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### INDUSTRIAL OPPORTUNITY ISSUE

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The Coffee Pot Experiment  
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Another Way of Looking at Entropy  
*HERSHEY*

Biotechnology Laboratory Methods  
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Triangular Diagrams Teach Steady and Dynamic Behaviour of Catalytic Reactions  
*KLUSACEK, HUDGINS, SILVESTON*

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**New Jersey Institute of  
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# NEW JERSEY INSTITUTE OF TECHNOLOGY

*Photo by Bill Wittkop*

GORDON LEWANDOWSKI  
*New Jersey Institute of Technology  
Newark, NJ 07102*

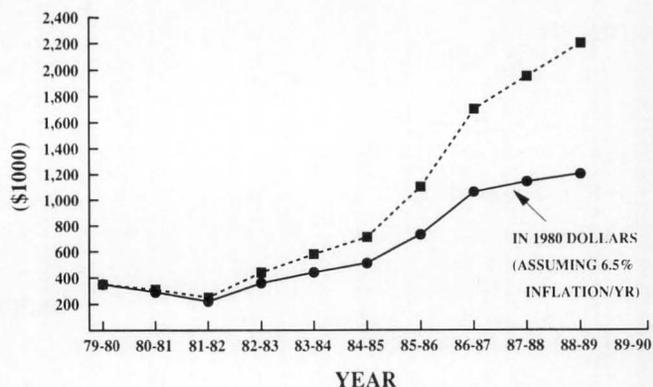
UNTIL ABOUT 1980, NJIT was largely an undergraduate teaching institute producing high quality bachelor's degree engineers. The focus of the undergraduate curriculum was (and still remains) a pragmatic program of study for the 95% of our students who go to work immediately after graduation.

More than 90% of our undergraduates commute to Newark from a radius of about thirty miles. They are attending a university with a very definite vocational objective in mind, namely to enter a well-paying profession. One out of every four engineers in New Jersey is a graduate of NJIT. About 10% of our undergraduate enrollment is black and another 11% is hispanic. In fact, NJIT ranks 12th nationwide in the number of engineering degrees awarded annually to minorities (black and hispanic) [1].

Over the years we have been fortunate in attracting bright, well-motivated students. Their leadership skills are reflected in the fact that our AIChE Student Chapter has received the Award of Excellence for eighteen consecutive years, which is far and away an AIChE record.

Although we continue to recognize the importance of our undergraduate program, over the past few years there has been a dramatic change in faculty emphasis on research (as shown in Figure 1). Research funding in the department has increased six-fold (approximately three-fold in uninflated dollars) over the past ten years, to a current level of \$2.2 million.

The increasing research effort has paralleled the



**FIGURE 1. Research Funding, Department of Chemical Engineering, Chemistry, and Environmental Science**

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**Although we continue to recognize the importance of our undergraduate program, over the past few years there has been a dramatic change in faculty emphasis on research . . . funding in the department had increased six-fold over the past ten years, to a current level of \$2.2 million.**

growth in our graduate program. In fact, we now have a higher enrollment in the graduate program (240 total) than in the undergraduate program (140 total). Approximately half of our graduate students are enrolled in the MS program in Environmental Science. A negative factor has been the low enrollments in our doctoral program; of the 240 full and part-time graduate students, only fifteen are doctoral students. This is clearly inconsistent with the level of research funding and as a result, we have embarked on a vigorous campaign to publicize our graduate program in order to recruit more qualified doctoral students.

#### **A BRIEF HISTORY**

NJIT began in 1881 as the Newark Technical School, which later evolved into the Newark College of Engineering. In 1975, with the incorporation of a School of Architecture, the name was changed to New Jersey Institute of Technology. NJIT now occupies a thirty-six acre campus in Newark, and has an annual budget of approximately \$85 million. About half of that amount comes from the State. Total enrollment includes about 4000 full-time (2700 undergraduate and 1300 graduate) and 3400 part-time students.

BS degrees in chemical engineering were first awarded in 1919, and the program has been accredited since 1950. The first female graduate was in 1930, making our department a pioneer in that regard (currently, about 20% of our undergraduates are female). The MS program has been in existence since 1948 and the DEngSc since 1961. The department also awards BS and MS in Applied Chemistry, and an MS in Environmental Science.

#### **INTERDISCIPLINARY NATURE**

The department combines faculty in chemical engineering and chemistry, and this affords many opportunities for interdisciplinary projects—both educational and research. In that respect, as well as in others, we have been old-fashioned enough to become modern. We began as an industrial chemistry department more than 100 years ago and have always maintained close ties between the two disciplines. The recent report on "Frontiers in Chemical Engineering Education" [2] has given renewed vigor to the thesis that chemical engineers need to be well-grounded in



*Photo by Bill Wittkop*

#### **Students at work in the senior chemical engineering lab.**

chemistry (as well as other sciences).

Although we do not have a biology department at NJIT, the Newark campus of Rutgers University (located across the street from NJIT) has an excellent Department of Biological Sciences. We currently have joint research projects with faculty in that department and have students enrolled there in an introductory course on microbiology. We also maintain close ties to the University of Medicine and Dentistry of New Jersey (UMDNJ) through both our biomedical engineering (MS) and environmental science (MS) programs.

#### **FACILITIES**

The department is principally located in Tiernan Hall, which was built in 1972. Departmental resources include two dedicated computer rooms containing a total of twenty-five terminals which are connected to a VAX 11/785 and a VAX 8800. We are also linked to the supercomputer facility at the John von Neumann National Supercomputer Center in Princeton, NJ. In addition, all freshmen at NJIT are provided with their

own personal computer.

Our undergraduate instructional facilities include an outstanding unit operations laboratory (comprised of about 6,500 ft<sup>2</sup> on three levels) with a multi-story high-head area, pilot-scale equipment, and a number of computer-driven process control experiments.

We also occupy about 20,000 ft<sup>2</sup> of research space in Tiernan Hall. Research labs include the analytical equipment normally expected of a serious research effort (GCs, GC/MS, HPLCs, AAS, NMR, *etc.*) as well as specialized research equipment (continuous and batch fermentors, a laser doppler velocimeter, a fully instrumented pilot-scale scrubber, UV/ozone reactors, *etc.*).

In 1988, an \$11 million building dedicated to hazardous waste research was built on campus. More

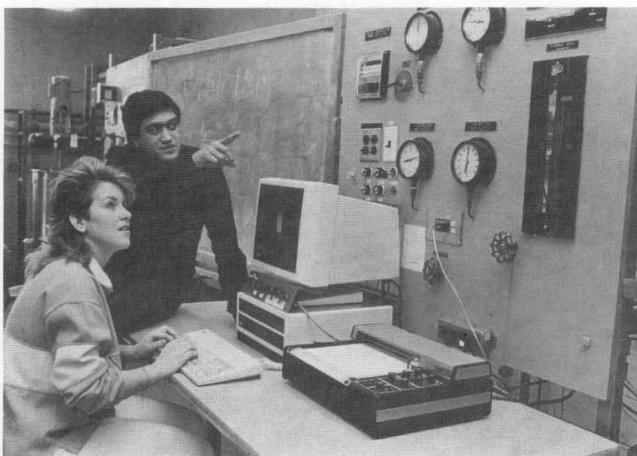


Photo by Bill Wittkop

**The process control lab at NJIT.**

than \$2 million of research equipment is being purchased for the new building, and many of our faculty have research labs and offices there.

## RESEARCH FOCUS

A principal research focus is hazardous waste treatment. In 1984, NJIT became the lead institute in an NSF Industry/University Cooperative Research Center in Hazardous and Toxic Substances. The Center was then designated an Advanced Technology Center by the State of New Jersey, and is now known as the Hazardous Substance Management Research Center (HSMRC). The other universities represented in the center are Rutgers University, Princeton University, Stevens Institute of Technology, and UMDNJ. HSMRC support comes from the State of New Jersey (\$3 million), NSF, the U.S. Army, and twenty-eight major corporations (each of which con-

tributes \$30,000/year and appoints a representative to the Industrial Advisory Board). In addition, the HSMRC, in conjunction with Tufts University and MIT, has been designated a regional center for hazardous waste research by the U.S.EPA, which provides an additional \$1 million in annual support. About 25% of the HSMRC research budget involves faculty from our department (Drs. Armenante, Baltzis, Bozzelli, Dauerman, Huang, Knox, Lei, Lewandowski, Shaw, and Sofer). Richard Magee (professor of chemical and mechanical engineering) is Executive Director of HSMRC, and Gordon Lewandowski is Director of the Biological/Chemical Treatment Division.

Through the efforts of the HSMRC, we have recently developed ties to the Institut National des Sciences Appliquees (INSA), in Lyon, France. We currently have both a graduate student and a post-doctoral student from that university in our MS program in environmental science.

Another important departmental resource associated with environmental research has been the Air Pollution Research Laboratory, directed by Drs. Bozzelli, Greenberg, and Kebbekus. They have received substantial funding for more than a decade from the N.J.DEP and U.S.EPA for the purpose of monitoring the concentration of air pollutants in the region.

A different research focus involves structural organic chemistry. Arthur Greenberg has a strong research program in strained organic molecules and is co-editor of the journal *Structural Chemistry*, published by VCH (New York). Drs. Venanzi and Gund direct the state-of-the-art molecular modeling computer graphics laboratory which examines the interactions between substrates and enzymes (or between drugs and receptors).

The biotechnology program is also supported by the engineering research of Drs. Armenante, Baltzis, and Sofer. Although geared primarily toward biodegradation of hazardous waste, their research also involves multiphase mixing phenomena, microbial competition, and conversion of biomass.

In addition, David Kristol (professor of chemistry) heads the interdisciplinary biomedical engineering program (which awards an MS in that field). As a result of that program, faculty in our department are involved in joint research projects with faculty at the nearby medical school (UMDNJ). Additional areas of research interest are given in Table 1.

## CURRICULUM

The undergraduate curriculum includes 139 credits: 41 in chemical engineering, 27 in chemistry, 16 in

**TABLE 1**  
**NJIT Faculty and Research Interests**

*Piero Armenante (University of Virginia)* • biodegradation of hazardous waste; mixing phenomena  
*Basil Baltzis (University of Minnesota)* • mathematical modeling of microbial systems  
*Joseph Bozzelli (Princeton University)* • gas phase reaction kinetics; air pollution analysis  
*Leonard Dauerman (Rutgers University)* • treatment of solid waste using microwaves  
*Arthur Greenberg (Princeton University)* • strained organic molecules; air pollution analysis  
*Teddy Greenstein (New York University)* • biochemical processes; fluid mechanics  
*James Grow (Oregon State University)* • production of thin films; surface analysis  
*Tamara Gund (Princeton University)* • molecular modeling of drug/receptor interactions  
*Deran Hanesian (Cornell University)* • reaction kinetics; plastics processing  
*Ching Huang (University of Michigan)* • photochemical oxidation of waste; transport phenomena  
*Barbara Kebbekus (Pennsylvania State University)* • air pollution analysis  
*Dana Knox (Rensselaer Polytechnic Institute)* • stabilization of solid waste; thermodynamic modeling  
*George Lei (Polytechnic University)* • polymers  
*Gordon Lewandowski (Columbia University)* • biodegradation of hazardous waste  
*Howard Perlmutter (New York University)* • organic synthesis  
*Angelo Perna (University of Connecticut)* • solid waste disposal  
*Edward Roche (Stevens Institute of Technology)* • computer modeling of chemical processes and distillation  
*Henry Shaw (Rutgers University)* • control of air pollutants  
*Sam Sofer (University of Texas)* • biochemical and biomedical processes  
*Lawrence Suchow (Polytechnic University)* • superconductivity; solid state materials  
*Reginald Tomkins (University of London)* • electrochemical processes  
*Richard Trattner (City University of New York)* • control of gaseous pollutants  
*Carol Venanzi (University of California, Santa Barbara)* • molecular modeling of enzyme/substrate interactions

**TEACHING FACULTY**

*Ernest Bart (NYU)* • *Vincent Cagnati (MS-Stevens)* •  
*Robert Conley (Brown)* • *Donald Getzin (Columbia)* •  
*Donald Lambert (VPI)* • *Avner Shilman (Polytechnic U.)*

**PROGRAM ADMINISTRATORS**

*Howard Kimmel (CUNY)* • Assistant Vice President for Academic Affairs; Director, Center for Precollege Programs  
*David Kristol (NYU)* • Director, Biomedical Engineering and Engineering Science Programs  
*Richard Magee (Stevens Institute)* • Executive Director, HSMRC  
*Richard Parker (U. Washington)* • Associate Dean, Engineering

mathematics, 12 in physics, 24 in liberal arts, and 19 in miscellaneous subjects and electives. The chemical engineering courses include: material and energy balances, a unit operations/transport sequence (fluid mechanics, heat transfer, mass transfer and stage separations), reactor design, thermodynamics, process control, process and plant design, and unit operations laboratory. Computer projects are required in all junior- and senior-level courses.

For many years now we have also been encouraging undergraduates to become involved in research.

**More than 90% of our undergraduates commute to Newark from a radius of about thirty miles. They are attending a university with a very definite vocational objective in mind, namely to enter a well-paying profession.**

Qualified students can satisfy two of their electives by working on a research project under faculty guidance.

We also want to make sure that we continue to produce professionals. This means educating our students to be more aware of the world around them and their place in that world. In this regard, we are fortunate in having an excellent program in Science, Technology, and Society (STS) at NJIT. Course materials have been developed in conjunction with STS and Humanities faculty that expand the educational base of our students into areas such as public policy, communication, and ethics.

NJIT also has a very strong co-operative education program with industry. This program involves both undergraduate and graduate students. For example, we are currently developing a co-op program with a local waste treatment company which would enable our environmental science students to gain practical experience before receiving their MS degrees.

At the graduate level, we have a required core curriculum which includes: mathematical methods, kinetics, thermodynamics, and transport phenomena. MS students receiving financial support are required to complete a thesis and eight courses (including the core and four electives). Students not receiving an assistantship are not required to complete a thesis and may take two additional courses instead. Doctoral students take eight courses beyond the MS, in addition to a thesis. Qualified students may also be admitted directly into the doctoral program with a bachelor's degree.

We are very interested in receiving more applications to our doctoral program. We have the research program to support a much larger doctoral population

*Continued on page 165.*

## EXTRINSIC VERSUS INTRINSIC MOTIVATION IN FACULTY DEVELOPMENT\*

*Higher education succeeds or fails in terms of motivation, not cognitive transfer of information. To teach implies a transfer of information, and that is not the main purpose of higher education. To profess means to confess one's faith in, or allegiance to, some idea or goal. An effective professor is one who is intrinsically motivated to learn, because he/she will have the best chance to educate others.*

**Csikszentmihalyi (1982)**

E. DENDY SLOAN  
*Colorado School of Mines  
Golden, CO 80401*

**I**F WE WISH TO address the question of faculty motivation and vitality we must follow the findings of Wergin, Mason, and Munson [1] who suggest that the factor most predictive of success in faculty motivation and development is depth of knowledge about the faculty members themselves and their personal characteristics. Bess [2] also indicates that the best effects of such motivation will be realized by accounting for individual differences. However, there appears to be a paucity of data concerning the select sample of engineering faculty on which we wish to concentrate. In addition, there are many components affecting faculty motivation which are too diverse to discuss, *e.g.*, health, family situation, *etc.* This need for data on the faculty sample leads to the initial conclusion of this paper; we would be much more comfortable with any of the following tentative conclusions if we had thorough research information on the faculty of interest. We initially suspect, however, that the means of motivating faculty may be radically different from

**Engineers draw upon sciences such as chemistry, physics, and mathematics for tools in application to technical problem solving, but here we must turn to softer sciences, *i.e.*, psychology and sociology, for tools in determining faculty characteristics.**

\*Modified from a portion of a paper "Enriching the Undergraduate Engineering Experience," originally presented at a workshop of the American Society for Engineering Education, sponsored by the National Science Foundation.

E. Dendy Sloan is a professor of chemical engineering at the Colorado School of Mines, where he has depended upon the magnanimity of students and colleagues for twelve years. He has served as Chairman of both the Chemical Engineering Division and the Educational Research and Methods Division of ASEE. He does research in natural gas hydrates, fluid properties, and pedagogical methods.



the means of motivating industrial workers.

But as engineers we typically have to make heuristic decisions based on incomplete data, accepting the risks involved and with the expectation that sequential heuristics, based upon more data, will be much better. Therefore we must make some inferences from the small data base on the collection of both engineering and science faculty, and hope to paint the silhouette of the faculty with a broad brush.

Engineers draw upon sciences such as chemistry, physics, and mathematics for tools in application to technical problem solving, but here we must turn to softer sciences, *i.e.*, psychology and sociology, for tools in determining faculty characteristics. Since the author has no formal training in either field, the examination should be considered somewhat cursory. In particular, I hope to show how the concept of stages in faculty growth and development are related to the motivation of faculty for effective professing.

### STAGES IN FACULTY GROWTH AND DEVELOPMENT

The mathematician/philosopher Alfred North Whitehead [3] postulated three stages of education.

