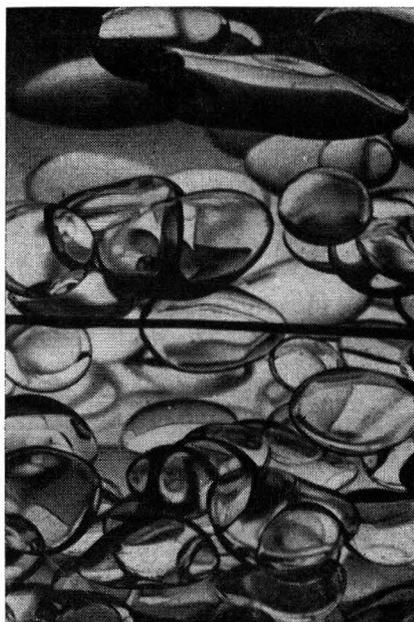
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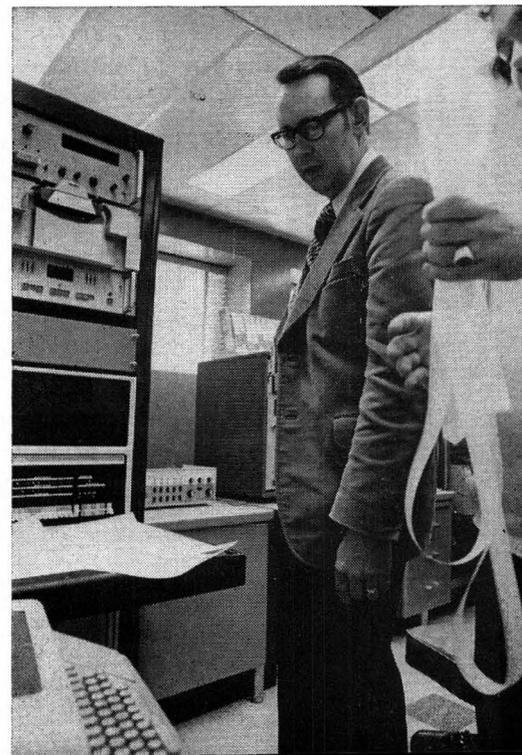
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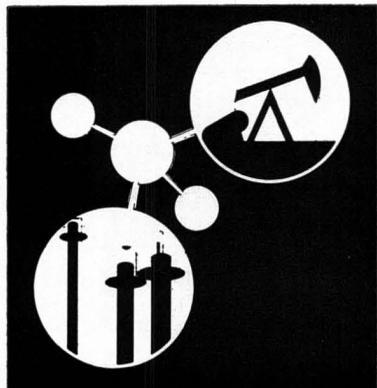
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For information contact

Dr. Richard J. Farris
Graduate Program Director
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Dr. R. L. Laurence
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Holy Cross, Cornell, Case
Edwin Young
Detroit, Michigan

THE RESEARCH PROGRAM

Laser Light Scattering
Reservoir Engineering
Thrombogenesis
Sterilization
Applied Numerical Methods
Dynamic Process Simulation
Ecological Simulation
Electroless Plating
Electrochemical Reactors
Polymer Physics
Polymer Processing
Composite Materials
Coal Liquefaction
Coal Gasification
Acidization
Gas Hydrates
Periodic Processes
Tertiary Oil Recovery
Transport In Membranes
Flow Calorimetry
Ultrasonic Emulsification
Heat Exchangers

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THE PLACE

Department Of Chemical Engineering
THE UNIVERSITY OF MICHIGAN
ANN ARBOR, MICHIGAN 48109

For Information Call 313/763-1148 Collect

Department of Chemical Engineering

UNIVERSITY OF MISSOURI — ROLLA

ROLLA, MISSOURI 65401

Contact Dr. M. R. Strunk, Chairman

Day Programs M.S. and Ph.D. Degrees

Established fields of specialization in which research programs are in progress are:

- (1) Fluid Turbulence Mixing and Drag Reduction Studies—Dr. G. K. Patterson and Dr. X. B. Reed
- (2) Electrochemistry and Reactions at Electrode Surfaces—Dr. J. W. Johnson
- (3) Heat Transfer Studies—Dr. J. J. Carr
- (4) Bioconversion of Agricultural Wastes to Methane—Dr. J. L. Gaddy and Dr. N. L. Book
- (5) Polymers and Polymeric Materials—Dr. H. K. Yasuda

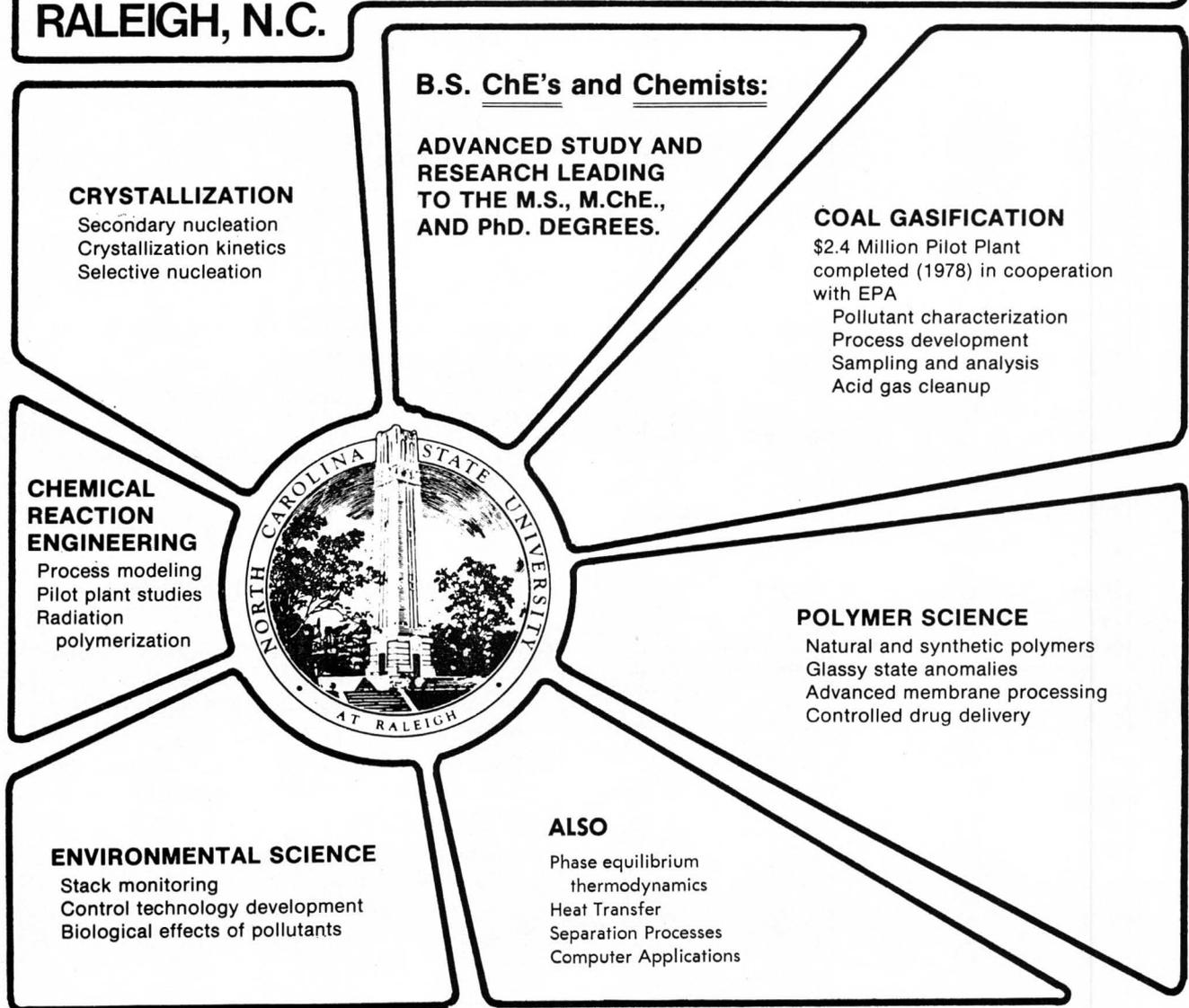
In addition, research projects are being carried out in the following areas:

- (a) Optimization of Chemical Systems—Dr. J. L. Gaddy
- (b) Design Techniques and Fermentation Studies—Dr. M. E. Findley
- (c) Multi-component Distillation Efficiencies and Separation Processes—Dr. R. C. Waggoner
- (d) Separations by Electrodialysis Techniques—Dr. H. H. Grice
- (e) Process Dynamics and Control; Computer Applications to Process Control—Drs. M. E. Findley, R. C. Waggoner, and R. A. Mollenkamp
- (f) Transport Properties, Kinetics, enzymes and catalysis—Dr. O. K. Crosser and Dr. B. E. Poling
- (g) Thermodynamics, Vapor-Liquid Equilibrium—Dr. D. B. Manley



Financial aid is obtainable in the form of Graduate and Research Assistantships, and Industrial Fellowships. Aid is also obtainable through the Materials Research Center.

CHEMICAL ENGINEERING AT NORTH CAROLINA STATE UNIVERSITY RALEIGH, N.C.