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The initial stage is the *Romance* stage in which the learner becomes enthralled with the potential of the subject area, but has only a fragmentary knowledge of what is involved in reaching that potential. The second stage is one of *Precision*, in which the learner fills in the detailed learning required to achieve the potential. Finally comes the stage of *Generalization*, when both the precise principles and romance are incorporated and connected to other areas of the learner's knowledge and life. While Whitehead's model of education was intended to describe optimal learning stages through the college years, similar learning stages may be postulated for other learners, such as faculty who encounter the field of teaching (for which they have had no formal training.)

Levinson, *et al.* [4] were somewhat more specific about stages of growth (particularly in the adult years), using a longitudinal study. It is worth noting that 20% of the Levinson group's sample was university faculty. That original work was supported and popularized by Gould [5] and Sheehy [6]. In their analysis, growth and development occur through a series of stable and transitional periods. During stable periods the adult pursues fairly clear goals. During transitional periods, however, individuals reorder priorities and change behavior in order to compensate for neglected dimensions.

There is a growing body of evidence that there are faculty career phases, especially in teaching and research components. Research phases appear to be bimodal in terms of productivity according to Blackburn, Behymer, and Hall [7] in their study of a large cross-sectional sample of 1,216 faculty. Productivity appears to increase from the entry level until the ages between 35 and 39, during which time faculty normally strive to obtain tenure and full professor status. There is a slight decline in productivity between the ages of 35-39 and 40-44 while faculty go through Levinson's mid-life transitional period. Productivity increases again with the resolution of the mid-life transition until the early fifties, and then there is a slow decline until retirement. Senior faculty still produce significantly more writings than junior faculty, even with this last decline. These findings are supported by Cole [8] who determined that roughly the same proportion of scientists in different age groups makes important discoveries. This is a direct refutation of the theory by Lehman [9] (brought about by questionable sampling) that most of the important discoveries are made by those faculty under thirty years of age.

Teaching development also appears to be bimodal (Baldwin and Blackburn [10]), although Blackburn

**Difficult times generally arise twice during [teachers' careers] . . . during the early years when they are first learning how to teach, [and during] periods of new or added responsibility which involve new coursework, additional committee work, administrative duties, etc.**

[11] appeals for more data before coming to conclusions on the initial, somewhat anecdotal evidence. Their findings of the characteristics of teacher development are summarized in Table 1. There is an approximate parallel of teaching development to the above research development. Difficult times generally arise twice during a career. Teachers have difficulty during the early years when they are first learning how to teach (Stage I of Table 1); in this respect the increase in teaching productivity lags the research productivity by 2-3 years. The second difficult period occurs with periods of new or added responsibility (Stages II to IV) which involve new coursework, additional committee work, administrative duties, *etc.*

Normally, career reassessment also occurs twice. The first period of reassessment is in the late assistant professor period (Stage II) when the faculty must explore contingency options in case tenure is not achieved. In the full professor period (Stage IV) there is also a time when he/she must decide whether to remain a classroom teacher or to try to diversify as a means of maintaining professional vitality.

The two periods of difficulty in teaching, the period of decline in research productivity, and the periods of career reassessment all provide clues for strategies to approach the problem of motivation, as discussed below.

## **FACTORS IN FACULTY MOTIVATION**

While there is a sizeable amount of data on other motivational theories, *i.e.*, expectancy theory and behavior modification theory, one of the clearest and most applicable motivational theories is the so-called "Needs Theory" derived from the work of Maslow [(12, 13]. In this concept, Maslow proposed a hierarchy of needs of the individual, shown below in successive degrees of fundamental needs:

1. Self-Actualization Needs
2. Esteem Needs
3. Belongingness Needs
4. Safety Needs
5. Physiological Needs

The Needs Theory suggests that the lower needs on the hierarchy (levels 4 and 5) are the first ones

encountered, and the higher needs are realized only after the lower needs are gratified. The stronger the deprivation of a need, the more it dominates; the more a need is gratified, the less important it is and the more important the next higher need becomes. Schneider and Zalesny [14] suggest that faculty, by their autonomous nature, appear to have the needs which are the most mature. The academic environment attracts people who tend to be oriented to self-initiated behavior. Aldefer [15] indicates that frustration of growth (self-actualization) needs increases the desires of relatedness satisfaction, and frustration of relatedness leads to the desire for existence gratification. In other words, frustrated researchers might turn to affiliation available through teaching; frustrated teachers might move to another institution, extend their education, or participate more in administration.

McKeachie [16], Csikszentmihalyi [17] and Deci and Ryan [18] all indicate that faculty are intrinsically motivated and have limited positive extrinsic motivation possibilities. Intrinsic motivation is coincident with the highest levels of Maslow's need hierarchy, while extrinsic motivators are appropriate for those on the lower levels of the hierarchy. Organizational

structure, external rewards (such as promotion and pay), and feedback are examples of extrinsic reward systems—which are seen as somewhat self-defeating when used in a controlling manner. If extrinsic rewards are used, then faculty may slacken their efforts once full professorship and tenure have been obtained; such administration may build in a never-ending spiral of salary increases in hopes of continuing faculty motivation.

Centra [19] suggests that when self-actualized people encounter a discrepancy between one's self-theory and other evidence, there is motivation to take action. Csikszentmihalyi [17], McClelland, *et al.* [20], and Litwin and Stringer [21] all suggest that intrinsic motivation is reinforced by slightly imbalancing (a) the challenges to the faculty, with (b) the skills the faculty have to meet the challenge. If the challenge severely outweighs the skills, then frustration occurs; if the challenge (such as teaching a course multiple times) does not require stretching the skills, then boredom occurs. Optimally, challenges are addressed which allow concerted efforts to lead to success.

Deci and Ryan [18] indicate that intrinsic motivation appears to work equally well for both teachers and learners. A teacher who is intrinsically motivated

TABLE 1  
Faculty Characteristics and Experiences at Five Stages of the Academic Career

I	II	III	IV	V
Assistant Professors in the first three years of full-time college teaching	Assistant Professors with more than three years of college teaching experience	Associate Professors	Full Professors more than five years from retirement	Full Professors within five years of retirement
<ul style="list-style-type: none"> <li>• Idealistic (sometimes unrealistic) career ambitions</li> <li>• Enthusiastic about the job</li> <li>• Adjusting to novel occupational demands</li> <li>• Concerned about succeeding as a teacher</li> <li>• Eager to engage in scholarship</li> <li>• Unfamiliar with informal operations and governance (power) structure in their higher education institution</li> <li>• Receptive to assistance from more experienced colleagues</li> </ul>	<ul style="list-style-type: none"> <li>• More confident of their skills than are novice professors</li> <li>• More politically sophisticated</li> <li>• Know how their institution works and how to get things done</li> <li>• Apprehensive about upcoming tenure evaluation</li> <li>• Seeking recognition and advancement (confirmed by receipt of tenure)</li> <li>• Experience disappointment if career does not measure up to original expectations</li> <li>• Question their future in higher education and occasionally consider career alternatives</li> </ul>	<ul style="list-style-type: none"> <li>• Enigmatic</li> <li>• Enjoy peer recognition associated with tenure and promotion</li> <li>• Becoming integral part of their institution. Actively involved in college activities, especially major committees</li> <li>• Generally satisfied with career progress to date</li> <li>• Sometimes nagged by fear that career has plateaued, that there is little room left to advance professionally</li> </ul>	<ul style="list-style-type: none"> <li>• At a career turning point</li> <li>• Reduced enthusiasm for teaching and research</li> <li>• Sometimes question the value of academic career</li> <li>• Must decide to continue same career activities or move in different directions (choice between stagnation and diversification)</li> <li>• Seek to extend career (influence) beyond own campus through consultation, professional organizations</li> <li>• Limited opportunities for change; advancement can lead to disillusionment at this stage</li> </ul>	<ul style="list-style-type: none"> <li>• Generally content with their career achievements</li> <li>• Quite limited goals for the remainder of their professional career</li> <li>• Gradually withdrawing from various responsibilities</li> <li>• Fear their knowledge is out-of-date</li> <li>• Somewhat isolated from younger colleagues</li> <li>• Try to cope with problems independently</li> <li>• Only half will take advantage of formal professional growth opportunities</li> <li>• Particularly comfortable with service to department or college</li> </ul>

After Baldwin & Blackburn [3]

seems to enjoy the activity for its own sake and has a good chance to get the student to seek the intrinsic rewards of learning. If a teacher is extrinsically motivated, students might conclude that learning is worthless in and of itself, and lacks inherent value. Whitehead [3] says that the ideal of a technical education is to be ". . . a commonwealth in which work is play and play is life." Two action systems are cited to yield intrinsic rewards in teaching: (1) changes in student performance attributable to teacher actions, and (2) the continuing integration of new information on the teacher's part.

The implicit assumption in this application of Needs Theory is that those attracted to engineering education are gratified by the relatively unstructured academic world, have strong self-actualization needs, and enjoy a moderate challenge and risk. Thus these individuals would take advantage of an opportunity to grow and develop, if that opportunity were made available, with some encouragement and no stigma.

#### IMPLICATIONS OF CAREER PHASES

The recognition of the clues provided by the phases in a career allows administrators to capitalize on a professor's knowledge, expertise, and interests in order to increase intrinsic motivation. There is also a severe caution against the use of extrinsic motivation such as occurs on an industrial scale; extrinsic motivational techniques appear to be hazardous to the long-term health of faculty.

For younger faculty, one might capitalize on up-to-date research knowledge by having novice faculty members teach advanced courses rather than introductory ones. Some of the responsibilities of younger faculty might be relieved while they are learning the art of teaching during the first difficult years. Younger faculty typically appreciate formal workshops and seminars on the state-of-the-art, both in research and in teaching methodology.

Funding, facilities, and release time reserved for mid-career faculty could generate new enthusiasm and halt professional entropic effects. Administrators could provide a challenge, or even retraining, for those faculty who have reached an easy, perhaps boring, part of a career. One could encourage career planning to assist in consciously and systematically examining the alternatives. In particular, a flexible leave and internship policy would allow resolution of some of the mid-life career uncertainty.

Senior faculty could play a major developmental role as a mentor or teaching consultant to beginning or adjunct faculty. Such mentorship has been indi-

cated to be a positive influence for both junior and senior faculty, provided there is eventual growth away by both parties (Levinson, *et al.*, [4]). Senior faculty, in particular, appear to like designing an individual program, rather than (say) partaking in a workshop with others. Such faculty could undertake "senior statesman" projects such as long range planning, studies of student attrition, or work with alumni groups. Temporary administrative jobs might be offered to those faculty. In some cases early retirement and outplacement should be considered as alternatives.

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**Senior faculty could play a major developmental role as a mentor or teaching consultant to beginning or adjunct faculty. Such mentorship has been indicated to be a positive influence for both junior and senior faculty provided there is eventual growth away by both parties.**

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#### IMPLICATIONS OF MOTIVATIONAL STUDIES

Motivational factors indicate the need for an environment which increases intrinsic motivation while supplying extrinsic motivators as informational tools only. Increasing amounts of administrative control and increased concern about promotion and tenure are both seen as counter-productive in the long run. Extrinsic rewards appear to reinforce intrinsic motivation only when they are given in a positive, informational sense.

Intrinsic gratification is gained by encouraging satisfying relationships with students and colleagues such as is brought about by small classes, by continued exposure to students beyond the normal single-term class, and by networking with colleagues for teaching discussions. Intrinsic satisfaction is also brought about by providing a sense of autonomy, perhaps from a sense of input to the curriculum, a choice concerning courses to be taught, and more formative and less summative evaluation procedures.

Intrinsic motivation also occurs when intellectual stimulation occurs. This stimulation must meet the criteria that it changes the way people think about the subject area. For example, stimulation may be gained by participation with industry, either in open-ended problem-solving courses, in team-teaching normal courses, or by consulting in ways which enrich the faculty's intellect and put him on the frontier of knowledge. Sabbaticals, summer work, workshops, and short courses to do research/teaching development can also provide such stimulation. Ultimately, elec-

*Continued on page 187.*

# CONTENT AND GAPS IN BSChE TRAINING\*

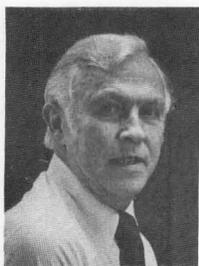
## *Value and Mystique in Engineering Economics*

JAMES B. WEAVER  
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**E**NGINEERING ECONOMICS is often taught to chemical engineering students by other engineering departments. Within ChE departments, economics is usually introduced into a design course as a major sub-topic and therefore receives student attention only for part of a semester. AIChE is planning a survey to clarify the current extent of economics training in BSChE curricula.

Thirty-eight texts on investment analysis from all sources have been reviewed by the author, and coverage of these is compared. The books include engineering economics, chemical engineering design/economics, cost engineering, and finance/business school sources. While coverage of many topics is consistent and adequate, omissions are remarkable. Some patterns seem related to differences among the four sources above. For instance, many engineering economics texts still omit proper coverage of working capital and corporate income taxes—apparently for historical reasons. Chemical engineering-sourced texts are consistent on these important topics, but rate lower on other important factors of investment analysis. Finance/business texts rate better overall.

The author believes engineers should receive consistent training in these topics, as a first step toward improving the image of investment analysis by top executives. (Now, investment analysis is often treated



**Jim Weaver** retired in 1980 as Vice-President for Venture and Capital Appraisal from ICI Americas, Inc. He earned his BS and MS degrees in chemical engineering from MIT. He has authored many articles on investment appraisal, including coauthorship of sections on "Cost and Profitability Estimation" for two editions of Perry's *Chemical Engineers' Handbook*. He is enjoying retirement in Florida, but continues to write and speak.

\*Paper presented at the AIChE meeting, Washington, DC, in December, 1988.

as a computer-dominated toy, or a sales tool for desired projects.) Additional consistent training could improve objectivity and appropriateness of investment analyses in corporations and the government.

### DISCUSSION

Industry does not generally use objective engineering techniques for investment appraisal. With the availability of computers, executives ask for more economic studies but usually use the many possible scenarios on a project to further their own goals—to fortify their intuition. Top management is playing with economic analysis more, but they are using it less. Unless curricula for analysts are improved, it will be difficult to improve industry's attitude.

Current practice and education for investment analysis has dominated much of my time since my 1980 retirement, because I feel that the available economics courses for chemical (and other) engineers are haphazard and inappropriate for what is one of the most important and all-encompassing aspects of engineering. Project evaluation is not an engineering specialty—it is a topic in which all specialties need a background, so that freshly-graduated engineers can (promptly) assist industry or government decisions on major investments. Few engineers now receive the proper education for this activity. And those that *are* trained get inconsistent training.

Between October 1987, and November 1988, I read 38 texts currently offered for courses dealing with investment analysis.\* I looked for the topics [1] that I found unsettled and continually debated during my 40-year career in investment appraisal. I also looked for important topics which I felt texts and courses were missing entirely—or, conversely, were overemphasizing. I was seeking useful discussion which might clarify unsettled problems for the student, not uniformity. Many non-economic engineering problems remain unsettled, and current status of studies is discussed in current engineering texts. As I feared, that

\*Texts published before 1980 are included only for highly-rated volumes not revised in this decade.

**Project evaluation is not an engineering specialty—it is a topic in which all specialties need a background, so that freshly-graduated engineers can (promptly) assist industry or government decisions on major investments. Few engineers now receive the proper education for this activity. And those that are trained get inconsistent training.**

was not the case in project-appraisal texts; each author has his own point of view, and only a few discuss other views or say that topics are unsettled.

Texts I reviewed were not all by chemical engineers—or even all by engineers. Investment analysis has recently become just as important a topic for business school students (in finance, for instance), and I wanted to compare their coverage of these topics. My conclusions are more favorable for the finance-oriented texts than for those by engineers! Their courses would probably be useful for chemical engineering undergraduates.

Chemical engineering (ChE) texts do rate higher than most traditional “engineering economics” (EE) texts, based on my criteria. That doesn’t help ChE students much, because most universities do not have a full course on project analysis in the chemical engineering department. In ChE, economics is considered part of design and is introduced into that course—if it is taught at all. That means part of a semester—usually less than half.

Many chemical engineering departments also offer (or require) a course in ‘Engineering Economics’ for their undergraduates (or graduates)—given by another engineering department (usually civil or industrial engineering). That is why I claim that problems of ‘EE’ texts are problems for many chemical engineering undergraduates.

Today, all we know about the current status of requirements is that different universities may or may not require any such courses. Others may require either, or both. With the help of an AIChE survey we expect to be more specific on current status in a year or two. For over a decade, Ed Eisen of McNeese State University has taken useful surveys on a wide range of ChE unit operations (including design) for AIChE’s Education Division. The 1989 survey will focus specifically on courses in investment analysis, and results should be available some time in 1990. The intent is to include courses (and texts) in the business schools at the same universities.