FOR ADDITIONAL INFORMATION, A CATALOG, AND APPLICATION MATERIALS, WRITE

Dr. James K. Ferrell, Head
Department of Chemical Engineering
North Carolina State University
Raleigh, North Carolina 27650

Graduate Study in Chemical Engineering at

NORTHEASTERN UNIVERSITY

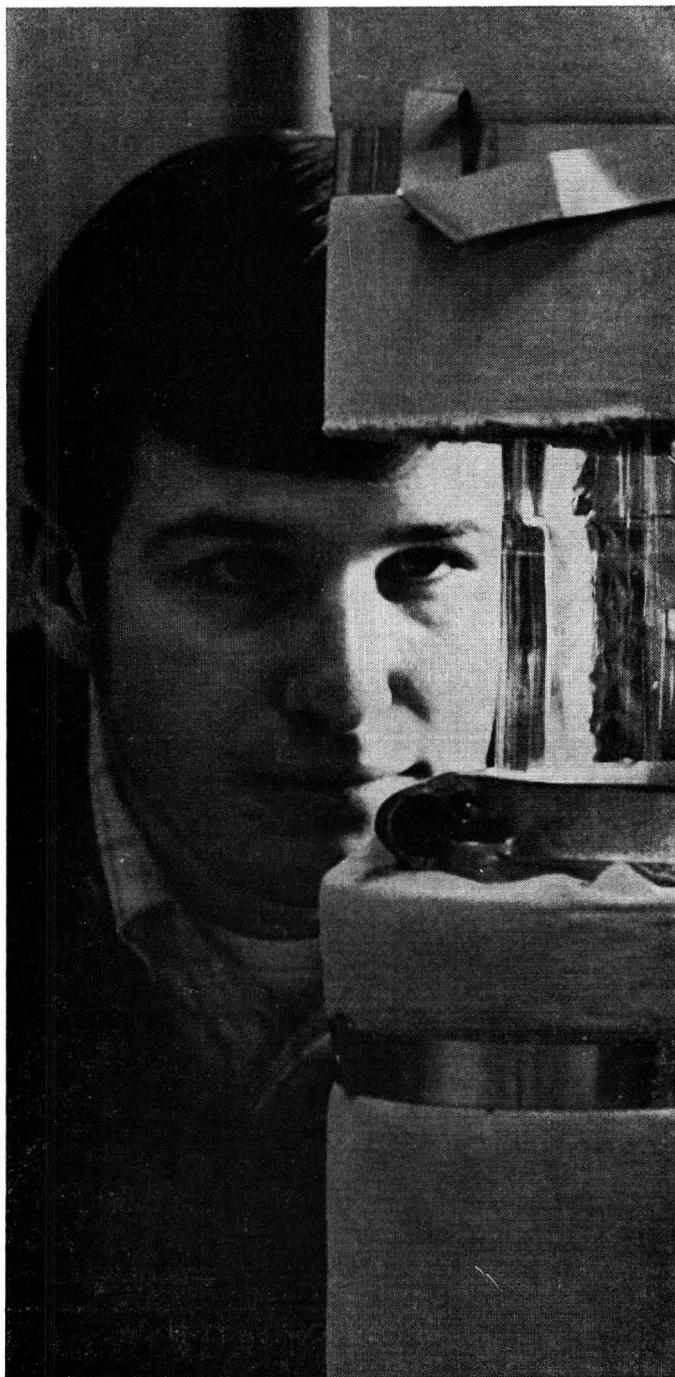
M.S., Ph.D., and D. Eng. programs are available at Northeastern University to qualified students with B.S. degrees in Chemical Engineering from accredited institutions. The M.S. programs are available on the Coop plan of alternate periods of work and study. Faculty research interests include energy conservation and conversion, process dynamics and control, light induced reactions, environmental control, process development and modeling simulation. Some financial support is available.

Location—Northeastern University is located in dynamic Boston close to major cultural, recreational, sports, and learning areas.

For further information please contact

**Dean George W. Hankinson
Graduate School of Engineering
Northeastern University
Boston, Mass. 02115**

LOOKING



WRITE TO

Prof. Lee C. Eagleton, Head
160 Fenske Laboratory
The Pennsylvania State University
University Park, Pa. 16802

for a
graduate education
in
Chemical Engineering ?
Consider

PENN STATE

Some Current M.S. & Ph.D.
General Research Areas:

BIOMEDICAL ENGINEERING

Physiological Transport Processes
Newborn Monitoring

ENVIRONMENTAL RESEARCH

Gaseous and Particulate Control
Atmospheric Modeling

REACTOR DESIGN AND CATALYSIS

Heterogeneous Catalysis
Cyclic Reactor Operations
Catalyst Characterization

TRANSPORT PHENOMENA

Analytical and Numerical Solutions
Polymer Rheology and Transport
Convective Heating and Mass Transfer
Mass Transfer in Cocurrent Flow

THERMODYNAMIC PROPERTIES

Property Correlations
Statistical Mechanics

PROCESS DYNAMICS AND CONTROL

Nonlinear Stability Theory
Optimal and Periodic Control

APPLIED CHEMISTRY AND KINETICS

Industrial Chemical Processes
Complex Reaction Systems

PETROLEUM REFINING

Process Development
Product Conversion

TRIBOLOGY

Properties of Liquid Lubricants
Boundary Lubrication Fundamentals

INTERFACIAL PHENOMENA

Adsorption Thermodynamics and Kinetics
Monolayer and Membrane Processes

ENERGY RESEARCH

Tertiary Oil Recovery
Nuclear Technology

university of

pennsylvania chemical and biochemical engineering

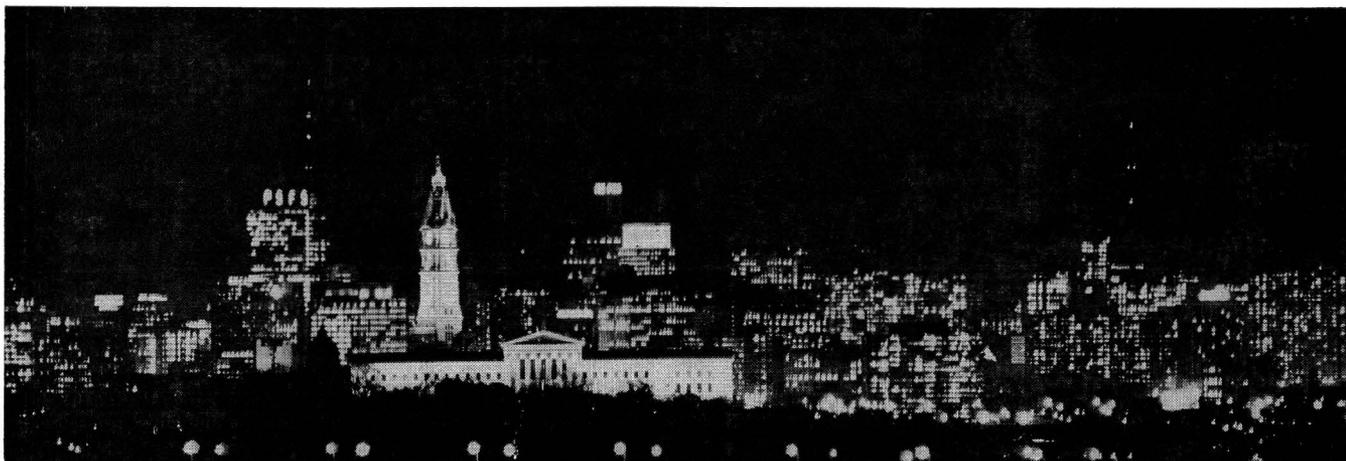
FACULTY

Stuart W. Churchill (Michigan)
Elizabeth B. Dussan V. (Johns Hopkins)
William C. Forsman (Pennsylvania)
Eduardo D. Glandt (Pennsylvania)
David J. Graves (M.I.T.)
A. Norman Hixson (Columbia)
Arthur E. Humphrey (Columbia)
Mitchell Litt (Columbia)
Alan L. Myers (California)
Melvin C. Molstad (Yale)
Daniel D. Perlmutter (Yale)
John A. Quinn (Princeton)
Warren D. Seider (Michigan)

RESEARCH SPECIALTIES

Energy Utilization
Enzyme Engineering
Biochemical Engineering
Biomedical Engineering
Computer-Aided Design
Chemical Reactor Analysis
Environmental and Pollution Control
Polymer Engineering
Process Simulation
Surface Phenomena
Separations Techniques
Thermodynamics
Transport Phenomena

The faculty includes three members of the National Academy of Engineering and three recipients of the highest honors awarded by the American Institute of Chemical Engineers. Staff members are active in teaching, research, and professional work. Located near one of the largest concentrations of chemical industry in the United States, the University of Pennsylvania maintains the scholarly standards of the Ivy League and numbers among its assets a superlative Medical Center and the Wharton School of Business.



PHILADELPHIA: The cultural advantages, historical assets, and recreational facilities of a great city are within walking distance of the University. Enthusiasts will find a variety of college and professional sports at hand. The Pocono Mountains and the New Jersey shore are within a two-hour drive.

For further information on graduate studies in this dynamic setting, write to Dr. A. L. Myers, Chairman, Department of Chemical and Biochemical Engineering, 220 S. 33rd Street, University of Pennsylvania, Philadelphia, PA 19104.