#### METHOD OF ANALYSIS

This is only a partial report on my survey, emphasizing strengths and weaknesses of ChE texts. The complexity of the survey (31 topics in 38 books)

**TABLE 1**  
**Chemical Engineering Texts**

Author/Year key	Citation
A&R86	Axtell, O., and J. Robertson, <i>Economic Evaluation in the Chemical Process Industries</i> , Edn. 1, Wiley (1986)
C&R86	Couper, J.R., and W. H. Rader, <i>Applied Finance and Economic Analysis for Scientists &amp; Engineers</i> , Edn. 1, Van Nostrand/Reinhold (1986)
HW&W83	Holland, F.A., F. A. Watson, and J. K. Wilkinson, <i>Introduction to Process Economics</i> , Edn. 2, Wiley (1983)
PG&M84	Perry, R.H., and D.W. Green, <i>Perry's Chemical Engineers' Handbook</i> , (Sec. 25 by Holland, et al., "Process Economics"), Edn. 6, McGraw-Hill (1984)
P&T80	Peters, M.S., and K. Timmerhaus, <i>Plant Design and Economics for Chemical Engineers</i> , Edn. 3, McGraw-Hill (1980)
U84	Ulrich, G.D., <i>Guide to Chemical Engineering Process Design and Economics, A</i> , Edn. 1, Wiley (1984)
V83	Valle-Riestra, F., <i>Project Evaluation in the Chemical Process Industries</i> , Edn. 1, McGraw-Hill (1983)

means each journal article will be incomplete. I have sent full draft reports to many authors. The American Association of Cost Engineers has agreed to publish complete results as a monograph.

Complete citations for the seven ChE texts are shown in Table 1. The ‘Author-Year Key’ is used in Tables 3-6 to identify each text. Tables 3-6 contain my key judgments. Note that in these tables, minus [-] is better than zero [0]. Table 2 discusses alphabetically the 31 topics which I used in analyzing the texts; most are covered in more detail in reference [1].

Unlike usual book reviews, my screening looked only at the specific topics discussed in Table 2. I have volunteered further specifics on my judgments to interested authors and several have accepted.

#### SUMMARY OF RESULTS

Two of these seven ChE books were ranked highest in the survey. For extensive coverage, Peters & Timmerhaus was best, although it is becoming out of date. For good (brief) coverage, Axtell and Robertson also ranked well. In fact, in spite of its brevity, A&R86 only missed nine of my topics (fewer than any

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**TABLE 2: Discussion of Topics Listed in Tables 3-6**

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**Accounting Systems** • Engineers need background about financial accounting systems, including product cost accounting and capital record-keeping. Accounting figures are estimates, approximations of history within legal constraints for use by shareholders and government authorities. However, approved systems permit wide variation in detail and any set can be misused by newcomers, outsiders, or untrained engineers. Texts should warn that such historical data is often not suitable as such for use in investment analyses.

**Acquisition Analysis** • Mergers and acquisitions represent important and frequent investments by major corporations. Texts should discuss whether or not the same investment appraisal techniques apply to them. Lack of discussion permits the inference that the same techniques are applicable. Authors should say they are not applicable to merger and acquisitions studies—or else discuss the many special considerations.

**After-Tax Analysis** • Because depreciation is tax deductible, capital investment alternatives must be compared after taxes. However, before-tax comparisons have not been abandoned, nor clearly vetoed, in many texts. Even for preliminary screening, before-tax comparisons may mislead. Many authors prefer the simplicity of deferring all consideration of taxes until late in the text. If they do, eventual need for considering taxes should be stressed in early pages. Even then, the occasional user may dip into the text and be misled by problem "solutions" in early pages which ignore taxes.

**Alternatives** • Investment appraisal must include alternative investments—not just a single proposal. For instance, mutually-exclusive alternatives solve the same problem with different capital investments. Choosing a process or the plant capacity represents this type of alternative. Restricted funds may also require comparison of non-mutually-exclusive alternatives which compete only for funds. All project forecasts should also be compared to an alternative set of forecasts for the "zero-investment" case.

**Break-Even Analysis** • This accounting-based concept was widely used in project, plant, and product studies before cash-flow investment analysis was widespread. It still may be useful if cash-flow breakeven is considered, but many texts discuss only breakeven at zero accounting profit. Limited usefulness of breakeven does not seem to warrant extensive coverage.

**Computer Short-Cuts** • An early criticism of discounting procedures was the effort and time consumed in calculation. Computers, large and small, and hand-held programmable calculators reduce the problem tremendously.

**Cost of Capital - Average or Project?** • Should all investment projects be compared to the same hurdle rate, or should the hurdle be lower where special financing is available to an investment project? Journal articles differ. Texts should discuss at least the author's view.

**Cost of Capital vs. MARR** • The hurdle rate (or minimum acceptable rate of return, MARR) is clearly related to cost of capital — but is it equal or higher? Some companies have higher hurdle rates (for some projects) to allow for risk. A higher hurdle rate might also allow for some projects justified on bases other than profitability — for instance, roads, office building, research facilities.

**Depreciation** • Several different concepts are included; the distinction may be particularly important for engineers who may think of the wrong meaning first. Estimates of depreciation may refer to: physical life of the equipment, due to deterioration (often most important to engineers); accounting allocations maintained in financial books for shareholders; and, often, different tax-deductible allocations acceptable to IRS. All should be discussed, including frequent IRS changes in the latter. Legality of separate tax and shareholder books (in the U.S.) should be recognized. Few engineers seem aware of the important distinction.

**Documentation** • For historical and legal purposes, records are needed about justification of major investments. Such records supply feedback for later proposals, both specific cost forecasts and from general approach to the justification. How detailed should such documentation be? Should records cover all stages if changes are made in project scope? Or in justification forecasts?

**Equity Basis for Analysis — 100%?** • (This relates to Cost of Capital-MARR above.) For comparability, most authorities believe all projects should be analyzed and compared on the basis of 100% equity, the full investment base, and financing should be considered separately. Others recommend including interest as a cost and reducing the investment base if borrowing is involved in the project or the company.

**Feasibility Studies** • For any large project, justification is a many-step procedure. How should early studies be handled? What data should be available before the first formal profitability calculation? How often should it be repeated?

**Forecasting** • Forecasts of key elements affect project profitability studies, and forecasts for 5 to 15 years are required. Are year-by-year forecasts useful? Are they possible?

**Handling Inflation** • Inflation affects some but not all aspects of project profitability studies, so it should be considered. High inflation rates of the 1970s brought this factor into almost every text; continuing attention is needed.

**Incremental Expansion** • Often a minor bottleneck can be broken to expand existing facilities, delaying major investment. Sometimes a minor investment will permit activation of larger, idle facilities. However, such alternatives introduce special hazards. The incremental investment may put the producer deeper in unprofitable businesses, unless some broader analyses are made.

**Learning Curves** • Correlations since World War II showed patterns of cost reduction on wide ranges of products as producers gained cumulative experience in manufacturing. This provided a means of cost and price forecasting which could help project appraisal studies in the 1950s and 1960s. However, cost reductions never approached high rates of inflation in the 1970s, and the technique no longer seems useful.

**Linear Programming of Rosters** • If suitable data on single best-estimate forecasts were available simultaneously on a roster of all foreseeable projects, and the projects are independent (or relationships are specified), linear programming could be used to choose the best set of alternatives. Data requirements are extreme, perhaps unrealistic.

**Multiple Rates of Return** • In DCF internal rate of return studies, unusual cash patterns can cause multiple and meaningless solutions. Mathematics are understood, and several means are available to avoid the problem.

**Payout Time** • This quick-and-dirty analytical technique remains a favorite with manufacturing companies. It has some advantages and many disadvantages. One overlooked disadvantage — it ignores working capital. Discounted payout time is recognized as an improvement and should be mentioned.

**Plant Location** • Costs differ by locality, so location has important (on occasion dominating) effects on investment appraisal studies. The nature of the effects and importance of analysis should be mentioned.

**Plant Sizing** • A key alternative (q.v.) is how big a plant to build, how much capacity, presumably based on sales forecasts. Building in several stages may show a higher profitability, even if total investment cost is higher. Some patterns of problems and solutions exist.

**Preliminary Engineering Approval** • Major projects often involve millions of dollars of engineering and design expenses — more than many other projects cost in total. If new markets or technology are involved, or unusual risk of any sort, some special management approval seems warranted before such expenditures, even if it's only internal engineering.

**Presentation Formats** • Standardized forms for project proposals are shown in some articles and books. Some may be obsolete, based on a single scenario which may not represent a management consensus. Multiple scenarios complicate the presentation but seem necessary to permit a real decision at top company levels.

**Project Audits** • Many companies prescribe formal review of some or all capital projects, after implementation. Feedback is said to justify the cost. There are problems; nature and extent of such audits should be discussed.

**Reinvestment Assumption (DCF)** • Although many feel the question has been resolved, some authors maintain that internal rate of return assumes that positive cash flows during a project must be reinvested during the project life at the solving rate of return to achieve the calculated return. Ideally, both points of view should be discussed.

**Replacement** • Special techniques were devised after World War II to assess replacement of existing facilities. Such problems can now be handled within more general project appraisal techniques. Some texts still include excessive details of the older special techniques.

**Risk Analysis** • This topic receives wide (if variable) coverage in engineering economy texts and articles. While of theoretical interest, industry has considered and rejected complex techniques. Detailed text coverage impinges on more important topics.

**Sensitivity Analysis** • Projects are often presented for corporate decisions based on a single "best estimate" scenario. Simple graphical and tabular means were developed to show project sensitivity to major variables. As a minimum, these should be discussed. With the computer, other possible scenarios can be calculated in full for further investigation of sensitivities.

**Sunk Costs** • Past investments should not (in general) influence current decisions. However, tax deductibility of depreciation means some past decisions affect timing and amount of future cash flows.

**Unequal Project Lives** • Most "alternatives" (q.v.) can be considered at equal project lives, which simplifies comparisons. Some cases necessarily involve unequal project lives, and several decision models have been developed.

**Working Capital** • Like a new company, almost every investment project requires initial cash to get under way, until incoming cash flows are sufficient to pay current bills. Inventories and accounts receivable are assets, but they require initial cash, too, partly offset later by accounts payable to others.

other), and rated a "+" on thirteen topics (better than any other).

Two other ChE texts also had satisfactory coverage. Couper & Rader was quite acceptable, in spite of a few gaps. It contains outstanding coverage of a couple of topics, as discussed below. The section on "Process Economics" in the 6th edition of Perry's *Chemical Engineers' Handbook* also rates satisfactory for handbook coverage.

The other three ChE texts have coverage which I feel is unsatisfactory, but each text had some strong points that I will mention later. And some non-engineering texts had better coverage on several topics.

The most flagrant omission, in all 38 books, was a lack of attention to working capital and to the impact of income taxes. Table 3 presents those results along with my over-all judgments. All the ChE texts had some discussion of both topics, unlike most of the EE texts (all fourteen omissions of working capital were in EE texts). Four ChE texts covered each of the two major topics adequately—but not the same four! Three tended to introduce taxes late and to give it low emphasis, even though taxes can have a dominating impact on choices. This makes the early examples and homework problems in those texts misleading. Delay in discussing taxes also prevents full discussion of several other key topics, including sunk costs, payout time, break-even analysis, and cost of capital, because of the impact of taxes on each of them.

Table 4 groups the topics most often omitted in texts on investment analysis. None of the seven ChE texts covered more than three of the ten topics.

I ranked C&R86 "outstanding" on coverage of feasibility studies. The sequence of early decisions on projects is ignored in the majority of texts reviewed. However, P&T80, A&R86, and V83 also covered feasibility studies well, so ChE texts ranked above the other engineering and non-engineering texts in

this respect. Are feasibility studies more important, for some reason, in chemical engineering? I think the answer is that the other specialties just have not seen ChE texts and forgot to mention the problem.

Another strong point in C&R86 is its coverage of computer short-cuts, and A&R86 also included the topic well. *None* of the other ChE texts discussed the important help that computers can give. Timing of publication cannot be given as an excuse for ignoring this topic; non-ChE texts as old as 1980 got good rankings, but many others, more recent, did not.

Documentation of major investment decisions is important in industry, but does not seem important to textbook authors. Only two of the ChE texts bring it up at all, and only one of the EE texts gives it adequate coverage. Likewise, presentation of proposals for decision is important. Both C&R86 and P&T80 ranked high in this respect, but none of the other ChE texts and only a handful of the other types did.

Note that three topics I would like to see covered were not mentioned by any of the seven ChE texts. One is acquisition analysis, a very important topic nowadays. The authors could at least say whether or not they feel the same techniques are applicable for appraising acquisitions!

Table 5 summarizes results for other important topics I felt were often inadequately covered. The ChE texts did not rate well here, either. Three of the books mentioned ten of the fourteen topics, but only two adequately covered more than three of the topics [C&R86 had 4, A&R86 had 7].

When texts mention audits of investment project

**TABLE 3**  
Dominating Topics and Overall Judgment  
(Chemical Engineering-sourced Texts Only)

	• Author/Year Code •						
	A&R 86	C&R 86	HW&W 83	PG&M 84	P&T 80	U 84	V 83
Working Capital	-	+	+	+	+	-	+
After Tax Analysis	+	-	+	+	+	-	-
My Total Judgment (All Topics)	OK- and brief	OK- and some gaps	Weak	OK- for handbk	OK- for extensive	Weak	Weak

+ coverage which is adequate or better  
- inadequate coverage

**TABLE 4**  
Topics Often Omitted

	• Author/Year Code •						
	A&R 86	C&R 86	HW&W 83	PG&M 84	P&T 80	U 84	V 83
Acquisition Analysis	0	0	0	0	0	0	0
Computer Shortcuts	+	+	0	-	-	-	-
Documentation	-	-	0	0	0	0	0
Feasibility Studies	+	++	0	0	+	0	+
Forecasting	-	0	0	0	0	0	0
Incremental Expansion	0	0	0	0	0	0	0
Plant Location	0	0	0	0	+	0	0
Plant Sizing	+	0	0	0	0	0	-
Preliminary Eng. Approval	0	0	0	0	0	0	0
Presentation Formats	-	+	0	0	+	0	0

+ coverage which is adequate or better  
++ outstanding coverage  
- inadequate coverage  
0 no coverage of important topics

performance after implementation, they all say such audits are important. But C&R86 was the only ChE text to bring it up, and all but three of the non-ChE texts also gave it short shrift.

How does one choose plant size to meet a given forecast? Few texts discuss this at all. A&R86 is the only ChE text with satisfactory coverage, although V83 gives it some coverage.

Table 6 groups another set of topics—those I felt were overemphasized in many EE texts. They are topics of considerable mathematical and research interest (or were at one time)—but I found that none

were widely used in industry. And I felt industry had good reason to ignore them. I don't believe academics have made progress not recognized by industry. So, for the first three items in this table, I feel that omission of any coverage is all right (an asterisk is used instead of a zero).

At the other extreme, "exag" shows (for any of the five topics) where I feel book space is wasted by extensive coverage. In all likelihood, valuable course time is also wasted on these topics at the expense of those topics in Tables 4 and 5.

ChE authors did better than the average from other sources on the Table 6 topics—particularly on break-even analysis. Nobody got carried away, and coverage by three was adequate. Three other ChE texts dealt only with accounting break-even concepts, instead of including cash-flow break-even.