**GRADUATE STUDY
IN CHEMICAL AND PETROLEUM
ENGINEERING**

University of Pittsburgh

Sixty graduate students, along with 300 undergraduates, pursue their education on three floors of Benedum Hall. The facilities are modern and excellently equipped. Graduate applicants should write:

Graduate Coordinator
Chemical and Petroleum
Engineering Department
School of Engineering
University of Pittsburgh
Pittsburgh, Pa. 15261

FACULTY

Charles S. Beroes
Alfred A. Bishop
Alan J. Brainard
Shiao-Hung Chiang
James T. Cobb, Jr.
Paul F. Fulton
George E. Klinzing
Alan A. Reznik
Yatish T. Shah
Edward B. Stuart
John W. Tierney

UNIVERSITY OF PITTSBURGH

The first school west of the Allegheny Mountains to offer engineering degrees, the University granted its first undergraduate engineering degree in 1846 and started the graduate program in 1914. Today, approximately 2,000 undergraduates and 600 graduate students are enrolled in the School of Engineering. Students have access to the George M. Bevier Engineering Library of 38,000 volumes; University libraries of over 2,500,000 volumes; libraries in 50 industrial research centers and universities nearby. University of Pittsburgh has a comprehensive computer system with both batch and time-sharing

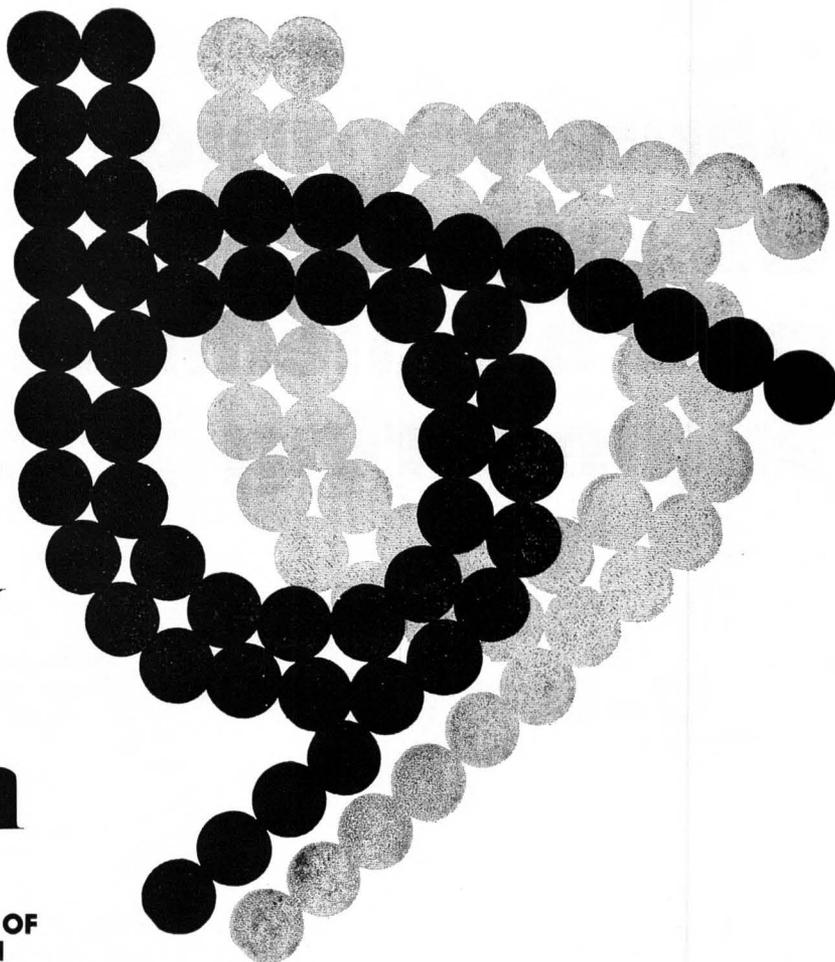
facilities to use in academic and research investigations.

PROGRAMS AND SUPPORT

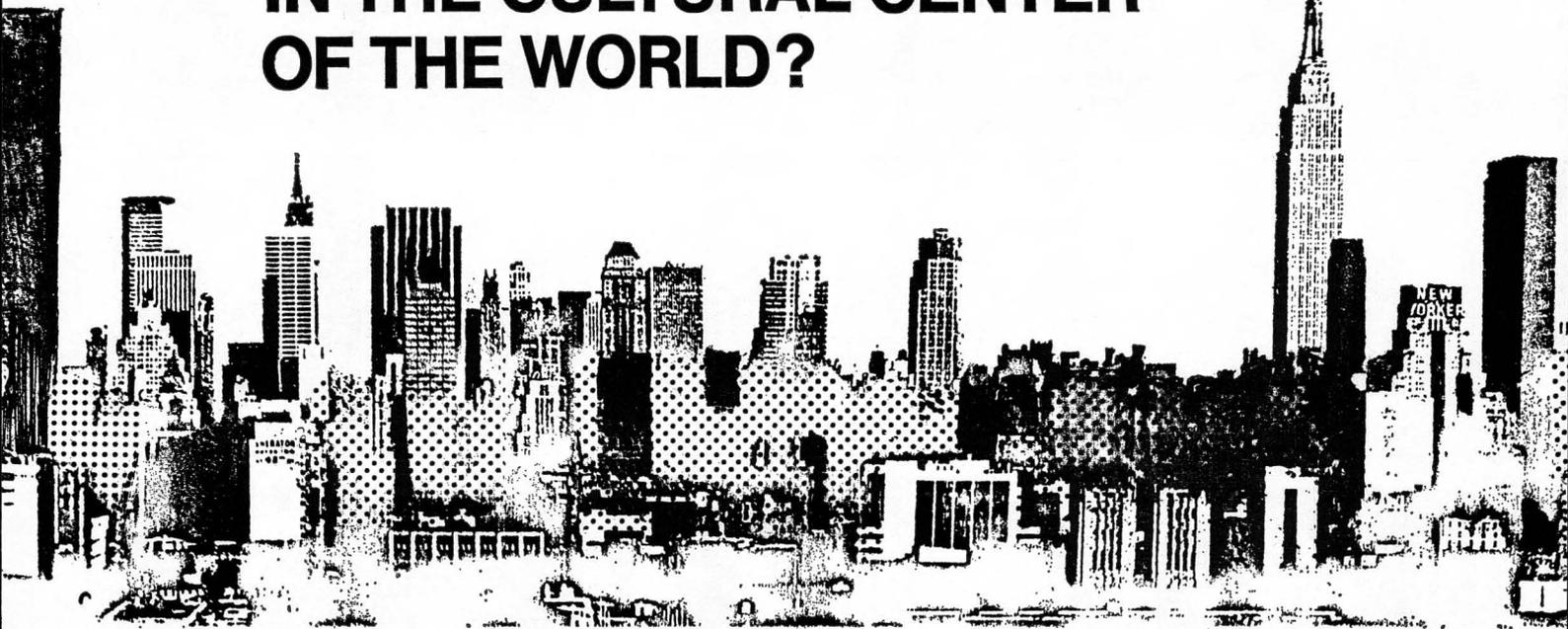
Master of Science and Doctor of Philosophy degrees in Chemical Engineering and Master of Science degree in Petroleum Engineering are offered. While obtaining advanced degrees, students may specialize in Biomedical, Energy Resources, Nuclear, and Environmental areas. A joint Master of Science degree with the Department of Mathematics is offered. Teaching and Research Assistantships and Fellowships are available.

PITTSBURGH

The city leads a rich cultural life in an exciting geographic and social setting. Pittsburgh Symphony Orchestra, under the direction of Andre Previn, ranks high. A wide range of musical events rocks Heinz Hall. Pittsburgh Laboratory Theatre and Pittsburgh Public Theatre take innovative approaches to drama. Natural history displays at Carnegie Museum and art exhibits at the new Sarah Scaife Gallery draw over a million visitors yearly. For sports followers, Pittsburgh offers Pirates, Steelers, Penguins. And skiers find a variety of slopes just a half-hour uphill drive from the city.



HOW WOULD YOU LIKE TO DO YOUR GRADUATE WORK IN THE CULTURAL CENTER OF THE WORLD?



CHEMICAL ENGINEERING POLYMER SCIENCE & ENGINEERING

FACULTY

R. C. Ackerberg
R. F. Benenati
J. J. Conti
C. D. Han
W. H. Kapfer
S. H. Lin
J. S. Mijovic
E. M. Pearce
P. F. Schubert
E. N. Ziegler

RESEARCH AREAS

Air Pollution
Catalysis, Kinetics and Reactors
Fermentation and Food Processing
Fluidization
Fluid Mechanics
Heat and Mass Transfer
Mathematical Modelling
Mechanical Behavior of Polymers
Morphology of Polymers
Polymerization Reactions
Process Control
Rheology and Polymer Processing

Polytechnic Institute of New York

Formed by the merger of Polytechnic Institute of
Brooklyn and New York University School of
Engineering and Science.

Department of Chemical Engineering

Programs leading to Master's, Engineer and
Doctor's degrees. Areas of study and research:
chemical engineering, polymer science and
engineering and environmental studies.

Fellowships and Research Assistantships
are available.