**TABLE 5**  
Other Topics Often Poorly Covered

	• Author/Year Code •					
	A&R 86	C&R 86	HW&W 83	PG&M 84	P&T 80	U V 84 83
Acctg. System Analysis	-	-	-	+	-	0 -
Alternatives	+	+	-	0	+	- -
Cost of Capital - Average?	0	0	0	0	0	0 0
Cost of Capital vs MARR	-	-	0	0	0	0 -
Depreciation	+	-	+	-	-	+ -
Equity Basis for Analysis	+	0	0	0	0	0 -
Handling Inflation	+	-	-	-	+	- +
Multiple Rates of Return	-	-	0	0	-	0 -
Payout Time	+	+	-	-	+	- +
Project Audits	0	+	0	0	0	0 0
Reinvestment Assumption	+	-	0	0	0	0 0
Sensitivity Analysis	+	+	+	+	0	- -
Sunk Cost	0	0	0	+	0	0 -
Unequal Project Lives	0	0	0	0	0	0 0

+ coverage which is adequate or better  
- inadequate coverage  
0 no coverage of important topics

**TABLE 6**  
Topics Often Overemphasized

	• Author/Year Code •					
	A&R 86	C&R 86	HW&W 83	PG&M 84	P&T 80	U V 84 83
Break-Even Analysis	+	+	+	-	-	* -
Learning Curves	*	*	-	exag	*	* +
Linear Programming of Rosters	*	*	*	*	*	* *
Replacement Analysis	+	0	0	0	+	0 +
Risk Analysis	0	exag	exag	-	0	- exag

+ coverage which is adequate or better  
- inadequate coverage  
exag exaggerated coverage, superfluous for real use in industry even if accurate  
0 no coverage of important topics  
\* no coverage where topic is not important; no criticism intended

## CONCLUSION

I hope this comprehensive review (admittedly, one man's judgment) will permit universities to improve their choice of books for courses being given in chemical engineering design-and-economics. But I must

**TABLE 7**  
Top Ranked Texts

Author/Year key	Citation
<b>Engineering Economics Texts</b>	
B78	Bussey, Lynn E., <i>The Economic Analysis of Industrial Projects</i> , Edn. 1, Prentice-Hall (1978)
GI&L82	Grant, E.L., G. Ireson, and R. Leavenworth, <i>Principles of Engineering Economy</i> , Edn. 7, Wiley (1982)
S87	Smith, G.W., <i>Engineering Economy: Analysis of Capital Expenditures</i> , Edn. 4, Iowa State University Press (1987)
S&W86	Sprague, J.C., and J. Whittaker, <i>Economic Analysis for Engineers and Managers</i> , Edn. 1, Prentice-Hall (1986)
S&S87	Stermole, Frank, and John M. Stermole, <i>Economic Evaluation and Investment Decision Methods</i> , Edn. 6, Engineering Press, Inc., San Jose, CA (1987)
S83	Stevens, G.T., <i>Economic Analysis of Capital Investments for Managers and Engineers</i> , Edn. 1, Reston Pub. Co. (1983)
<b>Business/Financial Texts</b>	
B&S88	Bierman, Harold, and Seymour Smidt, <i>The Capital Budgeting Decision Economic Analysis of Capital Investment</i> , Edn. 7, MacMillan (1988)
B&M84	Brealey, R., and S. Myers, <i>Principles of Corporate Finance</i> , Edn. 2, McGraw-Hill (1984)
H82	Herbst, A.F., <i>Capital Budgeting: Theory, Quantitative Methods, and Applications</i> , Edn. 1, Harper & Row (1982)

sadly add that even the best is none too good for teaching a consistent picture of the important elements of investment analysis to graduate and undergraduate students. The best I can say is that the chemical engineering authors have been more perceptive than many of the other engineering authors. The best group of texts is from the finance/business school sector. ChE undergraduates might benefit from wider use of those texts.

This paper cannot be stretched to cover the advantages and shortcomings of the 31 texts from non-ChE sources.

As a substitute, Table 7 lists the top ranked books (in my opinion) in each category. All the engineering-sourced books published since 1980 were included in my study. Therefore, if a book is not listed in the table, I recommend your school should not be using it. However, my coverage of finance/business tests is probably not so complete.

#### REFERENCES

1. Weaver, James B., "Persistent Problems in Investment Analysis," *Ind. Management*, **28** (4), p 7-12 (1986). Published by Institute of Industrial Engineers, Norcross, GA 30092 □

## ChE letters

### FLORIDA STATE/FLORIDA A&M ACCREDITATION ERROR NOTED

To The Editor:

With reference to our article, "General Education Requirements and Chemical Engineering Curricula," appearing in the Spring 1989 edition of *Chemical Engineering Education*, in Table 3 we referred to Florida State/Florida A & M as having an unaccredited Chemical Engineering program. This resulted from using the 1986 Annual Report of The Accreditation Board for Engineering and Technology, Inc. (ABET).

After the article was submitted, the 1987 Annual Report of ABET was released. Florida State/Florida A & M now has an *accredited* Chemical Engineering program. We humbly apologize for the mistake and take full responsibility for the error in our article.

Walden L. S. Laukhuf  
C. A. Plank  
James C. Watters  
*University of Louisville*

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## USING THE LABORATORY TO DEVELOP ENGINEERING AWARENESS

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The Professional Institutions Directorate of the Engineering Council (of the United Kingdom) issued guidelines in 1983 for the training of all undergraduate engineering students in Great Britain who wish to attain chartered engineering status. These proposals subsequently became mandatory in 1985 and included the requirements that all courses accredited by the Engineering Council contain a minimum level of Engineering Applications 1 (EA1) and Engineering Applications 2 (EA2) by the start of the 1988 academic year. For chemical engineering these are defined as:

- An introduction to the methods of fabrication, selection of materials of construction, and operation of chemical process plant hardware, giving due consideration to the interaction of these factors on costs, safety, operability, and reliability.
- The application of engineering principles to the solution of practical process engineering problems.

In the UK it has been common for most chemical engineering courses to integrate the practice of process



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engineering and to seek real solutions to practical problems. Thus, few modifications were necessary to meet the requirements of EA2. However all UK courses needed enhancement in order to meet the EA1 proposals of the Engineering Council. The focus of this paper is on the changes made to the undergraduate laboratory programme of the chemical engineering first degree course at the University of Bath. These changes have been introduced in order to meet the Engineering Council requirements and to develop a greater student awareness of engineering concepts.

### BACKGROUND

Before moving on to the detail, a contextual introduction is given. Most students entering the chemical engineering course at Bath have specialized in three sciences at the secondary school level and have attained at least three General Certificate of Education qualifications at the advanced level (usually in chemistry, physics, and mathematics). The student has little or no knowledge of engineering subjects, and practical experience is limited since the trend in recent years has been to reduce the amount of laboratory work at secondary schools (mainly because of financial considerations). Although the student may have visited companies or listened to talks from visiting engineers, his concept of engineering is often flawed. They are often unaware of the probability of multiple solutions to a problem and have no idea of the technical difficulties encountered in design and construction of processing units.

The Chemical and Bio Process Engineering degree course at Bath endeavours to provide a solution to some of the problems and to instill engineering awareness in the student. For most students, a year-long industrial placement is an integral part of the degree scheme. The placement is undertaken as the third year of a four-year course, and a position as a trainee engineer within a company or research establishment is found by the University. Not only is the relevance of

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the academic course highlighted for the students, and knowledge consolidated, but valuable practical experience is also gained. During this period progress of the student is monitored both by the company and by his industrial tutor. An improved appreciation of financial constraints and the importance of communication skills is obtained, and the student's subsequent development during the final year of the degree scheme is enhanced.

### THE BATH APPROACH

Engineering awareness is developed from the very beginning. Students entering the department are given a week-long course which introduces them to the various core subjects of chemical engineering and their relation to the "process dimension." The process dimension is seen to be the main characteristic of chemical engineering and can be defined as "the ability to break down into its component parts a manufacturing process in which matter is transformed or chemically changed to provide a specification for each subdivision, and to recombine the whole into an economical, workable, and maintainable plant." This is achieved by means of overview lectures, a preliminary design assignment, and industrial visits.

In the third term of each year the students undertake a design project which has been chosen to show the relationship between chemical engineering fundamentals, engineering practice, and the enabling science (mathematics, economics, chemistry, *etc.*) which they have been taught during the year. The design projects are chosen to complement the courses, to provide experience in teamwork, and to develop awareness of the practice of chemical engineering.

The first year design project is usually a mass and energy balance and flow sheeting exercise on a well-documented process. The second year design is used to draw comparisons between existing processes and less conventional routes, *e.g.*, the production of n-butanol by chemical and biochemical routes. In the final year, senior chemical engineers from industry suggest the original problem specification, provide technical input when information is not available in the open literature, and lead discussion groups. This work involves projects requiring the latest technology, *e.g.*, off-shore gas-oil separation, destruction of toxic wastes, and microbial production of *cis*-1,4-polyisoprene.

A major element in developing engineering awareness during the first two years of the degree scheme is the undergraduate laboratory programme. The rest of this paper is devoted to those elements of the programme which relate to EA1.

### UNDERGRADUATE LAB: EA1 Experiments

The experiments relating to the EA1 requirements, which comprise approximately 30% of the total first and second year laboratory programme, can be summarized as follows:

#### 1st Year Experiments

- The design and construction of a pumping circuit involving leak testing, calibration of instruments, and characterization of the pump
- Start-up, operation, manual control, and monitoring of pilot plant equipment, *e.g.*, double effect evaporator and batch packed distillation column
- The problems of measurement and choice of transducer, *e.g.*, temperature, pressure, and viscosity measurements using various measuring devices

The object of these experiments is to demonstrate the difficulties that can be encountered in "simple" measurements and relatively "straightforward" processing equipment, and to establish the need for engineering input.

#### 2nd Year Experiments

- Start-up and operation of a steam boiler (capacity 2000 lbs per hour steam at 150 psig)
- Hazard and operability study (HAZOP) of a batch distillation column
- Disassembly and reassembly in a different configuration of a plate heat exchanger and analysis of thermal performance
- Work permit preparation for the modification of a number of pieces of process equipment, *e.g.*, cooling tower and distillation unit

Process safety has deliberately been included in the experimental programme to complement the lecture courses on process design and development and loss prevention, and to emphasize the need for chemical engineers to be aware of, and to actively include, safety in all aspects of their work.

## FIRST YEAR EA1 EXPERIMENTS

The experiment (see Table 1) requiring the calibration of certain devices for temperature measurement and for viscosity measurement was introduced in 1982 because students had misconceptions about the meaning of accuracy, particularly with reference to the calibration of instruments.

The first part of this experiment requires the calibration of a number of temperature measuring devices against a standardized National Physics Laboratory thermometer and, if possible, comparison of the values obtained with theoretical values from the literature, *e.g.*, e.m.f.s of thermocouples. The equipment consists of a thermostatically controlled water bath, a multimeter, and various temperature measuring devices which can all be purchased for approximately £1300. The students invariably report the results in terms of the accuracy of one device, *i.e.*, deviation from a straight line or a smooth curve when compared to the others, without consideration of the sensitivity of the device or the limits on reading the scales on the instrument.

The second part of the experiment is the determination of the viscosity of carboxy-methyl-cellulose solution using three different techniques. The only expensive item of equipment is the rotating cup viscometer, which costs approximately £1000. Students are given references for the different methods, but are not told that the fluid is non-Newtonian. The apparatus for the falling sphere method was chosen to give very small fall times, thus making the main experimental error the timing of the fall of the sphere. Typical conclusions drawn by the students were that only the rotating cup method was "accurate" and that the other techniques were not suitable for determining viscosities, in spite of the fact that they were given the literature references and informed that these are standard methods for determining viscosity. Only about 10% of the students concluded that the techniques being used might not be suitable for the range of viscosities being studied.

Oral presentation of results (in the presence of their fellow students) is required for these experiments, and it enables us to make students aware of the difference between errors resulting from the calibration of an instrument, the accuracy of an instrument based on theory, and the method of calibration. It also illustrates some of the pitfalls to be avoided when using results from measurement devices and fosters discussion of the limitations of the various measurement techniques and the problems of departure from ideality.

The experiment dealing with the operation of a double effect evaporator (see Table 2) was designed

to give experience in start-up, steady-state operation, and shut-down of a pilot plant. The equipment, which would have cost in the region of £40,000 to purchase, was donated to the department. Only manual control is provided on the equipment, and hence the students experience difficulty in obtaining and controlling the unit at steady-state. This experiment gives most students their first hands-on experience with equipment of a reasonable size, and their reactions have been mixed. Generally they have found it enjoyable to operate a pilot scale unit. However, the difficulties already referred to limit the amount of meaningful data on the performance of the evaporator, and this has been frustrating. In reporting their results, nearly all the students refer to the need for better control so that steady-state operation can be obtained.

The operation of a packed, batch distillation column, 80mm diameter, with a packed height of 1.7m, gives the students their first exposure to distillation on any pilot or larger scale. Their experience has usu-

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**TABLE 1**  
**Calibration of Temperature Measuring Devices and Measurement of Viscosity**

*Time allowed for experimentation:* 4 hours

Experiment requires:

- Part A:
- Calibration of the following devices using a standardised National Physical Laboratory thermometer:
    - Mercury-in-glass thermometer
    - Thermistor
    - Platinum resistance thermometer
    - Type T and type K thermocouples
  - Comparison of results with data from literature
- Part B:
- Measurement of viscosity
  - Preparation of a carboxy-methyl-cellulose solution (range 0.5 to 1.5 w/w%)
  - Determination of viscosity at 20°C and 35°C using
    - Falling sphere method
    - Rotating cup
    - Ostwald viscometer

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**TABLE 2**  
**Operation of Double Effect Evaporator**

*Time allowed:* 7 hours  
(Capacity of evaporator - nominal 800 kg<sup>h</sup><sup>-1</sup>)

Experiment requires:

- Start-up of evaporator
  - Steady-state operation using manual control
  - Mass and energy balances over evaporator
  - Shut-down of evaporator
-

ally been limited to small scale bench distillations in chemistry practicals, using standard glassware. They are asked to start-up the column and to operate at total reflux to determine heat losses. Then they must choose a reflux ratio and carry out a mass balance for the time of operation. Their main reaction is surprise at both the length of time required ( $\approx 3$  hours) to reach equilibrium at total reflux and the poor thermal efficiency. The latter is mainly due to the large heat losses from the unlagged reboiler.

Written reports in the form of a technical letter giving a brief outline of the experiment, together with the results, a brief discussion, conclusions, and recommendations are required for the above two experiments. The students are graded by evaluating the report and by monitoring their approach during the experimentation.

The experiment in which the students design, construct, and test a pumping circuit is detailed in Table 3. The equipment consists of standard "off the shelf" items and costs approximately £1250 per rig. The items provided enable a number of different circuit configurations to be constructed.

The experiment has been invaluable in demonstrating the problems involved in the design of even simple

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**Since an engineer is effective through what he does rather than through what he knows or could do, it is important that engineering students acquire not only understanding and practical experience, but also speaking, writing, and calculation skills.**

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rigs. This is particularly true for students who have little or no previous practical experience who make mistakes in the design and construction of the pumping circuit. We hold discussions with each student pair to point out errors in their design construction and to suggest improvements before they attempt to construct the rig. After the rig is built, tests are carried out to leak test, to characterize the pump, and to carry out the other tasks detailed in Table 3.

The lessons learned by the students during their first year laboratory sessions on EA1 can be summarized as follows:

- Instruments are only as accurate as their calibration
- Instruments must be chosen with a particular task in mind
- Effective control of a unit must be carefully thought out; the effect of altering one parameter may have considerable effect on other parameters and the overall operation of the unit.
- Manual control can be satisfactory but is limited to some simple systems
- The time for a system to reach steady-state conditions can be long
- Multiple solutions exist even for simple design problems
- An appreciation is gained of the practical difficulties encountered in the construction of units consisting of a variety of materials and components
- The importance of effective communication skills is demonstrated

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**TABLE 3**  
**Design and Construction of Pumping Circuit**

*Time allowed:* 15 hours

*Experiment requires:*

- Design of circuit
- Construction of circuit
- Leak testing
- Determination of flow rate versus head characteristics of pump

*The following components are provided:*

- Rotameter
- Pump (dismantled)
- Borden pressure gauge and pressure transducer and indicator
- 'V-Reg' valve and globe valve
- Two tanks and framework
- Q.V.F. pipe sections, elbows, tees, hose connectors and couplings
- Various pipe fittings and flexible hose

*The student must determine:*

- The circuit design for characterisation of pump and leak testing
  - Calibrate one of the pressure measuring devices using a 'dead weight tester' before inserting in circuit
  - Use calibrated pressure gauge to calibrate other gauge *in-situ*
  - Calibrate *in-situ* the rotameter
  - Determine flow rate versus head characteristics of pump
- 

**SECOND YEAR EA1 EXPERIMENTS**

Although it can reasonably be argued that students have already acquired a good level of understanding of safe working procedures, this key area is now emphasized, through both existing and new experiments. The expenditure for the following experiments was less than £250 since most of the necessary equipment was already installed.

The batch distillation of an organic mixture in a steam heated boiler is undertaken by all students, working in pairs. In addition to the traditional analysis (for example the calculation of the HTU of the packing), a hazard and operability study is required [2, 3, 4]. The latter forms the main focus of the reports produced by the students.

The Work Permit assignment (Table 4) requires the students to read four official Health and Safety Executive (HSE) guidance notes [5, 6, 7, 8]. They must then prepare a work programme and issue a work permit for 1) the replacement of a condenser on a batch distillation column and the repair of a weld fracture on the vapour return line of the reboiler, and 2) entry into an induced draught cooling tower to inspect the fan.

Students are not required to produce a formal report of this assignment, but they must submit material which would reflect the way in which the information could be presented at a preliminary meeting of the plant supervisor, the plant engineer, the maintenance supervisor, and the safety officer. In common with the previous assignment this is undertaken, in turn, by all of the second year students.

A third task, undertaken by some students, is to witness the start-up of the department's package steam boiler, to report on the start-up and shut-down procedures currently used, to identify the hazards, and to note key operating parameters (see Table 5). By way of preparation, a HSE guidance note on the operation of automatically controlled steam and hot water boilers [9] is studied.

The fourth and last task relating to EA1 illustrates how a traditional experiment can be modified to include an EA1 component. In the past, students have used a small plate heat exchanger to evaluate the dependency of heat transfer coefficients and the pressure drop on fluid flowrates. The practical exercise of changing the plates and leak testing was introduced two years ago. The students complete the performance analysis, devise and discuss a safe procedure for changing the plates, and then carry out the task. As with the other EA1 assignments, it is relevant and is enjoyed by the students, making them more receptive to the lessons embodied in the experiment.