For further information contact

Professor C. D. Han
Head, Department of Chemical Engineering
Polytechnic Institute of New York
333 Jay Street
Brooklyn, New York 11201



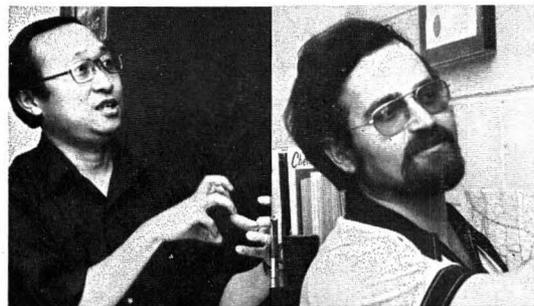
PURDUE



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Barile
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Chao
Delgass
Eckert
Emery

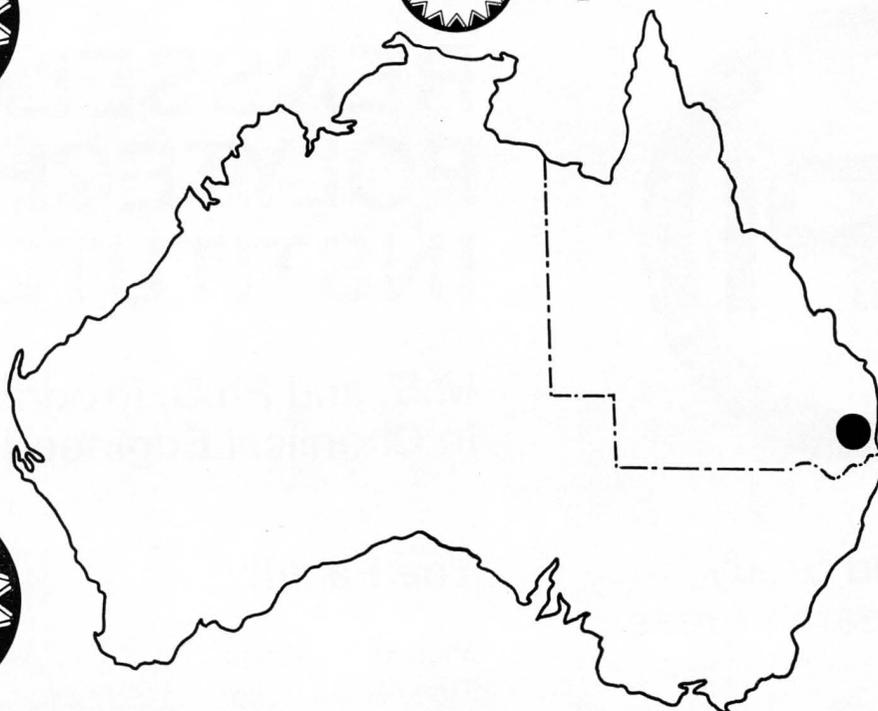
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Hanneman
Houze
Kessler
Koppel
Lim
Peppas

Ramkrishna
Reklaitis
Squires
Theofanous
Tsao
Wankat
Weigand



Graduate Information
Chemical Engineering
Purdue University
West Lafayette, Indiana 47907





UNIVERSITY OF QUEENSLAND POSTGRADUATE STUDY IN CHEMICAL ENGINEERING

★ POSTGRADUATE SCHOLARSHIPS AVAILABLE ★

STAFF AND RESEARCH AREAS

D. J. Nicklin (Cambridge)
Two-phase Flow, Fluidization

P. C. Brooks (M.I.T.)
Process Dynamics and Control

P. F. Greenfield (N.S.W.)
Biochemical and Enzyme Engineering,
Mass Transfer and Catalysis, Waste
Treatment

G. J. Kelly (Tasmania)
Corrosion, Electrochemical
Technology

L. S. Leung (Cambridge)
Fluidization, Gas-solid Flow, Thermo-
dynamics

R. G. Rice (Pennsylvania)
Column Flotation, Mass and Heat
Transfer, Adsorption

R. H. Weiland (Toronto)
Fluid Dynamics, Mass and Heat
Transfer

E. T. White (Imperial College)
Crystallization, System Analysis,
Computer Control

R. J. Wiles (Queensland)
Particulate Conveying, Rheology

R. Y. K. Yang (Princeton)
Reaction and Enzyme Engineering,
Numerical Methods, Stability Analysis

THE DEPARTMENT

The Department occupies its own new building and is well supported by research grants and modern equipments including a multi-purpose Varian mini-computer system. It has maintained an active postgraduate programme, which involves course work and research leading to M. Eng. Studies, M. Eng. Science and Ph.D. degrees.

THE UNIVERSITY AND THE CITY

The University is one of the largest in Australia with more than 18,000 students. Brisbane, with a population of about one million, enjoys a pleasant climate and attractive coasts which extend northward into The Great Barrier Reef.



**FURTHER
INFORMATION**

For further information write to:
Co-ordinator of Graduate Studies, Department of Chemical
Engineering, University of Queensland, Brisbane, Qld. 4067,
AUSTRALIA.





RENSSELAER POLYTECHNIC INSTITUTE

M.S. and Ph.D. Programs in Chemical Engineering

Advanced Study and Research Areas

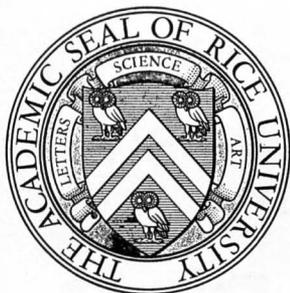
- Thermodynamics
- Heat Transfer
- Kinetics—Catalysis
- Fluidization
- Fluid—Particle Systems
- Interfacial Phenomena
- Polymer Materials
- Polymer Processing
- Biochemical Systems
- Air Pollution Control
- Atmospheric Chemistry
- Water Resources
- Environmental Studies

The Faculty

Michael M. Abbott *Ph.D., Rensselaer*
Elmar R. Altwicker *Ph.D., Ohio State*
Donald B. Aulenbach *Ph.D., Rutgers*
Georges Belfort *Ph.D., California—Irvine*
Henry R. Bungay III *Ph.D., Syracuse*
Chan I. Chung *Ph.D., Rutgers*
Nicholas L. Clesceri *Ph.D., Wisconsin*
Dady B. Dadyburjor *Ph.D., Delaware*
Charles N. Haas *Ph.D., Illinois*
David Hansen *Ph.D., Rensselaer*
Arland H. Johannes *Ph.D., Kentucky*
Clement Kleinstreuer *Ph.D., Vanderbilt*
Peter K. Lashmet *Ph.D., Delaware*
Howard Littman *Ph.D., Yale*
Charles Muckenfuss *Ph.D., Wisconsin*
Rajamani Rajagopalan *Ph.D., Syracuse*
George P. Sakellaropoulos *Ph.D., Wisconsin*
William W. Shuster *D.Ch.E., Rensselaer*
Sanford S. Sternstein *Ph.D., Rensselaer*
Hendrick C. Van Ness *D.Eng., Yale*
Peter C. Wayner, Jr. *Ph.D., Northwestern*
Stephen W. Yerazunis *D.Ch.E., Rensselaer*

For full details write

Dr. David Hansen, Chairman
Department of Chemical and Environmental Engineering
Rensselaer Polytechnic Institute Troy, New York 12181



Graduate Study in Chemical Engineering at Rice University

Graduate study in Chemical Engineering at Rice University is offered to qualified students with backgrounds in the fundamental principles of Chemistry, Mathematics, and Physics. The curriculum is aimed at strengthening the student's understanding of these principles and provides a basis for developing in certain areas the necessary proficiency for conducting independent research. A large number of research programs are pursued in various areas of Chemical Engineering and related fields, such as Biomedical Engineering and Polymer Science. A joint program with the Baylor College of Medicine, leading to M.D.-Ph.D. and M.D.-M.S. degrees is also available.

The Department has approximately 30 graduate students, predominantly Ph.D. candidates. There are also several post-doctoral fellows and research engineers associated with the various laboratories. Permanent faculty numbers 12, all active in undergraduate and graduate teaching, as well as in research. The high faculty-to-student ratio, outstanding laboratory facilities, and stimulating research projects provide a graduate education environment in keeping with Rice's reputation for academic excellence. The Department is one of the leading 42 Chemical Engineering Departments in the U.S., ranked by graduate faculty quality and program effectiveness, according to recent evaluations.

MAJOR RESEARCH AREAS

Thermodynamics and Phase Equilibria
Chemical Kinetics and Catalysis
Chromatography
Optimization, Stability, and Process Control
Systems Analysis and Process Dynamics
Rheology and Fluid Mechanics
Polymer Science

BIOMEDICAL ENGINEERING

Blood Flow and Blood Trauma
Blood Pumping Systems
Biomaterials

Rice University

Rice is a privately endowed, nonsectarian, coeducational university. It occupies an architecturally attractive, tree-shaded campus of 300 acres, located in a fine residential area, 3 miles from the center of Houston. There are approximately 2200 undergraduate and 800 graduate students. The school offers the benefits of a complete university with programs in the various fields of science and the humanities, as well as in engineering. It has an excellent library with extensive holdings. The academic year is from August to May. As there are no summer classes, graduate students have nearly four months for research. The school offers excellent recreational and athletic facilities with a completely equipped gymnasium, and the southern climate makes outdoor sports, such as tennis, golf, and sailing year-round activities.

FINANCIAL SUPPORT

Full-time graduate students receive financial support with tuition remission and a tax-free fellowship of \$400-460 per month.