## DISCUSSION

At Bath all EA1 learning is woven into the degree scheme, and it is apparent that the students are receptive to this approach. Not only are additional demands on the students' time minimized, but also the relevance of the EA1 and EA2 material to process engineering is clear.

An alternative approach reported by others [10] includes an EA1 module on the dismantling, inspection, reassembly, adjustment, and testing of a safety valve. However, most students see this as a task where the principal objective is simply overhauling and testing a safety valve as quickly as possible. The originators

of this task had thought that the principles underlying the activity would be an appreciation of the construction and functioning of the valve, and not the manual task itself. This problem indicates that if EA1 learning is to be educational (as opposed to mere training), then it must be an integral part of the course.

Since an engineer is effective through what he does rather than through what he knows or could do, it is important that engineering students acquire not only understanding and practical experience, but also speaking, writing, and calculation skills. The engineering application tasks outlined above have proved to be efficient learning experiences. Through the setting of education tasks it has been possible to assess students in this area. Previously, the development of engineering awareness was a valued but unquantified by-product of a traditional course of study. The students' experimental and design reports now reflect a better understanding of engineering practice (as well as engineering principles), and they are more fully prepared for their industrial placement and final year of study.

The inclusion and integration of EA1 and EA2 material into the Chemical and Bio Process engineering degree course at Bath has met the requirements of the Engineering Council, and re-accreditation of the course has recently been granted. Students graduating with an Honours degree are exempt from educational requirements for Chartered Engineer status and Cor-

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**TABLE 4**  
**Work Permit**

*Time allowed:* 4 hours

Assignment requires:

- Study of Health and Safety Guidance Notes
- Familiarisation with proposed maintenance work
- Familiarisation with use and application of flammable gas detectors
- Production of report proposing work programme

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**TABLE 5**  
**Steam Boiler Operation**

*Time allowed:* 4 hours

Assignment requires:

- Study of Health and Safety Guidance Notes
  - Study of manufacturer's instruction manual
  - Witnessing of boiler start-up
  - Production of report: start-up and shut-down procedures, identification of hazards, and record of key operating parameters
-

porate membership of the Institution of Chemical Engineers.

## CONCLUSIONS

A number of Engineering Applications related experiments have been introduced into the course by modifying existing equipment and by provision of new items at a cost of  $\approx$  £6000. The changes have given the students more hands-on experience in the laboratory and have encouraged an engineering approach to problems. The pumping circuit equipment allows the students to develop their own thinking on the construction and functioning of a simple rig, and it lets them make their own mistakes under carefully controlled and safe conditions.

Overall it has been found that the students are responding to this approach and are more receptive to the laboratory sessions. Their laboratory reports reflect both an increasing awareness of a practical engineering approach and improved communication skills.

## ACKNOWLEDGEMENT

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development of the laboratory programme.

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## ChE book reviews

### CHEMICAL REACTION AND REACTOR ENGINEERING

edited by James J. Carberry and Arvind Varma  
Marcel Dekker, Inc., New York, NY 10016; 1088 pages,  
\$150 (1987)

Reviewed by  
Anthony G. Dixon  
Worcester Polytechnic Institute

This book is made up of fifteen chapters on various topics in reaction engineering, by leading workers in the field. It is similar in concept to the Wilhelm memorial volume of ten years ago (*Chemical Reactor Theory. A Review*, L. Lapidus and N. R. Amundson, eds., Prentice-Hall, 1977), but strikes a much more even balance between theory and application. The editors claim the book to be "hardly a textbook or a handbook," but most chapters have aspects of both functions. Practitioners will find it a useful reference, while teachers will want to assign particular chapters as collateral reading for graduate courses in reactor design and related areas. The production of the book is high quality, with uniform type and illustrations for all chapters, which has had some trade-

offs in terms of the high price and the delay in publishing—the almost complete lack of references after 1983 belies the 1987 publishing date.

General topics are covered first. Villadsen and Michelsen open with a chapter on numerical methods, beginning with a short review of basic techniques. Most of the chapter emphasizes collocation methods, especially newer developments. A section on parameter estimation is most welcome. Shinnar's chapter on residence-time distributions gives a clear exposition of the limitations of the method, marred only by the many typographical errors. The author eschews mathematical complexity in favor of conceptual understanding and common sense.

In their chapter on catalytic surfaces, Delgass and Wolf provide an excellent guide to the alphabet soup of surface analysis and catalyst characterization techniques. They explain what each technique is used for, basic principles, equipment, interpretation of data, and difficulties. Both surface and adsorbed species methods are covered.

Diffusion and reaction in catalyst pellets is covered by Luss in a chapter that provides a comprehensive literature survey. The emphasis is less on physical insight and more on the mathematical development. A good section on effectiveness factors is provided. Doraiswamy and Kulkarni cover gas-solid noncatalytic reactions, beginning with single pellet models and moving to reactor

*Continued on page 153*

# THE COFFEE POT EXPERIMENT

## *A Better Cup of Coffee Via Factorial Design*

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Undergraduates have little exposure to statistical experimental design. For some time we had been searching for a means of introducing senior lab students to the concepts of this important topic. We needed a process with numerous variables on which many experiments could be run within a short time frame, yet which was safe, simple, and satisfied the space constraints of our laboratory setting. It was also important that any new experiment illustrate chemical engineering principles beyond those of our existing unit operations facilities. This article describes an undergraduate experiment that has successfully met the above objectives and yielded several extra benefits—some totally unexpected.

Experimental design involves the use of statistical methods in the planning and analysis of experiments so that valid results with known and generally smaller ranges of uncertainty are obtained in an efficient man-

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**Sandra Harris** received her PhD from the University of California at Santa Barbara in 1978. Since that time she has been a member of the chemical engineering department at Clarkson University. She has been director of the senior unit operations laboratory several times and is active on the Curriculum Committee and on the Laboratory Improvement Committee. Other interests include process dynamics and control.



ner. Adherents of experimental design often emphasize its ability to reduce the number of required experiments, but its greatest value lies in forcing an experimenter to use more forethought in the scheduling of runs and greater rigor in interpretation of their results. The likelihood of an unhappy conclusion to an experimental program, *i.e.*, uninterpretable or meaningless results, is thereby considerably reduced.

Applications for experimental design range from the comparison of two treatments to more esoteric subjects such as model identification and time series analysis. Since the majority of our students have had no formal training in statistics, the goals of our experiment are quite limited. The aim is to expose students to useful references on applied statistics and to require them to carry out simple two-level factorial and fractional factorial designs. These elementary designs illustrate key statistical concepts, are usually the first designs encountered in any sequential strategy of experimentation, and serve as a foundation for various more specialized designs (*e.g.*, surface response designs).

Several texts offer explanations of factorial designs [1-3], and some recent articles [4, 5] extolling the merits of experimental design are listed with our references. A continuing series on experimental design in Chemtech [6] is also recommended, particularly for those familiar with matrices.

### THE EXPERIMENTAL PROGRAM

Our senior laboratory course is organized along the following lines. Students work together in three or four member teams. Each student receives a lab manual containing experiment descriptions and additional references. Experiments are outlined in a manner that encourages creative approaches; cookbook procedures are kept to a minimum. All experiments are performed during two weekly six-hour lab periods. Students turn in a pre-lab report a day before the start of any experiment; prior to the second week of lab,

they make an oral progress report to the faculty member serving as experiment director; and a final report is due a week after completion of the experiment.

The problem posed to the students is excerpted below:

*Consider your lab group as a team of engineers hired by the Peyton Hall Coffee Company to develop a process for making coffee. The prospective customers are a discriminating lot who are unwilling to pay more than \$.20 per cup. The company has invested a considerable sum in a Norelco Dial-A-Brew II coffee maker, so this production unit must be used. Don't break it. Process options that should be considered are*

1. The type of coffee:  
Coffee C1 (\$.2/lb) and Coffee C2 (\$.4/lb)
2. The type of filter:  
Filter F1 (\$.01/sheet) and F2 (\$.02/sheet)
3. The type of water:  
W1, from the water fountain at no cost  
W2, distilled water at \$.01/cup
4. At least two other process changes or variables of your choice.

In their final report students are asked to present a process cost summary, to discuss recommendations for further process development, and to explain any discrepancies in their mass and energy balances.

The apparatus for the experiment consists principally of the drip coffee maker, four pint-size thermos bottles, a household thermometer, a water jug, a dish-washing bucket, and many styrofoam cups. Other instruments the students are expected to use include a spectrophotometer, an ammeter, balances, a magnifying glass, and a microscope.

A week before starting the experiment, students are given the operating instructions for the coffee maker and a copy of a statistics text. We find the book by Box, Hunter, and Hunter to be highly readable, and pages 306-328 plus pages 374-386 are a sufficient reading assignment for our purposes.

During the first lab session, students perform a  $2^3$  factorial experiment. This consists of eight runs (pots of coffee, 3 cups/pot) covering all possible combinations of three variables at two different settings. Encouragement is given to replicate at least one run. With each pot of coffee, students must do overall mass and energy balances, measure several characteristics of the product, and obtain samples for a taste test. Property measurements normally include spectrophotometric percent transmission on a sample diluted with three parts water and a residual weight obtained from a Mettler balance with an infrared dryer attachment. pH measurement is convenient, but usually shows only minor variation with type of coffee. To date, no groups have taken on the challenge of a

**We needed a process with numerous variables on which many experiments could be run within a short time frame, yet which was safe, simple, and satisfied the space constraints of our laboratory setting.**

chromatographic analysis.

Students are forewarned that reliable taste test results are obtained only with difficulty. Taste test procedures are left entirely as their responsibility.

After using the first lab period to refine their experimental procedures and to acquaint themselves with factorial experiments, students have an opportunity to meet with the experiment director before attempting a  $2^{5-1}$  fractional factorial design during the second week of lab. The effects of five different variables are now to be evaluated from the results of sixteen runs. The variables are chosen by the students. Some fairly obvious choices are the "brew control" setting on the coffee maker and the change of coffee grounds. Other parameters that have been investigated include: addition of salt to the coffee grounds, pre-wetting the bed of grounds, comparison of fine versus coarse ground coffee, and use of stainless steel versus glass carafe.

#### SAFETY

Normal precautions for use of any electrical appliance need to be followed. Students are also cautioned that the glass carafe is fragile and cannot withstand significant thermal shock. We have kept a stainless steel carafe on hand as a substitute, but have not had to use it.

The foremost hazard that we guard against is chemical contamination. To that end, the apparatus is stored in a nearby faculty member's office rather than in the lab stockroom, we deal exclusively with black coffee, and the experiment is set up in an area removed from the rest of the lab.

#### THEORY

For a  $2^3$  factorial experiment involving three variables each at two levels or settings (arbitrarily denoted by + and -), the basic model for interpreting any product characteristic,  $Y$ , is Eq. (1).

$$Y_{+++} = \langle Y \rangle + \frac{A + B + C + ab + ac + bc}{2} + \text{error} \quad (1)$$

where  $Y_{+++}$  is the value obtained in the experiment with the first, second and third variables at their + setting;  $\langle Y \rangle$  is the average  $Y$  value for all experi-

ments; A, B, and C represent the "main effects" of the three variables; ab, ac, and bc are the "two factor interaction effects" of the respective variable sets; and the error term is assumed to be an independent and normally distributed random variable.

The main effect, A, is defined as  $\langle Y_{A+} \rangle - \langle Y_{A-} \rangle$ , where  $\langle Y_{A+} \rangle$  is the average result for all experiments with the first variable at a + setting. The interaction effect, ab, is defined as  $\langle Y_{AB+} \rangle - \langle Y_{AB-} \rangle$ , where  $\langle Y_{AB+} \rangle$  is the average for all experiments in which the product of the first two variable settings is positive, *i.e.*

$$\langle Y_{AB+} \rangle = \frac{(Y_{+++} + Y_{++-} + Y_{--+} + Y_{---})}{4} \quad (2)$$

ab is a measure of the non-additivity of the response to changes in the first and second variables.

A much fuller discussion of factorial designs is presented in applied statistics texts [1-3]. Eq. (1) is presented to illustrate that the primary goal is determining which variables give large main effects and which variables may strongly interact. Note the above concepts apply whether a variable is quantitative, such as the mass of coffee grounds, or qualitative, such as the type of coffee.

Luckily, there is a convenient technique, known as Yates Algorithm [2, pp. 323-324], for computing each of the main and interaction effects. All of the terms in Eq. (1) can be easily calculated from a table of Y values. Variables whose main and interaction effects are small can be eliminated from consideration, and process development efforts can focus on those variables giving large effects. Early identification of unanticipated synergism (*i.e.*, large interaction effects) can speed efforts of process optimization, or, even better, serve as a basis for obtaining a patent.

Nonetheless, experimenters must always be cautious in interpretation of their results. If unexplained interaction is encountered, it is wise to redo the analysis using a simple transformation of Y, *e.g.*,  $\ln Y$  or  $1/Y$ . It may be that a model strictly additive in main effects is adequate for the transformed data.

The error term in Eq. (1), what statisticians call the residual, should also be examined to see if it is approximately normally distributed. An unusually large residual may indicate a flawed experiment that needs to be repeated. Also, if residuals vary in relation to the magnitude of Y, there is a need for data transformation of the type mentioned above. In order to do such an analysis in a  $2^3$  design, some experiments must be repeated. If there are only eight experiments, the error has but one degree of freedom and is equal

to  $(\langle abc+ \rangle - \langle abc- \rangle)/2$ , where  $\langle abc+ \rangle$  is the average of all experiments in which the product of the variable settings is positive, *i.e.*

$$\langle abc+ \rangle = \frac{(Y_{+++} + Y_{+--} + Y_{--+} + Y_{---})}{4} \quad (3)$$

## PITFALLS

Students are prone to concentrate on the taste testing and lose sight of their overall objective—development of a process for the Peyton Hall Coffee Co. Also, taste test results are apt to be indecisive for a number of reasons: taste bud fatigue, lack of contrast between samples, or simply too few examiners for such a subjective test. A positive aspect to this is that process decisions can then be made on the basis of economics and more reliable measurements of coffee strength. The taste test still serves as a safeguard against concocting an unpalatable product.

Review of initial student reports disclosed their unfamiliarity with cost analysis, standard errors, and use of microscopes. It is now explicitly mentioned that labor costs must be included in their analyses. Following the oral progress report, a lengthy discourse is made on procedures for estimating standard errors and the advantages of visual comparison.

## DISCUSSION

A motivating factor behind this experiment was the increasing number of our graduates finding employment in the food processing or consumer products industries, where consumer preference testing and statistical analysis of data are commonplace. The experiment drives home the points that many chemical engineers work outside the chemical industry and that you need go no further than your own kitchen to do interesting chemical engineering research.

The taste testing also introduces a social component absent in our other experiments. As expected, offering coffee samples to volunteers led to greater alertness at the end of our six-hour lab period, particularly when students had been up late the night before completing final reports on prior weeks' experiments. An unexpected plus was the willingness of faculty members, who had never before participated in lab, to throw open their office doors and take part in the taste testing.

Computational burdens associated with analysis of factorial experiments are avoided by providing students with a Multiplan software file that calculates all main and interaction effects using Yates Algorithm.

We have not considered espresso or gourmet cof-

fees, and it has been difficult locating common brands that give substantial taste differences. We will be happy to share our knowledge of which brand is unusually distasteful with anyone who writes. A copy of the write-up appearing in our lab notebook is also available.

This experiment, like all good research projects, has numerous facets worthy of additional exploration. Fundamental modeling of the drip making process, scale-up considerations, and effects of aging are all topics of interest. Another possible extension would have students report on the commercial processing of coffee beans [7]. Furthermore, there remains a controversy over whether professors' taste buds differ significantly from those of undergraduates.

In summary, our experience with this experiment has been quite positive. Almost all lab groups are able to sort through many process variables and make a reasonable recommendation to the Peyton Hall Coffee Co. Some students come away with an appreciation of factorial experiments and some do not. They all share the experience of utilizing dollar signs in the evaluation of their results. Operation of the experiment goes well, and, importantly, most students report they have fun.

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## REVIEW: Reactor Engineering

Continued from page 149

models, which somewhat anticipates the next two chapters. This chapter also covers the literature extensively, but the authors give good physical explanations of the models.

The next few chapters deal with some old favorites. The task of covering fixed-bed gas-solid catalytic reactors falls to Froment and Hofmann, who present a range of

models. This chapter is not as comprehensive as the corresponding one in Froment and Bischoff's book (*Chemical Reactor Analysis and Design*, Wiley, 1979). The authors emphasize uncertainties in reaction kinetics and reactor transport parameters, and deal mainly with phenomena actually seen under industrial conditions. In a well-written chapter, Rowe and Yates give a very clear description of the bubbling bed model and bubble behaviour in fluidized beds. They also emphasize the importance of the distributor and freeboard regions in reactor design. Denn and Shinnar cover the area of coal gasification with a strong emphasis on reactor efficiency and energy analysis. Some of their references may be difficult for students to find, and some familiarity with specialized terms is assumed.

In the longest chapter, Carra and Morbidelli give an extensive catalog of correlations, model equations, and solutions for gas-liquid reactors. Some interesting comments on scale-up and reactor power requirements are made at the end.