APPLICATIONS AND INFORMATION

Address letters of inquiry to:

Chairman
Department of Chemical Engineering
Rice University
Houston, Texas 77001

Houston

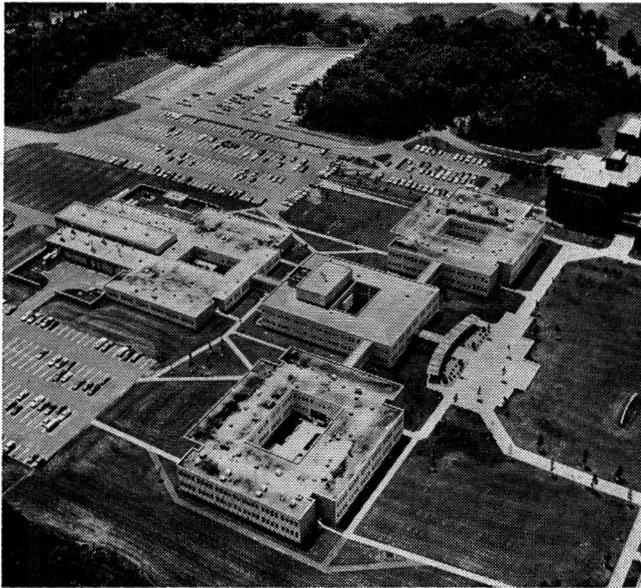
With a population of nearly two million, Houston is the largest metropolitan, financial, and commercial center in the South and Southwest. It has achieved world-wide recognition through its vast and growing petrochemical complex, the pioneering medical and surgical activities at the Texas Medical Center, and the NASA Manned Spacecraft Center.

Houston is a cosmopolitan city with many cultural and recreational attractions. It has a well-known resident symphony orchestra, an opera, and a ballet company, which perform regularly in the newly constructed Jesse H. Jones Hall. Just east of the Rice campus is Hermann Park with its free zoo, golf course, Planetarium, and Museum of Natural Science. The air-conditioned Astrodome is the home of the Houston Astros and Oilers and the site of many other events.



RUTGERS

THE STATE UNIVERSITY
OF NEW JERSEY



College of Engineering

M.S. and Ph.D. PROGRAMS

IN THE DEPARTMENT OF
**CHEMICAL AND
BIOCHEMICAL
ENGINEERING**

AREAS OF TEACHING AND RESEARCH

CHEMICAL ENGINEERING FUNDAMENTALS

- THERMODYNAMICS • TRANSPORT PHENOMENA • KINETICS AND CATALYSIS • CONTROL THEORY, COMPUTERS AND OPTIMIZATION • POLYMERS AND SURFACE CHEMISTRY • SEMIPERMEABLE MEMBRANES

BIOCHEMICAL ENGINEERING FUNDAMENTALS

- MICROBIAL REACTIONS AND PRODUCTS • SOLUBLE AND IMMOBILIZED ENZYMES • BIOMATERIALS
- ENZYME AND FERMENTATION REACTORS

ENGINEERING APPLICATIONS

- | | | |
|--|------------------------------|-----------------------------------|
| • BIOCHEMICAL TECHNOLOGY | • CHEMICAL TECHNOLOGY | • WATER RESOURCES ANALYSES |
| • INDUSTRIAL FERMENTATIONS | • FLAMMABILITY OF MATERIALS | • OCEANS AND ESTUARIES |
| • ENZYMES IN THERAPEUTIC MEDICINE,
PHARMACEUTICAL PROCESSING
AND WASTE TREATMENT | • PACKAGING | • QUALITY MANAGEMENT |
| • FOOD PROCESSING | • POLYMER PROCESSING | • WASTES RECOVERY |
| | • PLANT DESIGN AND ECONOMICS | |

**FELLOWSHIPS AND
ASSISTANTSHIPS
ARE AVAILABLE**

For Application Forms and Further Information Write To:
Graduate Admissions Office
542 George Street
Rutgers, The State University
New Brunswick, N.J. 08903

University of South Carolina

The College of Engineering offers M.S., M.E. and Ph.D. degrees in Chemical Engineering. Graduate students have the opportunity to work closely with the faculty on research projects. Research and teaching stipends are available from \$3000 to \$7200.

The University of South Carolina, with an enrollment of 23,800 on the Columbia campus, offers a variety of cultural and recreational activities. Columbia is part of one of the fastest growing areas in the country.

The Chemical Engineering Faculty

B. L. Baker, Distinguished Professor Emeritus, Ph.D., North Carolina State University, 1955 (Process design, environmental problems, ion transport).

M. W. Davis, Jr., Professor, Ph.D., University of California (Berkeley), 1951 (Kinetics and catalysis, chemical process analysis, solvent extraction, waste treatment).

J. H. Gibbons, Professor, Ph.D., University of Pittsburgh, 1961 (Heat transfer, fluid mechanics).

J. G. Goodwin, Jr., Assistant Professor, Ph.D., University of Michigan, 1977 (Kinetics and catalysis, reactor engineering).

F. P. Pike, Professor Emeritus, Ph.D., University of Minnesota, 1949 (Mass transfer in liquid-liquid systems, vapor-liquid equilibria).

T. G. Stanford, Assistant Professor, Ph.D., The University of Michigan, 1977 (Chemical reactor engineering, mathematical modeling of chemical systems, process design, thermodynamics).

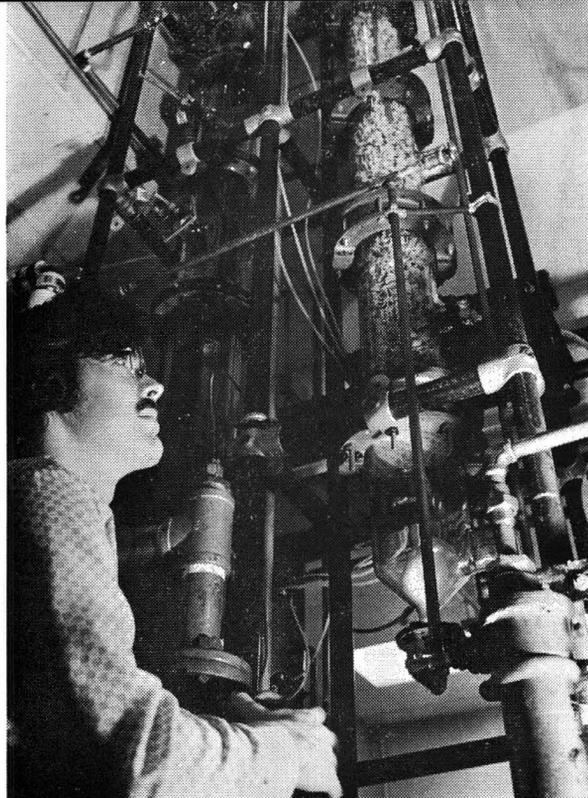
G. B. Tatterson, Assistant Professor, Ph.D., Ohio State University, 1977 (Turbulence, mixing, multi-phase flow, real-time computing).

J. A. Trainham, Assistant Professor, Ph.D., University of California (Berkeley), 1978, (Electrochemical systems).

V. Van Brunt, Assistant Professor, Ph.D., University of Tennessee, 1974 (Mass transfer, computer modeling, fluidization).

For further information contact:

Prof. J. H. Gibbons
Chairman, Chemical Engineering Group
College of Engineering
University of South Carolina
Columbia, South Carolina 29208



Chemical Engineering at Stevens Institute of Technology

Master's—Chemical Engineer—Doctoral Programs in Chemical Engineering Science Design and Polymer Engineering Research in

Transport Processes — Turbulence — Multiphase Systems

Pollution Modeling and Control — Combustion

Chemical Reaction Engineering — Energy Conversion

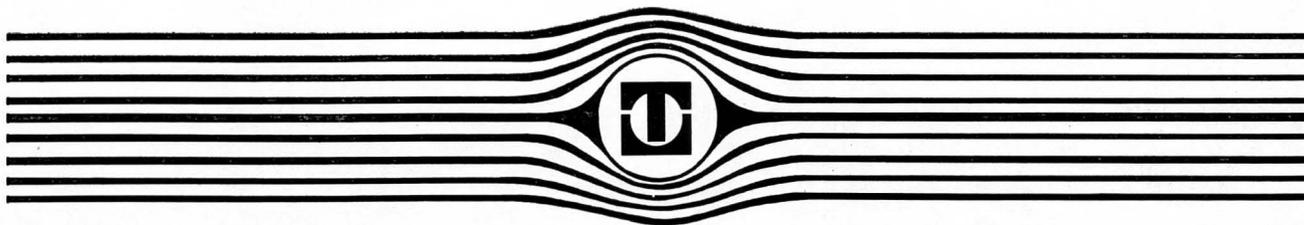
Membrane Separation Processes — Absorption — Extraction

Polymerization Kinetics — Polymer Rheology and Processing

Polymeric System Structure — Property Relationships

For further information contact:

Dean of Graduate Studies
Stevens Institute of Technology
Castle Point Station
Hoboken, New Jersey 07030
201-420-5234



THE UNIVERSITY OF TENNESSEE, KNOXVILLE

Graduate Studies in Chemical, Metallurgical, and Polymer Engineering

Programs

Programs for the degrees of Master of Science and Doctor of Philosophy are offered in chemical engineering, metallurgical engineering and polymer engineering. The Master's program may be tailored as a terminal one with emphasis on professional development, or it may serve as preparation for more advanced work leading to the Doctorate.

Faculty

William T. Becker
Donald C. Bogue
Charlie R. Brooks
Duane D. Bruns
Edward S. Clark
Oran L. Culberson
John F. Fellers
George C. Frazier
Hsien-Wen Hsu
Homer F. Johnson, Department Head
Stanley H. Jury
Carl D. Lundin
Peter J. Meschter
Charles F. Moore
Ben F. Oliver, Professor-in-Charge
of Metallurgical Engineering
Joseph J. Perona
Joseph E. Spruiell
E. Eugene Stansbury
James L. White, Professor-in-Charge
of Polymer Engineering

Research

Process Dynamics and Control
Sorption Kinetics and Dynamics of Packed Beds
Chromatographic and Ultracentrifuge Studies of Macromolecules
Development and Synthesis of New Engineering Polymers
Fiber and Plastics Processing
Chemical Bioengineering
X-Ray Diffraction, Transmission and Scanning Electron Microscopy
Solidification, Zone Refining
Welding
Cryogenic and High Temperature Calorimetry
Flow and Fracture in Metallic and Polymeric Systems
Corrosion
Solid State Kinetics



Financial Assistance

Sources available include graduate teaching assistantships, research assistantships, and industrial fellowships.

The University and Surroundings

Close to the center of Knoxville, the 397 acre campus combines a spacious environment with urban convenience. The proximity of the Oak Ridge National Laboratory and the headquarters of the Tennessee Valley Authority encourages constructive interchange with the activities of this 30,000 student campus.

The moderate Knoxville climate with the nearby Great Smoky Mountain National Park, Appalachian Trail, ski slopes and TVA lakes provides year round recreational challenges. The university and area communities offer a substantial program of cultural activities including a symphony orchestra, several theater companies and fine art museums as well as a wide assortment of rock concerts, folk music, mountain festivals, etc.

Write

Department of Chemical, Metallurgical
and Polymer Engineering
The University of Tennessee
Knoxville, Tennessee 37916



TEXAS A&M UNIVERSITY

Texas A&M is a land-grant and sea-grant university, and the oldest public institution of higher learning in Texas. The current enrollment is about 30,000. The university location is Bryan/College Station, Texas—twin cities with a combined population of 122,000 (including students). The surrounding country is deciduous forest—Houston is 95 miles Southeast and Dallas is 160 miles North.

CHEMICAL ENGINEERING DEPARTMENT

The ChE department has an enrollment of about 850 undergraduates and 70 graduates. ChE has excellent facilities in the Zachry Engineering Center. All graduate students have desk space. Graduate stipends are currently \$575/month.

Admission to The Texas A&M University System and any of its sponsored programs is open to qualified individuals regardless of race, color, religion, sex, national origin or educationally handicaps.

FACULTY AND RESEARCH INTERESTS

C. D. Holland (department head)—distillation
R. G. Anthony—catalysis
J. A. Bullin—pollution
R. Darby—rheology
R. R. Davison—solar energy
L. D. Durbin—control
P. T. Eubank—thermodynamics
C. J. Glover—oil recovery
K. R. Hall—thermodynamics
D. T. S. Hanson—biochemical
W. B. Harris—methanol fuel
J. C. Holste—polymers
A. I. Liapis—adsorption
A. D. Messina—heat transfer
R. D. Ostermann—bio-mass
A. T. Watson—simulation
R. E. White—electrochemical

FOR INFORMATION CONTACT:

**Graduate Advisor
Chemical Engineering Dept.
Texas A&M University
College Station, TX 77843**



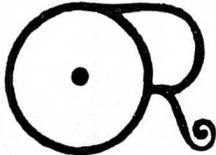
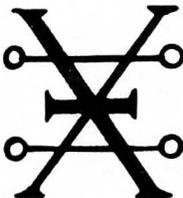
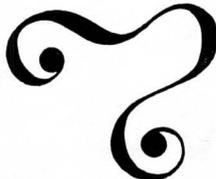
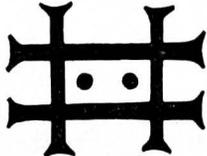
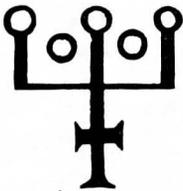
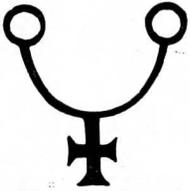
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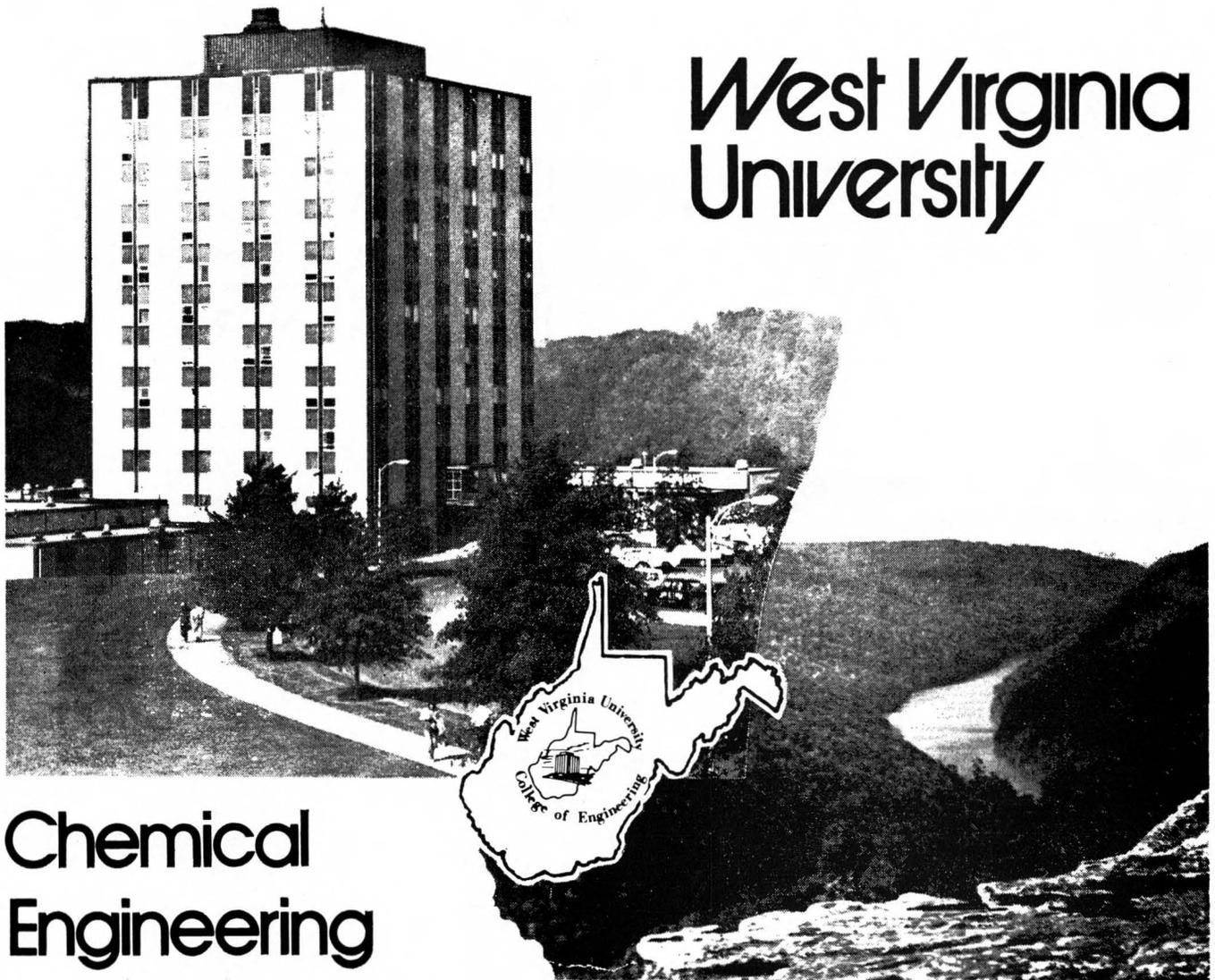
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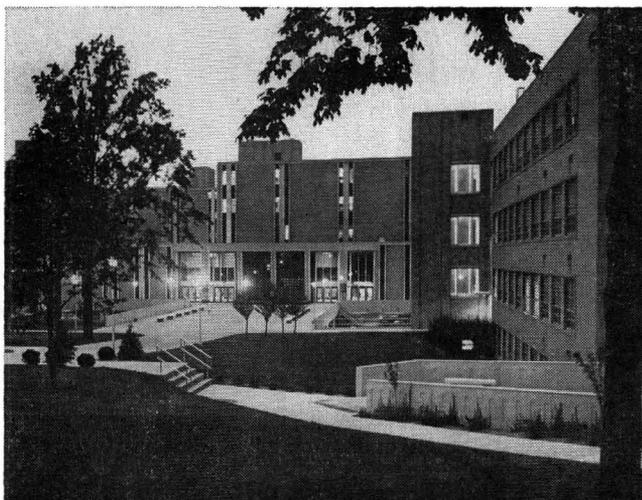
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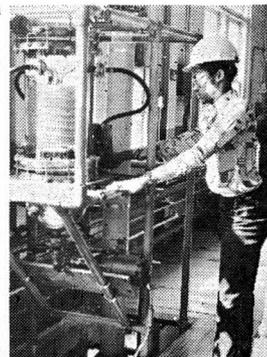
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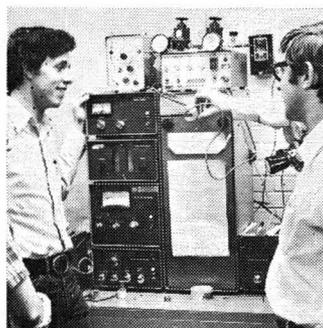
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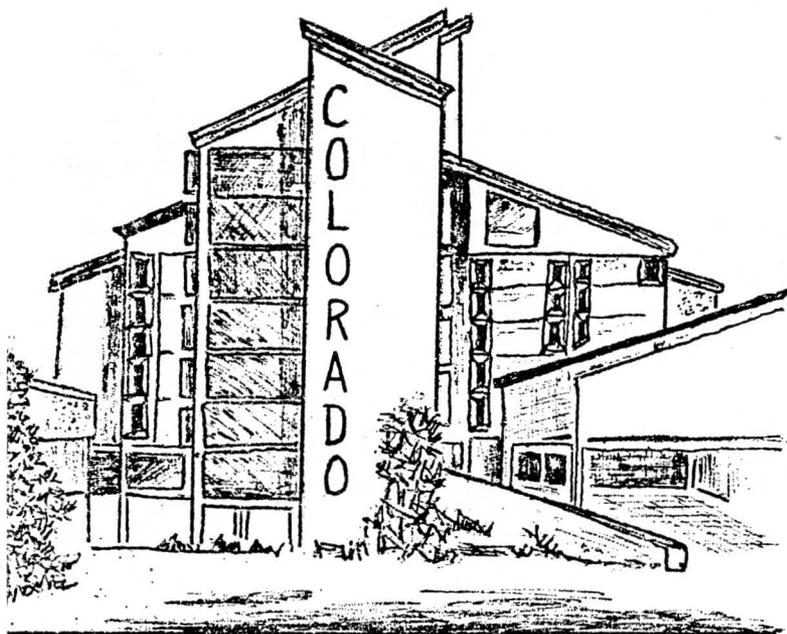
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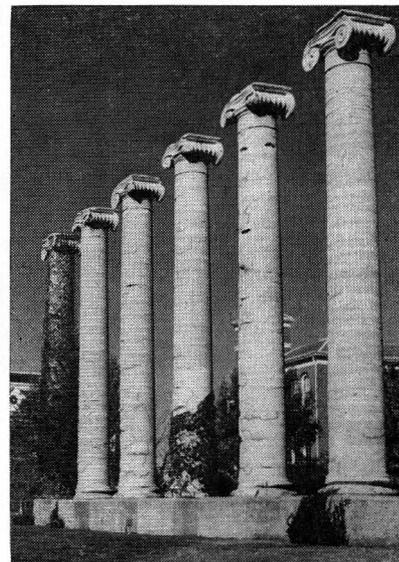
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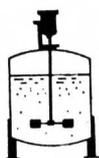
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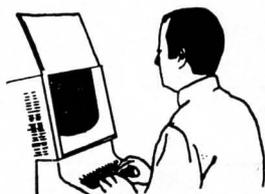