Shah and Sharma treat trickle bed and slurry reactors under the heading of gas-liquid-solid reactors. Again, many references and results are given. The part on slurry reactors contains many typographical errors, but also provides a useful worked example of slurry reactor design.

Some newer and more specialized reactor types are the subject of the concluding chapters. Tyrell, Galvan, and Laurence provide a short chapter that tries to make clear the focus of polymer reaction engineering, rather than being comprehensive. They concentrate on modeling the product distribution by step-growth and chain-growth mechanisms. There is relatively little on actual reactor design.

Erickson and Stephanopoulos give an introduction to biological reactors that is reasonably accessible for non-specialists. A short introduction to microbial growth concepts and a review of mass transfer ( $O_2$  supply) set the stage for an interesting chapter on reactors. In possibly the first treatment in a reaction engineering book, DeBarnardez, Claria, and Cassano give a necessarily expository view of photochemical reactors. They stress the differences between these and more traditional reactor designs, especially the need for proper models of emission and absorbance of radiation. Several examples of photoreactor design are presented.

Trost, Edwards, and Newman give a very readable survey of electrochemical reactors, with strong emphasis on porous electrode systems, following a general introduction.

There is unfortunately no chapter in this book on deposition reactors, such as are used in the semiconductor industry. Maybe next time!

The final chapter is by Morbidelli, Varma, and Aris, and is somewhat different from the rest of the book in that it is completely theoretical, covering reactor steady-state multiplicity and stability. The two limiting cases of CSTR and plug-flow reactor are analyzed extensively. □

# ANOTHER WAY OF LOOKING AT ENTROPY

## *Entropy and Aging, Evolving Systems*

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I TEACH A DUAL-LEVEL thermodynamics course which reflects my non-traditional interest in the subject, *i.e.*, I am fascinated with the concept of entropy, dissipative systems, stability through fluctuations, stationary states and equilibrium. I apply these ideas to my major preoccupation—aging, evolving systems, longevity analysis, and structural complexity. I examine living systems and so-called inanimate systems such as corporations. I find in the classroom that teaching this “new” thermodynamics engages student interest and enthusiasm to a degree which, amazingly, seems to match my own. I challenge the class to analyze the aging process in humans, in corporations and cities, from an entropic point of view. We examine the structure of organizations, as to which are most entropically efficient. We extend the boundaries of knowledge into regions where there are no apparent right and wrong answers, which means that sometimes I give the entire class an A grade to reflect my pleasure in their accomplishments.

Entropy, of course, is not something tangible, not something capable of being seen or touched. Hence, entropy is a difficult concept to grasp. It is not a solid, it is not hot or cold and does not have a physical consequence, such as temperature. We can say that entropy is a measure of the disorder of a system and show that more disorder means higher entropy content [3]. Real processes tend to go in the direction of increasing entropy. Aging can be envisioned as an ir-

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**Entropy . . . is not something tangible, not something capable of being seen or touched. Hence, entropy is a difficult concept to grasp . . . We can say that entropy is a measure of the disorder of a system and show that more disorder means higher entropy content.**

reversible process of entropy accumulation. Getting older means having less control of body functions, being more disordered. Death is the ultimate disorder, a state of maximum entropy. This point has been speculated upon by many scientists, including Jones [18] and Von Bertalanffy [35].

The second law of thermodynamics essentially says that systems will run down of their own volition if left to themselves. In other words, the entropy content tends towards a maximum. Thus, increasing entropy could be an indication of the direction in which the system is inclined to go. Unless there is outside intervention, the second law of thermodynamics codifies the one-sidedness of time, or time's arrow. We can only move forward; that is, time is irreversible.

Everything we know is tending towards chaos (unless there is outside intervention), towards an equilibrium with the environment. To quote Von Bertalanffy [35]:

**The significance of the second law can be expressed in another way. It states that the general trend of events is directed toward states of maximum disorder, the higher forms of energy such as mechanical, chemical, and light energy being irreversibly degraded to heat, and heat gradients continually disappearing. Therefore, the universe approaches entropy death when all energy is converted into heat of low temperature, and the world process comes to an end.**

### AGING, EVOLVING LIVING SYSTEMS

It was not until the 1950s that entropy started to seriously emerge in discussions of living phenomena. Complicated biological processes such as cell differen-

tiation, growth, aging, *etc.*, were now analyzed from the second law of thermodynamics and entropy calculations made [6, 36]. Bailey [1] wrote: "Entropy is a very viable concept for the biological and social sciences. It applies to both open and closed systems. It can be discussed in terms of organization or order." Jones [18] said: "One common feature of biological processes is their unidirectionality in time, that is, they are not reversible, except under special circumstances. Since entropy is the only physical variable in nature which generally seems to parallel the direction and irreversibility of time, these should be fertile areas for the effective use of entropic models."

Much of the historical development of entropy has dealt with isolated or closed systems. A closed system is one which can exchange energy but not matter with the surrounding environment. The second law of thermodynamics states that a closed system must evolve to a state in equilibrium with its environment—a condition of maximum entropy. Open systems are those which can exchange both matter and energy with the surroundings. Obviously we, the living, are examples of open systems. Open systems must maintain the exchange of energy and matter in order to sustain themselves, or slow the approach to the final state, death.

We can say that entropy accumulation within the living system is composed of two parts, one being the internal entropy production based on the myriad of irreversible chemical reactions which constitute the chemistry of life. Secondly, there is the entropy flow through our boundaries, such as in the food consumed, air inhaled and exhaled, biological waste products, heat from the skin, *etc.* The internal entropy production derived from our chemical reactions always proceeds in the direction of increasing our entropy content, since the chemistry of life is inherently irreversible. However, the food in, air in and out, waste products out, and heat out may in total contribute positive or negative entropy flows through our boundaries, which then affect the rate of accumulation of entropy in our living body.

Zotin [37] proposed that we evolve towards a final state, death, by a series of changes, each change called a stationary state. We settle into a stationary state and stay for a while until pushed to the next, and the next. This is clearly seen in the transformation of butterfly larvae and pupae, dramatic physical changes. Balmer [2] applied entropy concepts to the study of an aging annual fish. This species displays all the characteristics of birth, growth, aging, and senile death, over a short twelve-month period. Balmer identified entropy flows into and out of the fish, such as food, excrement and body heat dissipation.

### Aging as an Entropy Driven Process

We can consider the aging process as a series of steps, proceeding from one stationary state to the next and the next. We can talk of an entropy driving force, causing the evolution from one stationary state to the next. Each time we achieve a stationary state, we "rest" for a "moment" and then go on to the next. In each stationary state we hunker down, collect ourselves, minimize our entropy production, smooth out our chemistry, and await the next push. And so we age. Thus the stationary state can be characterized as an entropy (disorder) producing state, where this entropy production is drawn down to a minimum before going on to the next stationary state where a new minimum is established. The theorem of minimum entropy production is a fundamental concept of the stationary state, first developed by Prigogine and Wiame

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**I challenge the class to analyze the aging process in humans, in corporations and cities, from an entropic point of view . . . We extend the boundaries of knowledge into regions where there are no apparent right and wrong answers . . .**

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[30]. Death is the final state to which we are drawn, where there no longer exists a tension for life; the driving forces have been reduced to nothing or some minimum level, below which life cannot be supported.

### Excess Entropy (EE) and Excess Entropy Production (EEP) Driving Forces for Aging

Having introduced the idea of longevity as an entropy driven process involving an evolution through innumerable stationary states, we can now explore the nature of the entropy driving force for life. If death represents the ultimate disorder (and our maximum entropy content) then we can characterize our longevity potential and vitality by the distance we are from the "black hole" of death. We can calculate a difference in entropy content, from the present (where we are) to where we're heading (towards death). This difference is called Excess Entropy (EE) and may be a driving force for life. By tracking EE versus age, we can see our life unfolding, or winding down, as EE approaches zero, the end of the journey. Not only is EE an important parameter in tracing our lifespan, but so too is the rate of change of EE. In other words, how quickly EE is diminishing with age is another key marker. We call this second parameter Excess Entropy Production (EEP).

EEP is the rate of change of EE with time. From Prigogine's theory of minimum entropy production in

the stationary state, we can surmise that EEP should not only become a minimum in the vicinity of death (a stationary state) but EEP should indeed become zero since that final stationary state is also the final equilibrium state where all thermodynamic forces and flows become zero. Thus we can trace life's course by EE and EEP tracks [11].

Our life's course is considered stable, so long as the positive-valued EEP is descending to zero and the negative-valued EE is ascending to zero. From the stability theory developed by Liapunov [19], we can say that if both EE and EEP are positive, the living system becomes unstable. Thus we have another criterion for death: that is, when the EE line passes into the positive-valued domain (it crosses the zero axis). In other words, instability in the life process prevents us from exercising the control required to maintain a proper tension of life. And so we die.

Internal entropy production for a chemical reaction system is given by Prigogine and Wiame [30]

$$\frac{dS}{dt} = \frac{Ar}{T} \quad (1)$$

where

- S = internal entropy content
- A = chemical affinity, a chemical driving force
- r = reaction velocity, a chemical flow
- T = temperature
- t = time

Eq. (1) can be more generally written as

$$\sigma(S) = \frac{dS}{dt} = \sum_{j=1}^n J_j X_j \quad (2)$$

where

- $\sigma(S)$  = internal entropy production at any time, t
- $J_j$  = a thermodynamic flow, for component, j
- $X_j$  = a thermodynamic driving force, for component, j

For a reference state, from Eq. (2), we can write

$$\sigma^0(S) = \sum_{j=1}^n J_j^0 X_j^0 \quad (3)$$

and

$$\sigma(S) = \sigma^0(S) + \delta\sigma(S) \quad (4)$$

where

- $\delta\sigma(S)$  = a small deviation of internal entropy production from the reference state. Prigogine has shown [28] that  $\sigma^0(S)$  in Eq. (3) is a minimum in the reference state (the equilibrium or stationary state).

From Eq. (2), Lee [19] showed

$$\frac{d(\delta^2 S)}{dt} = 2 \sum_{j=1}^n \delta J_j \delta X_j \quad (5)$$

and

$$S - S^0 = \frac{1}{2} \delta^2 S = \text{Excess Entropy} = \text{EE} \quad (6)$$

where

- $\delta J_j$  =  $J_j - J_j^0$ , the deviation of the flow from the reference state
- $\delta X_j$  =  $X_j - X_j^0$ , the deviation of the force from the reference state
- $S^0$  = entropy of the system, in the reference state
- $\delta^2 S$  = second entropy deviation from the reference state

It is this difference between the entropy content, S, at any time and that of the reference state,  $S^0$ , which is defined as Excess Entropy, *i.e.*,  $\text{EE} = S - S^0$ , a thermodynamic driving force for the life process. If the reference state is an equilibrium or final stationary state,  $S^0$  is a maximum. Thus EE is always negative and approaches zero in the negative domain as the system ages and evolves towards the final reference state.

From Eqs. (5) and (6), Excess Entropy Production (EEP) can be written [12] as

$$\text{EEP} = \frac{d\text{EE}}{dt} = \frac{d\left(\frac{1}{2}\delta^2 S\right)}{dt} = \sum_{j=1}^n \delta J_j \delta X_j \quad (7)$$

Lee [19] demonstrated that EEP approaches a minimum, or zero, as the system approaches the final stationary state or equilibrium. EEP describes the rate of approach of EE to the final state.

For a chemically reacting system



and with the definitions

- A = chemical affinity  $\cong \log[Z Y / C D]$
- = chemical force, X

and

- r = chemical reaction velocity  $\cong Z Y$
- = chemical flow, J

we can obtain Eq. (9), using Eq. (7) and assuming Y, C, D are constants [19]

$$\text{EEP} \cong \frac{(\delta Z)^2}{Z} \quad (9)$$

Although the influences of free radicals, vitamins, minerals, and other nutrients are essential in establishing longevity, nevertheless in a living system the chemistry of life is basically the metabolism of carbohydrates, fats, and protein. In general, in a homogeneous population the proportions of these food components in the diet tend to remain approximately

fixed. Thus, it is useful to focus on only one of these, protein, for example. Eq. (8) now becomes: protein + oxygen → carbon dioxide + water + urea + energy, and Eq. (9) is as follows:

$$EEP \equiv \frac{(\delta[\text{Protein}])^2}{[\text{Protein}]} \quad (10)$$

where

[Protein] = Daily Protein Consumption  
 $\delta[\text{Protein}]$  = Daily Protein Consumption minus the Minimum Protein Required (in the reference, equilibrium or final stationary state of maximum disorder)

### Life and Death

Aging may be the evolution towards a more probable state, the equilibrium state. As the body ages (returns to equilibrium) the EE driving force weakens or diminishes. Schrodinger [32] wrote, "Living systems survive by avoiding the rapid decay into the inert state of equilibrium." Jones [18] proposed, "The approach to equilibrium is a sign of death. Death may also be thought of as the attaining of a critical, maximum state of entropy during our journey towards equilibrium." Schrodinger further stated, "Thus a living organism continually increases its entropy . . . and tends to approach the dangerous state of maximum entropy, which is death."

Death can be when a critical amount of randomness is attained, when a certain amount of disorganization is suffered. Thus aging is a randomizing process, a disorganizing process. In terms of stability theory, equilibrium is the point or region of attraction; we are drawn relentlessly towards equilibrium. Life may be considered analogous to the spring-wound watch, where the timepiece may stop by one of two possible mechanisms. It can simply wind down (approach equilibrium), or the internal mechanism can somehow fail and the watch "dies" prematurely. Thus we can describe equilibrium deaths and instability or a catastrophic deaths.

Life may be considered a temporary upset from or perturbation of equilibrium. Equilibrium is absolutely stable, a universal attractor. Equilibrium always wins. Aging is a spontaneous process, where the body dissipates its EE. The various theories of aging (cross-linking, wear and tear, free radical, *etc.*) all imply a declining metabolic rate with age, and by extension, a diminishing EE and EEP. Evolution may be the natural process of prolonging the time that an organism spends in the far-from-equilibrium state. Genetics still plays its role in determining longevity potential, but is not in conflict with the ideas presented here. The tendency to return to equilibrium

**We can consider the aging process as a series of steps . . . In each stationary state we hunker down, collect ourselves, minimize our entropy production, smooth out our chemistry, and await the next push. And so we age.**

will always apply. Death will always have a probability of absolute certainty.

### AGING, EVOLVING, INANIMATE, CORPORATE-STYLE SYSTEMS

The concept of entropy has been widely discussed in many scientific and social arenas [4, 7, 14, 15, 20, 27, 33] and its application to organizational structure is a logical extension of the work done previously by Prigogine [24, 28], Georgescu-Roegen [5], Shannon [33], Quastler [31], Horowitz [15, 16, 17] and others [14, 24, 25].

One of the most famous uses of the entropic concepts in chemistry was by Ilya Prigogine [28, 29], recipient of the 1977 Nobel Prize in chemistry. He correlated non-equilibrium phenomena and disorder (entropy). He studied systems near equilibrium and systems with minimum entropy production. However, beyond a certain critical distance from equilibrium, entirely new structures could emerge. These new systems, far from equilibrium, Prigogine referred to as dissipative structures. In addition to his work in chemical thermodynamics, Prigogine has also been an innovator in the field of social thermodynamics [24]. He has adapted many of the principles of thermodynamics to social organizations, recognizing that each organization is itself an open system. Another contributor to the interdisciplinary analysis of open systems was economist and thermodynamicist, Nicholas Georgescu-Roegen [5] who believed that the notion of entropy had great utility in economics, that the earth is an open system with irreversible processes occurring within it.

### Emerging States Driven by Nonequilibrium Conditions

The behavior of nations and other human organizations illustrates the recondite dynamics of the nonequilibrium open system [14]. States, living cells, economic processes, ecological systems, and even transportation networks demonstrate the bridges between the physical and social sciences [9]. Prigogine studied self-organization under conditions of fluctuations and change, an evolutionary process in systems pushed far from equilibrium. Whether the fluctuations impinge on a household or a nation, the belief is that

they can be explained. He examined oscillating phenomena and sought a basis for predicting order from the perspective of entropy production (regarded by some as the reification of the arrow of time since entropy production describes in general the direction spontaneous processes must go). Use of the term, entropy, is derived from the Greek, meaning evolution [7]. Systems near equilibrium can be buffeted by small perturbations in energy and mass pressures, but no new organizations, no new structures, are formed. Imposing stronger gradients from the outside world could force the appearance of new, dissipative, nonequilibrium stationary states. Examples cited by Prigogine are a town and the living cell. Georgescu-Roegen wants economics, which ignores entropy, to begin to mark the existence and applicability of nonequilibrium dynamics and irreversibility. Economists, he says, have a blind faith in reversibility (we can restore original conditions by invoking the same laws, backwards and forwards, and ignoring time). Georgescu-Roegen states that matter is subjected to entropy degradation, from higher order to lesser, and hence becomes less useful. What he is stressing is an evolutionary philosophy. If driven hard enough we see new structures developing, nurtured by energy and matter fluxes [24]. Entropy, applied to the economic process, adds important new perceptions to the interactions of humans, technology, the market system, and limited resources—ideas spawned by Georgescu-Roegen. He proposed we think in terms of irreversibilities, limits on resource availability, and a more parsimonious society. Most current economic policy tinkers with prices, taxes, or the market in some way. Until now, we have stressed economic balances of energy and matter—what comes in must equal what goes out—rather than an understanding that something is lost in every transaction (in entropy terms). The real world dictates the transformation in one direction only: low entropy to high entropy. The consumer takes in high-grade, ordered energy and matter and exhausts low-grade, disordered wastes. The wastes must not injure or render inoperative the feedback and control mechanisms which affect the stability of the open, temporary state. Consumers may be individuals, cities, governments, corporations, or civilizations [10, 12, 13, 26].

#### Informational Entropy: Shannon's Approach

The mathematical definition of informational entropy was derived by C. E. Shannon [33] in 1949. With molecules in motion, colliding and rebounding, different molecules will occupy a given space at various times and hence many molecular arrangements, called

microstates, are possible. We associate the concepts of greater freedom, uncertainty, and more configurational variety with an increased number of microstates and higher entropy. If one had to guess where a particular molecule would be at a given time, the probability of error would be greater in the higher entropy state. Thus ordering of a system implies a lower entropy, which carries with it a certain reliability and smaller probability of error.

From the preceding discussion we know that as the number of microstates,  $W$ , increases, the state entropy,  $H$ , increases. Hence we can write [4],

$$H = K \log_a W \quad (11)$$

where  $a$  is the logarithmic base.

If we assume that all the microstates are equiprobable, then the probability of achieving each individual microstate,  $p_i$ , is simply one out of the total number of the microstates,  $W$ , or

$$p_i = \frac{1}{W} \quad (12)$$

or

$$H = -K \log_a (p_i) \quad (13)$$

We can extend this idea to non-equiprobable systems with the use of the Expectation Value,  $E_x$  [22], which is by definition the probability of each outcome,  $p_i$ , multiplied by the value of that individual outcome,  $X_i$ , summed over all possible outcomes, as indicated in Eq. (14)

$$E_x = \sum_i p_i \cdot X_i \quad (14)$$

With the probability,  $p_i$ , and the associated  $H$  value,  $-K \log_a p_i$ , from Eq. (13),  $E_x$  (also called  $S$ , the entropy of the system) is

$$S = -K \sum_i p_i \cdot \log_a p_i \quad (15)$$

Thus, Eq. (15) expresses the entropy of a system in terms of probabilities. It takes the concept of entropy from the thermodynamic setting to the domain of general probability theory. It can be shown that  $S$  in Eq. (15) achieves a maximum value if and only if all the  $p_i$ 's are equal [26]. If for convenience the constant  $K$  is taken to be unity, then Eq. (15) reduces to

$$S = - \sum_i p_i \log_a p_i \quad (16)$$

This is Shannon's formula for informational entropy.

#### The Meaning of Stored Information

As Weaver [33] states, ". . . the word 'information' in communication theory relates not so much to what

you say, as to what you can say." Potential message variety, freedom of choice, and a large vocabulary are the desired ends of communication and information transmission. A library obviously contains stored information. The information is stored in a linear sequence of symbols organized to the constraints of a language. The sequences are organized into books and periodicals, and these are carefully ordered on shelves. Everywhere order and constraints are associated with the information storage process. This is a state of low entropy. If we take each page of each book, cut it into single-letter pieces and mix them in one jumbled heap, the entropy would increase and stored information would decrease. In entropy terms, stored information is the divergence from the state of maximum disorder (when all  $p_i$  terms are equal). In other words, stored information is the difference between entropy content for the equally probable state,  $S^{\max}$  (maximum disorder) and that for the unequally probable present,  $S$ , and is denoted by  $D$ . Therefore, stored information is

$$D = S^{\max} - S \quad (17)$$

### Entropy and Corporate Structure

Shannon's informational entropy formula [33] has in the past found application by Gatlin [4], who computed genetic stored information, by Horowitz and Horowitz [15, 16] and Herniter [8] in marketing, by Lev [21] in accounting, by Thiel [34] and Georgescu-Roegen [5] in economics, by Philipatos and Wilson [27] in securities analysis, and by Murphy and Hasenjaeger [23] in organizational decentralization.

These authors extended the definition of  $p_i$  from the probability that a system will be in a particular microstate to such related considerations as: (1) the probability that a customer will purchase a product; (2) the degree of competition in the marketplace; (3) a measure of the dispersion in a securities portfolio; (4) the degree of market share; (5) the degree of organizational decentralization; and (6) the bits of stored genetic information.

One can generate a Power Index [10, 12, 26] to be used in Shannon's formula, analogous to  $p_i$ , in order to characterize the overall structure of a corporation. Since each unit controls those beneath it, one can also define a Cumulative Power Index for each unit,  $C_i$ , where

$$C_i = P_i + \text{sum of all } P_i \text{ controlled by this unit, } i$$

Finally, a Fractional Cumulative Power Index,  $f_i$ , is introduced as the unit's  $C_i$  divided by the sum of all  $C_i$  in the organization. Thus Eq. (16) is transformed to

$$S = - \sum_i f_i \log_2 f_i \quad (18)$$

We can define an entropic distance from disaster,  $D$ , for the actual structure, by Eq. (19):

$$D = S^{\max} - S \quad (19)$$

and the distance from disaster for an ideal structure,  $D^0$ , as

$$D^0 = S^{\max} - S^0 \quad (20)$$

and a structural efficiency,  $\eta$ , by Eq. (21):

$$\eta = \frac{S^{\max} - S}{S^{\max} - S^0} \times 100 \quad (21)$$

The distance from disaster,  $D$ , is also stored information, Eq. (17), as well as EE for the inanimate system, the corporate-style organization,

$$EE = S - S^{\max} \quad (22)$$

where  $S^{\max}$  = maximum entropy content for the organization, if all the units have the same budget, are at the same level, and are completely independent. A prescription for disaster. ( $S^{\max} = \log_2 n$  and  $f^{\text{disaster}} = 1/n$ , where  $n$  is the number of units in the organization [10].)

From Eqs. (7), (18) and (22) and recognizing that EEP is expressed as the product of thermodynamic forces and flows, we can write [12]

$$EEP = \delta S EE \quad (23)$$

where

$$\begin{aligned} J &= \text{flow} = S \\ X &= \text{Force} = EE \end{aligned}$$

and where previously, for the living system, flow =  $r$  and force =  $A$ . It can be shown [12, 26] that

$$EE = S - S^{\max} = S - \log_2 n \quad (24)$$

and

$$EEP = \left[ \sum_{i=1}^n \left( f_i - \frac{1}{n} \right) \log_2 f_i \right]^2 \quad (25)$$

For each year of a corporation's history,  $f_i$  can be computed for each unit and the summing process of Eq. (18) accomplished to produce  $S$  and then efficiency,  $\eta$ , from Eq. (21). The EE is obtained from Eq. (24) and EEP from Eq. (25). Thus EE and EEP longevity tracks can be constructed, just as they can

be (and have been) for the living system.

## CONCLUSION

In the classroom I offer undergraduate and graduate students the opportunity to explore another meaning of entropy, applied to: open systems; dissipative systems; stationary states exhibiting minimum entropy production; stability through fluctuations; entropy driving forces; excess entropy and excess entropy production concepts; the entropy nature of living systems; the entropic evolution of inanimate systems such as corporations; the meaning of life as an entropy-driven process; the finality of death from an equilibrium viewpoint; change processes which can affect entropy content of systems; aging, evolving systems and increasing disorder and entropy.

This leads our discussions into diverse fields such as gerontology and geriatrics, systems research, corporate planning, history, economics and process control. We become interdisciplinary for one quarter at least. Or longer.

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**INTRODUCTION TO MATERIAL AND ENERGY BALANCES**

by G. V. Reklaitis

John Wiley &amp; Sons, New York, NY (1983)

**Reviewed by****Gerald B. Westermann-Clark**

University of Florida

Several textbooks are available for an introductory course on chemical engineering calculations. Such texts share similar goals, including bridging from pre-engineering courses to the chemical engineering curriculum, illustrating the broad applicability of chemical engineering concepts, even outside chemical plants, and developing skills used later in the curriculum. If achieved, these goals can show students who still may be unsure about continuing in chemical engineering how chemical engineering is related to, but different from, other areas.

Despite the similarity of goals, one of two different approaches usually emerges in introductory texts: 1) a survey of chemical engineering calculations, including not only steady state material and energy balances, but also a sampling of other topics, such as unsteady state mixing in stirred tanks and plug-flow reactors; and 2) a development of strategies for material and energy balance calculations—an approach that usually adopts a notational system that is easily adapted to more complex, multi-unit processes than are usually seen in approach number one.

The first approach typically draws more heavily on dynamics concepts, while the second gives students a deeper perspective on process synthesis and design. Either approach can illustrate the diversity of problems amenable to chemical engineering analyses, and in fact, most introductory courses are a mixture of the two perspectives mentioned. As examples of these approaches, *Introduction to Chemical Engineering Analysis* (T. W. F. Russell and M. M. Denn, Wiley, 1972) may be cited as an example of the first, *Process Synthesis* (D. F. Rudd, G. J. Powers, and J. Sirola, Prentice-Hall, 1973) as an example of the second, and *Elementary Principles of Chemical Processes* (R. M. Felder and R. W. Rousseau, Wiley, 1986) as an example of a mixed approach.

The present textbook is divided about equally between material and energy balances, with each type of balance treated in nearly parallel fashion. After presenting the appropriate balance equations, each half of the text contains chapters on balances for nonreacting and reacting systems. Each half also contains a chapter on the use of balances in process flowsheets, with sections on strategies for manual and machine computations. The discussion of material balances also contains a beneficial

chapter on the relation between elemental and species balances, and the final chapter shows how material and energy balances can be solved simultaneously by means of a discussion of computational strategies. Overall, topics are very logically presented, and the parallel presentation of topics assists assimilation of the more difficult energy balances.

Although instructors will appreciate the degrees-of-freedom analyses, it is unusual for students (who generally try to solve a problem without first ascertaining whether it has a solution) to fully appreciate their value. However, the chapters on strategies for manual and machine calculations, which discuss linearizing nonlinear problems and simultaneous methods for solving systems of linear and nonlinear equations, show students that they can tackle relatively large problems with techniques from numerical methods courses. The discussion also apprises students of the limitations of the methods presented.

In each section consistent notation is developed, with  $N_j$  (or  $F_j$ ) denoting the molar (mass) flowrate of species  $j$  throughout, for example, and with summation signs frequently used to obtain more compact equations. The very useful open system analysis, consistent with that in *Chemical and Engineering Thermodynamics* (S. I. Sandler, Wiley, 1988), is developed for energy balances.

Numerous examples serve as excellent aids to discussions of concepts. The homework problems amply illustrate ideas advanced in each chapter. For use in problems and examples, the appendix contains a relatively large compilation of physical properties, including heat capacities, heats of formation, Antoine constants, and steam tables. Most obvious by their omission are unsteady state problems. Furthermore, the problems tend not to give students a representative cross-section of the range of problems that they can solve; rather, the emphasis is on problems encountered in chemical plants.

The content of this textbook places it between the books mentioned previously by Rudd *et al.* and by Felder and Rousseau. This text would fit very well into a curriculum in which numerical techniques are presented prior to or even concurrently with the material presented. The use of the open system energy balance, the most useful form of this balance for process calculations, makes this text consistent with what students are likely to need later. Although the author, an eminent process design engineer, has put forward a text that leans toward process design, this is a very readable, substantial contribution that, with minor adaptations to the needs of particular curricula, would be welcomed enthusiastically by students in introductory courses. □

***EDITORIAL NOTE:***

**The following detachable pages describe some industrial employment opportunities for graduating chemical engineers. Please post the information in a conspicuous place for the benefit of your students, or distribute the pages to students who may be interested. These companies have expressed a definite interest in hiring chemical engineers in the areas described, and we strongly encourage students seeking employment to respond as indicated.**

***Ray W. Fahien***

**Editor**

***Chemical Engineering Education***

# CH2M HILL

P.O. Box 22508  
Denver, CO 80222-0508

## ● GENERAL INFORMATION ●

CH2M HILL was founded in Corvallis, Oregon, in 1946 by three students and a professor from Oregon State University. It was originally called CH2M, as an acronym of the founders' last names: Cornell, Howland, Hayes, and Merryfield. In 1971, the firm merged with Clair A. Hill & Associates and became CH2M HILL.

The company provides comprehensive consulting, planning, and design services in water and wastewater management, water resource and agricultural development, transportation systems, hazardous- and toxic-waste management, and energy systems. A staff of 3,600 employees in more than 57 offices throughout the United States, Canada, and abroad provides full support and complementary services in economics, environmental sciences, construction/program management, mining infrastructure planning, and general planning, surveying, photogrammetry, and mapping. CH2M HILL is one of the 10 largest consulting engineering firms in the United States.

### CITIZENSHIP REQUIREMENTS

U.S. Citizenship or Permanent Resident Visa

### HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW

Write: Manager of Recruiting  
CH2M HILL  
P.O. Box 22508  
Denver, CO 80222-0508

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

Positions require a traditional BS in CE, ChE, or ME and a MS in Sanitary/Environmental Engineering. Experience is essential and varies from two to ten-plus years. Submit your credentials for evaluation. FE or PE required.

## ● POSITIONS ●

- Industrial Process Engineer •
- Industrial Water/Wastewater Engineer •
- Hazardous Waste Engineer •

## ● ADDITIONAL INFORMATION ●

CH2M HILL is an employee-owned firm which offers flexible benefits and a salary commensurate with experience.

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# MERCK & CO. INC.

P.O. Box 2000  
RAHWAY, NJ 07065

## ● GENERAL INFORMATION ●

Merck & Co. is a worldwide, research intensive health products company that discovers, develops, produces, and markets human and animal health products and specialty chemicals. The company has 32,000 employees and had sales of over \$5 billion in 1988.

**CITIZENSHIP REQUIREMENTS:** U.S. citizen or permanent visa

**REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED:** We recruit on campus nationwide (U.S.)

**HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW:** Please submit resume or application which clearly states educational background, objectives, and work experience to:

**Theresa Marinelli, Manager College Relations**  
Merck & Co., Inc  
P.O. Box 2000  
Rahway, NJ 07065

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

	<u>Functional Area</u>	<u>Degree Level</u>	<u>Major Hiring Locations</u>
	Corporate Division	BS	Rahway, NJ; Woodbridge, NJ
	Merck Sharpe & Dohme Research Labs	BS/MS	Rahway, NJ; West Point, PA
	Merck Chemical Manufacturing Division	BS/MS	Rahway, NJ; Danville, Pa; Elkton, VA
	Merck Chemical Manufacturing Division	MS	Rahway, NJ; Danville, PA
	KELCO Division	BS/MS	San Diego, CA
	Calgon Water Management Division	BS/MS	Pittsburgh, PA

### PhD

<u>Fields of Special Interest</u>	<u>Tech Center Locations</u>
<ul style="list-style-type: none"><li>• Process changes which address the environmental aspects of plant operations</li></ul>	Merck Chemical Manufacturing Division Rahway, NJ; Danville, PA
<ul style="list-style-type: none"><li>• Process development—from conception through to scale-up and eventual plant start up</li></ul>	Merck Sharpe & Dohme Research Labs Rahway, NJ; West Point, PA
<ul style="list-style-type: none"><li>• Chemical modification and analysis of natural polymers</li></ul>	KELCO San Diego, CA

## ● ADDITIONAL INFORMATION ●

*Merck hires chemical engineers in several divisions to play a critical role in the implementation of our business.*  
*In each division we have highly skilled chemical engineers and we will continue to hire highly qualified applicants in the chemical engineering field.*



# MILLIKEN & COMPANY

College Relations Department, M-260E  
P.O. Box 1926  
Spartanburg, SC 29304

## ● GENERAL INFORMATION ●

Milliken is a major manufacturer of textile products for apparel, commercial, home and industrial markets. Milliken Chemicals operates two modern Specialty Chemicals plants in South Carolina. The company was founded in 1865 and now has 50 plants and 15,000 associates in the US (16,000 worldwide). The Milliken environment is characterized by challenge, accomplishments, innovation, advanced technology, promotion from within based on individual performance, and extensive education and training opportunities. The chemical engineering jobs are in South Carolina and Georgia.

**CITIZENSHIP REQUIREMENTS:** U.S. citizenship or Permanent Resident Visa

**REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED:** Southeastern United States

**HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW:** Send cover letter with functional area interests and geographic preference statement, resume, and a copy of your transcript to the above address.

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

**Process Engineering:** Provides technical support in textile dyeing and finishing operations and in Specialty Chemicals production. Responsibilities include manufacturing compliance with customer product quality specifications and process efficiency/improvement project assignments.