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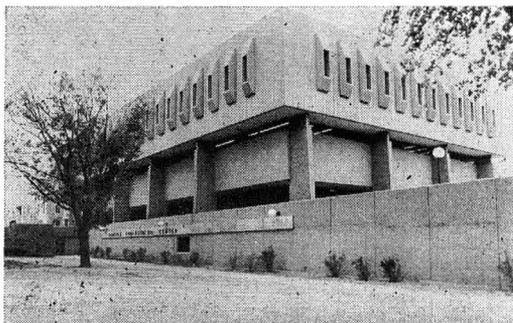
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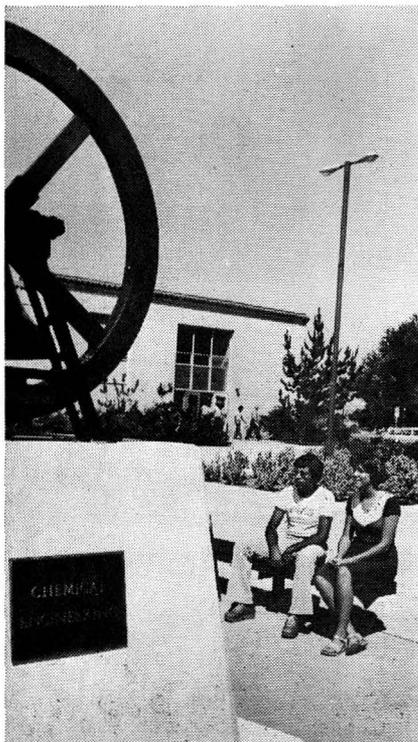


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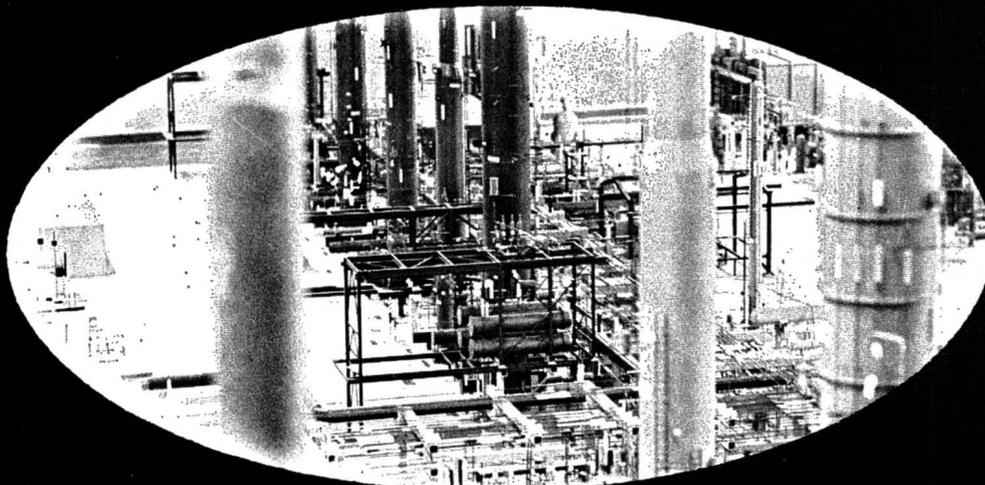
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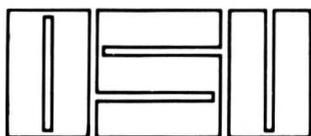
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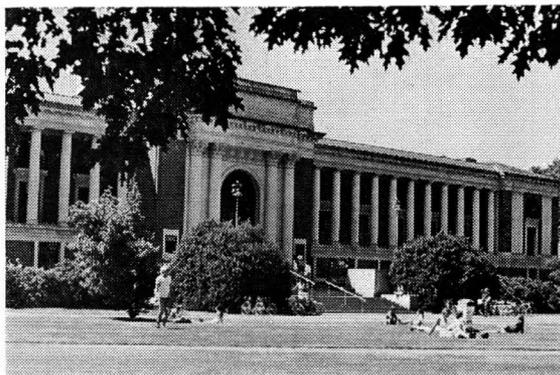
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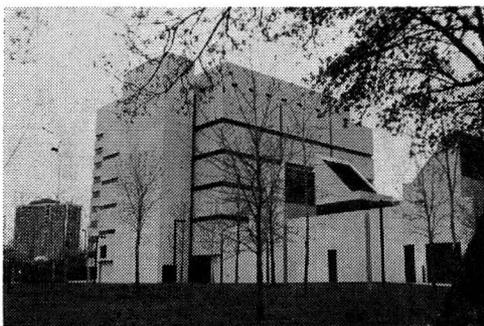


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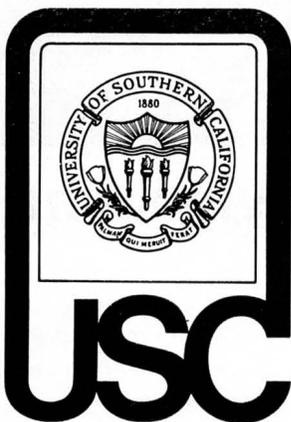
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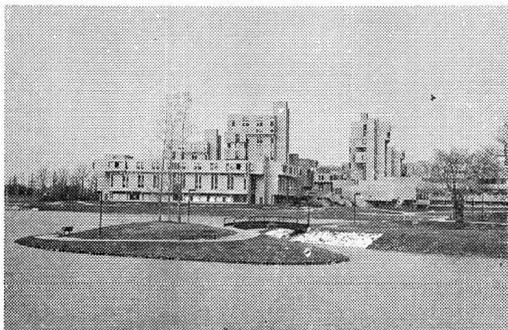
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FOR FURTHER INFORMATION on admission and financial aid contact:

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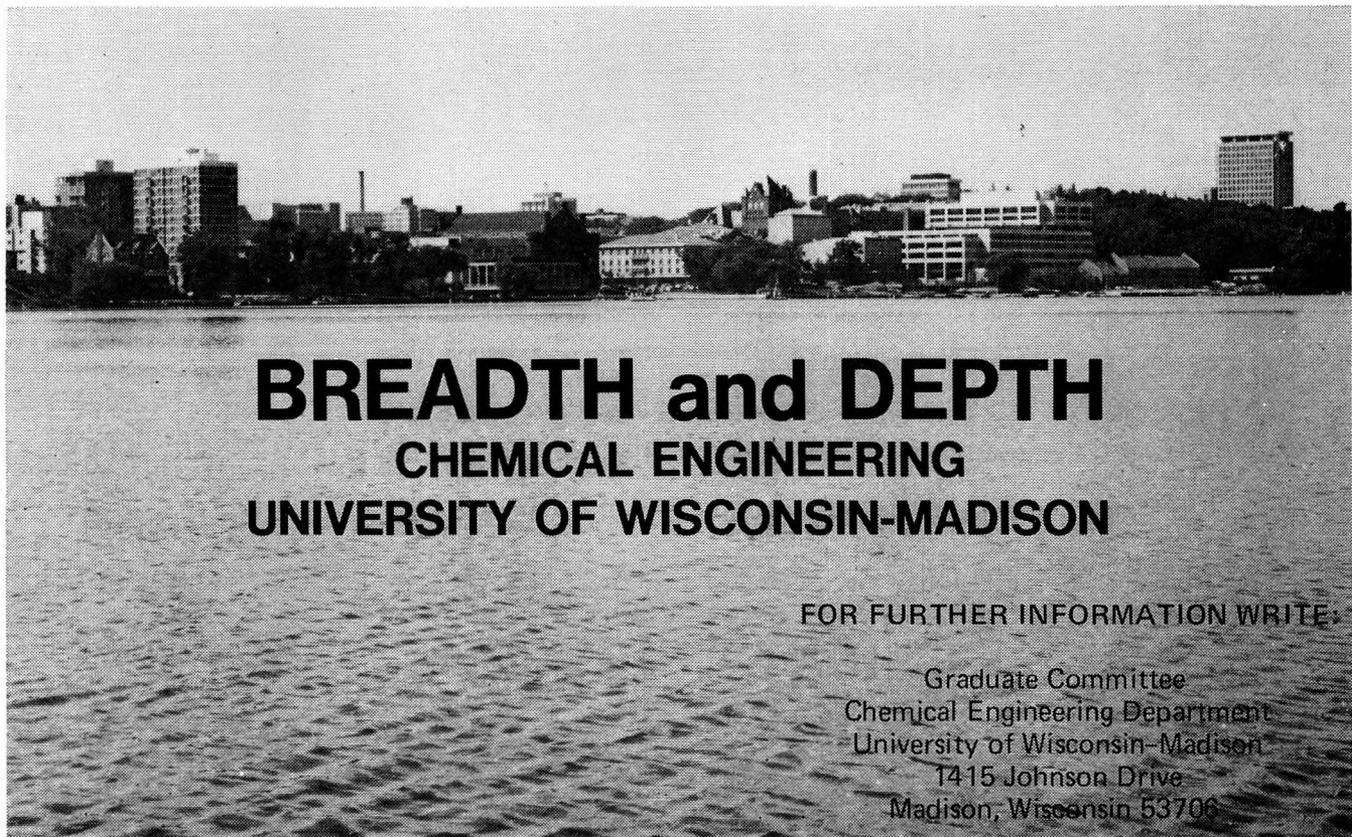
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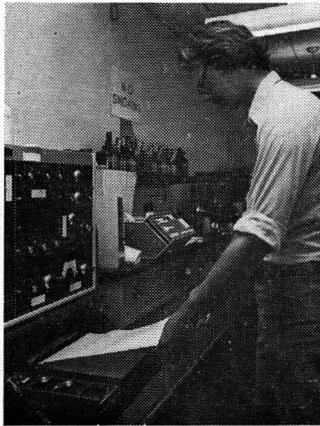
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PROGRAM OF STUDY: Thesis and non-Thesis programs leading to the M.S. degree are available. A full-time student can complete the program in a calendar year. Research and Teaching assistantships are available.

LIGNITE LIQUEFACTION PROJECT: UND's Chemical Department is engaged in a major research program under the U.S. Department of Energy on conversion of lignite coal to upgraded energy products. Students may participate in project-related thesis problems, or be employed as project workers while taking course work in the department.

ERDA: The Department of Chemical Engineering and the Grand Forks Energy Technology Center offer a cooperative program of study related to coal technology. Course work is taken at the University and thesis research performed at the Center under DOE staff members. Fellowships are available to U.S. citizens.

FOR INFORMATION WRITE TO:

**Dr. Thomas C. Owens, Chairman
Chemical Engineering Department
University of North Dakota
Grand Forks, North Dakota 58201**

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Address inquiries to:

Dr. John R. Collier
Chemical Engineering Department
Ohio University
Athens, Ohio 45701

University of Rhode Island Graduate Study

Chemical Engineering MS, PhD Nuclear Engineering MS

AREAS OF RESEARCH

Adsorption	Mass Transfer
Biochemical Engineering	Materials Engineering
Boiling Heat Transfer	Membrane Diffusion
Catalysis	Metal Finishing
Corrosion	Metal Oxidation
Desalination	Metallurgy
Dispersion Processes	Nuclear Technology
Distillation	Phase Equilibria
Fluid Dynamics	Polymers
Heat Transfer	Process Dynamics
Ion Exchange	Thermodynamics
Kinetics	Water Resources
Liquid Extraction	X-ray Metallography

APPLICATIONS

Apply to the Dean of the Graduate School, University of Rhode Island, Kingston, Rhode Island 02881. Applications for financial aid should be received not later than February 15. Appointments will be made about April.

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Dr. R. M. Bethea
Graduate Advisor
Department of Chemical Engineering
Texas Tech University
Lubbock, Texas 79409

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Noel de Nevers
Director of Graduate Studies
Department of Chemical Engineering
University of Utah
Salt Lake City, Utah 84112

UNIVERSITY OF VIRGINIA

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M.S., and Ph.D. Programs in Chemical Engineering. Chemical Engineering with a Biomedical /Biochemical Minor is available.

RESEARCH INTERESTS: Mass transfer phenomena, surface chemistry, fluid mechanics and rheology, fluidization, parameter estimation, process dynamics and control, solar energy conversion, crystallization, air pollution control, fermentation processes, immobilized biomolecules, biological mass transfer and disease, and modeling of biological processes.

FOR ADMISSION AND FINANCIAL AID INFORMATION

Graduate Coordinator
Department of Chemical Engineering
University of Virginia
Charlottesville, Virginia 22901

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Y

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ACKNOWLEDGMENTS

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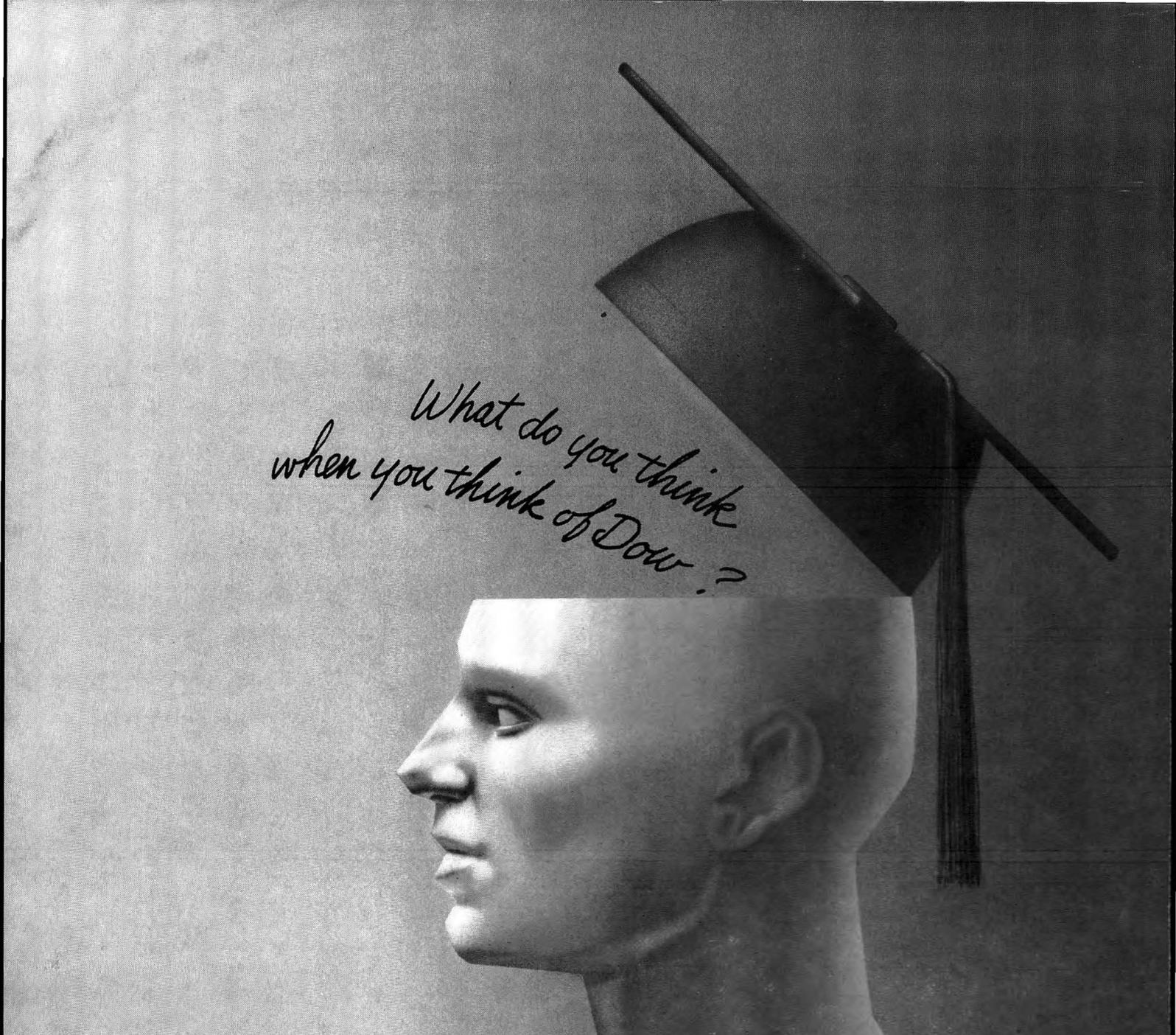
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