**Manufacturing Management:** Responsible for the production resources of people and machinery. The first line production manager may be promoted to either Advanced Production Manager or Process Engineer in the dual career ladder.

**Research:** Develops new products and associated machinery or processes. Prefer PhD, but will consider MS.

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# ASHLAND PETROLEUM COMPANY

P.O. Box 391  
ASHLAND, KY 41114

## ● GENERAL INFORMATION ●

Ashland Petroleum Company is the largest operating division of Ashland Oil, Inc., a Fortune 60 company with 37,600 employees and \$8.2 billion in annual sales. Recognized as the nation's largest independent refiner and leading supplier of petroleum products, the company also manufactures and markets fuel oils, lubricants, asphalt, jet fuels, and many other specialty products for both industrial and governmental customers.

**CITIZENSHIP REQUIREMENTS:** U.S. Citizen or authorized to work in the U.S.

**REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED:** Midwest, Southeast

**HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW:** Contact: Marc E. Washington, Manager of Professional Employment, at the above address.

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

<u>Functional Area</u>	<u>Degree Level</u>	<u>Major Hiring Locations</u>
• <i>Process</i>	BS	Catlettsburg, KY
• <i>Technical Services</i>	BS	Catlettsburg, KY
• <i>Control Systems</i>	BS	Catlettsburg, KY
• <i>Research</i>	BS	Catlettsburg, KY

### PhD

<u>Fields of Special Interest</u>	<u>Tech Center Locations</u>
• <i>Catalysis</i>	Catlettsburg, KY
• <i>Reaction Kinetics</i>	Catlettsburg, KY



# E. I. DU PONT DE NEMOURS & CO, INC.

Employee Relations Department  
1007 Market Street, N-13451  
Wilmington, DE 19898

## ● GENERAL INFORMATION ●

Established in 1802, Du Pont today is a diversified international company, strongly backed by scientific and engineering capabilities, with business operations in more than 48 countries, with approximately 140,000 employees worldwide, and with sales exceeding \$30 billion.

**CITIZENSHIP REQUIREMENTS:** U. S. Citizenship or permanent resident

**REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED:** Continental U.S.

**HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW:** Send resume and cover letter to:

Professional Staffing Section  
Employee Relations Department  
E. I. Du Pont de Nemours & Co., Inc.  
Wilmington, DE 19898

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### > BS/MS

	<u>Functional Area</u>	<u>Degree Level</u>	<u>Major Hiring Locations</u>
	Process/Project	BS/MS	Continental United States
	Design/Manufacturing	BS/MS	Continental United States
	Construction/Distribution	BS/MS	Continental United States
	Technical Sales and Service	BS/MS	Continental United States
	Research and Development	BS/MS	Continental United States
	(Other)	BS/MS	Continental United States

### > PhD

	<u>Fields of Special Interest</u>	<u>Tech Center Locations</u>
	Process, Project, Research and Development	Mid-Atlantic Region

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# OLIN CORPORATION

120 Long Ridge Road  
Stamford, CT 06904

## ● GENERAL INFORMATION ●

Olin Corporation is a diversified company with core business in chemicals, metals, and ammunition. A Fortune 200 company headquartered in Stamford, Connecticut, Olin employs 16,000 people worldwide and has annual sales exceeding \$2 billion.

### CITIZENSHIP REQUIREMENTS

U.S citizenship or permanent resident visa is required for employment

### REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED

Nationwide—undergraduate and PhD

### HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW

Resume and cover letter to  
Ms. Leah Lethbridge  
Regional Supervisor, College Relations  
Olin Corporation  
120 Long Ridge Road  
Stamford, CT 06904

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

<u>Functional Area</u>	<u>Degree Level</u>	<u>Major Hiring Locations</u>
• Sales	BS	Stamford, CT
• Business Evaluation	BS/MBA	Stamford, CT
• Development, Process, Maintenance, Production, Project	BS	Lake Charles, LA; Charles- ton, TN; Doe Run, KY; McIntosh, AL

### PhD

<u>Fields of Special Interest</u>	<u>Tech Center Locations</u>
• Research and Development and Process/Production	New Haven, CT; Charleston, TN; Lake Charles, LA; Joliet, IL; Rochester, NY; Doe Run, KY; Cheshire, CT



# UNION CARBIDE CORPORATION

CHEMICALS & PLASTICS GROUP

Section D3226

39 Old Ridgebury Road

Danbury, CT 06817

## ● GENERAL INFORMATION ●

Fortune 50 Company, recognized globally for leadership in its three business groups: Chemicals & Plastics; Industrial Gases; and Carbon Products. Founded in 1917, Carbide employs 44,000 worldwide, with 24,000 in USA. Annual sales for Chemicals & Plastics Group exceeded \$5.5 billion in 1988. Key C&P products include polyethylene, latex and specialty polymeric resins; ethylene oxide/glycol and derivatives; urethane intermediates; silicones; alcohols and organic solvents; and polycrystalline silicon.

**CITIZENSHIP REQUIREMENTS:** U.S. citizenship or Permanent Resident Visa (for BS/MS)

**REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED:** Gulf coast, northeast, midwest, southeast, southwest, and Rocky Mountain

**HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW:** Send resume and photocopy of transcript(s) to above address "Attention: Chemical Engineering Employment Coordinator." Be sure to include a cover letter specifying your functional and location preference(s). (*See below*)

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

<u>Functional Area</u>	<u>Degree Level</u>	<u>Major Hiring Locations</u>
Design (Process; Control Systems)	BS,MS	Charleston, WV; Tarrytown, NY
Environmental/Safety Engineering	MS	Charleston, WV
Manufacturing and Process/Project Engineering	BS,MS	Bound Brook, NJ; Charleston and Sistersville, WV; New Orleans, LA; Houston and Victoria, TX; Moses Lake, WA
Purchasing and Distribution	BS	Charleston, WV
R&D (Polymer Applications/Tech Service; Process Development)	MS	Bound Brook, NJ; Charleston, WV; Tarrytown, NY
Technical Sales	BS	Metropolitan areas, nationwide

### PhD

<u>Fields of Special Interest</u>	<u>Tech Center Locations</u>
Catalysis, Polymers, Separations	Bound Brook, NJ; Charleston, WV

## ● ADDITIONAL INFORMATION ●

UCC has been recognized for its innovative technologies by receiving several prestigious Kirkpatrick Awards (sponsored by *Chemical Engineering Magazine*). Two of these, UNIPOL (polyolefins) and Low Pressure Oxo (alcohols), are licensed internationally and account for >15 billion lbs/yr of plastics and solvents.

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# SHELL OIL COMPANY

AND SUBSIDIARIES

## ● GENERAL INFORMATION ●

Shell began operations in the United States in 1912. Emphasizing innovative technology and sound engineering, it has grown to be a major company employing in excess of 30,000 people throughout the United States. Chemical engineers are utilized in the recovery of oil and natural gas, refining and chemical plant operations, and sales activities.

**CITIZENSHIP REQUIREMENTS:** Candidates must be legally authorized to work in the United States. Will not consider candidates with student visas.

**REGIONS OF USA AND/OR CANADA WHERE BS/MS CAMPUS RECRUITING IS GENERALLY CONDUCTED:** Primary work locations include the Gulf Coast, California, Illinois, and Washington state.

**HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW:** Send resume and transcripts to  
Manager Recruitment  
Shell Oil Company  
Department D2  
P.O. Box 2463  
Houston, TX 77252

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

**Process Engineering:** Provide technical support to petrochemical operating units, plan and develop new facilities plus major and minor revisions to existing facilities.

**Computer Process Control:** Provide technical support to petrochemical process control systems, including systems modification/enhancement.

**Production Engineering:** Optimization of oil/gas wells and reservoir performance, design and application of enhanced recovery programs, thermal recovery processes, planning and economic evaluation of operations and multiple flow analysis and application.

**Chemical Sales:** Provide market intelligence and customer service in support of sales efforts. Perform market research and development and market chemical and polymer products.

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# ROHM AND HAAS COMPANY

CORPORATE STAFFING DEPARTMENT

Independence Mall West

Philadelphia, PA 19105

## ● GENERAL INFORMATION ●

Rohm and Haas Company is a highly successful multinational chemical company producing over 2,500 products for use in industry and agriculture. Most of our annual sales of over \$2.5 billion come from complex specialty chemical products designed for specific applications: plastics and modifiers for PVC resins, electronics chemicals, biocides, additives for motor oils, polymeric finishes for leather and textiles, acrylic resins for paints, and agricultural pesticides. We have offices and manufacturing facilities in 30 countries and employ over 13,000 people.

**CITIZENSHIP REQUIREMENTS:** U.S. citizens and those who have a legal right to work and remain permanently in the U.S., or who qualify as "Intending Citizens" under the Immigration Reform and Control Act of 1986.

**REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED:** Nationwide in Continental U.S.

**HOW TO APPLY IF UNABLE TO SCHEDULE CAMPUS INTERVIEW:** Send your resume and cover letter to the above address.

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

<u>Functional Area</u>	<u>Major Hiring Locations</u>
Research Process Engineering	Philadelphia Area
Plant Development	Philadelphia and Bristol, PA; Houston, TX; Louisville, KY; Knoxville, TN
Process Design	Philadelphia Area
Technical Sales	Major Cities Nationwide

### PhD

<u>Fields of Special Interest</u>	<u>Tech Center Locations</u>
Process Engineering	Philadelphia Area
Process Design	Philadelphia Area
Separations	Philadelphia Area
Materials	Philadelphia Area
Polymer Science	Philadelphia Area

## ● ADDITIONAL INFORMATION ●

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# DOW CHEMICAL USA

University Relations  
Box 1713-CH  
Midland, MI 48674

## ● GENERAL INFORMATION ●

Dow manufactures and markets chemicals, plastics, metals, consumer products, pharmaceuticals, specialty products and services, and agricultural products. Dow USA will hire over 275 chemical engineers in 1989 and has over 2400 chemical engineers working in all functions and geographic locations. In a 1988 magazine survey, chemical engineering students named Dow as the number-one company for which they would like to work.

**CITIZENSHIP REQUIREMENTS:** Only U.S. citizens, aliens who have a legal right to work and remain permanently in the U.S. or aliens who qualify as "Intending Citizens" under the Immigration Reform and Control Act of 1986 are eligible for employment.

**REGIONS WHERE BS/MS CAMPUS RECRUITING IS CONDUCTED:** Nationwide

**HOW TO APPLY IF UNABLE TO SCHEDULE A CAMPUS INTERVIEW:** Send resume and letter to above address, stating your job interests and geographic preferences.

## ● ENTRY LEVEL OPPORTUNITIES FOR CHEMICAL ENGINEERS ●

### BS/MS

<u>Functional Area</u>	<u>Degree Level</u>	<u>Major Hiring Locations</u>
Design	BS,MS	Michigan, Texas, Louisiana, Ohio, California
Process Engineering	BS,MS	Michigan, Texas, Louisiana, Ohio, California
Manufacturing	BS,MS	Michigan, Texas, Louisiana, Ohio, California
Research and Development	BS,MS	Michigan, Texas, Louisiana, Ohio, California
Sales	BS,MS	Offices in over thirty major cities

### PhD

<u>Fields of Special Interest</u>	<u>Tech Center Locations</u>
Math Modeling	Michigan, Texas, California
Polymer Processing	Michigan, Texas, California, Ohio
Polymer Characterization	Michigan, Texas, California, Louisiana
Catalysis	Michigan, Texas

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

## A PRACTICAL APPLICATION OF MASS BALANCES

WILLIAM F. FURTER<sup>1</sup>, MICHAEL J. PEGG<sup>2</sup>  
and PAUL R. AMYOTTE<sup>2</sup>

A COURSE IN MASS (and energy) balances is essentially a course in solving a large number and variety of problems. This has been our approach to teaching mass balances, and many of the problems we assign can be described by *given this and this, calculate that*. This seems reasonable in light of the fact that one of the primary reasons for doing mass balances is to determine unknown flowrates and compositions from a limited amount of data.

Another application of the mass balance technique is in checking the consistency of measured data from a process. It is, therefore, also useful to assign problems which demonstrate this concept. The problem presented here is one such example.

### PROBLEM

(a) A process steam boiler (operating at steady state) at a coal conversion plant fires coal gas from a continuous vertical retort. The fuel analysis is given in Table 1. An environmental test crew has made measurements of the flue gas emissions in the stack; the measured dry flue gas analysis is given in Table 2. Over the duration of the testing, the molal humidity of the combustion air supply was 0.05 mole moisture per mole dry air. Using the law of conservation of mass, check the consistency of the data.

(b) The boiler described in part (a) operates at a thermal input of 25 MW, and the higher heating value of the fuel gas has been determined as 17.97 MJ/m<sup>3</sup> at 15°C and atmospheric pressure. In addition to deter-

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TABLE 1  
Fuel Analysis

<u>Component</u>	<u>Volume %</u>
CH <sub>4</sub>	22.0
CO	18.0
H <sub>2</sub>	49.4
O <sub>2</sub>	0.4
CO <sub>2</sub>	4.0
N <sub>2</sub>	6.2

TABLE 2  
Dry Flue Gas Analysis

<u>Component</u>	<u>Volume %</u>
CO <sub>2</sub>	10.0
CO	0.8
O <sub>2</sub>	4.0
N <sub>2</sub>	85.2

mining the dry flue gas analysis, the environmental test crew has made several other measurements. The temperature of the flue gas was found to be 325°C. A particulates traverse revealed negligible stack solids, a flue gas moisture content of 38% by volume, and a stack gas velocity of 5.75 m/s. The chimney diameter is known to be 2.06 m, and the burners were thought to be operated with about 17% excess air over the duration of the testing. Using the law of conservation of mass, check the consistency of the data.

## SOLUTION

(a) The flow diagram is shown in Figure 1, with the system defined as the boiler plant. The basis for subsequent calculations is 100 mol of fuel gas fed to the boiler (actually the time required to fire this quantity of fuel gas).

The solution strategy follows that outlined for this type of problem by Lewis *et al.* [1]. Their procedure first calls for the assumption that there is a balance between input and output of all major elements in the process except one. The data consistency check is then achieved by seeing if an equality exists between input and output of the last element.

To systemize the choice of elements and balances, the following scheme is recommended in ref. [1] for this sort of process:

1. carbon balance to relate fuel to dry flue gas
2. nitrogen balance to relate dry flue gas to air supply
3. oxygen balance to determine moisture in flue gas
4. hydrogen balance to check data consistency

The parameters for these balances are shown in Table 3. The amounts of dry flue gas (X), dry air (Y) and flue gas moisture (Z) calculated from Table 3 via



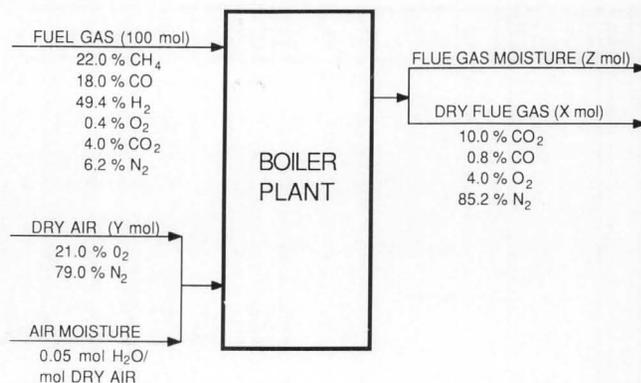
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**FIGURE 1.** Flow diagram for process steam boiler plant.

the carbon, nitrogen and oxygen balances are 407.4 mol, 431.5 mol, and 112.3 mol, respectively. The hydrogen balance yields an input of 115.0 mol  $H_2$  and an output of 112.3 mol  $H_2$  (less than 3% difference). Considering that all measurement errors have been lumped in the hydrogen balance [1], the input and output of hydrogen show good agreement. The data from this part of the problem are considered to be consistent.

(b) The data which are to be checked for consistency in this part are the percent excess air, flue gas moisture content, and stack gas velocity. Table 4 shows the calculations for the theoretical oxygen (77.3 mol),

**TABLE 3**  
Mass Balance Parameters on a Basis of  
100 mol Fuel Gas (equating volume % and mole%)

STREAM	CARBON (mol)	NITROGEN (mol)	OXYGEN (mol)	HYDROGEN (mol)
Fuel gas	22.0 (as $CH_4$ ) 18.0 (as CO) 4.0 (as $CO_2$ )	6.2 (as $N_2$ )	0.4 (as $O_2$ ) 9.0 (as CO) 4.0 (as $CO_2$ )	49.4 (as $H_2$ ) 44.0 (as $CH_4$ )
Dry air	-----	0.79 Y (as $N_2$ )	0.21 Y (as $O_2$ )	-----
Air moisture	-----	-----	0.05 Y/2 (as $H_2O$ )	0.05 Y (as $H_2O$ )
Dry flue gas	0.008X (as CO) 0.1X (as $CO_2$ )	0.852X (as $N_2$ )	0.04 X (as $O_2$ ) 0.008 X/2 (as CO) 0.1 X (as $CO_2$ )	-----
Flue gas moisture	-----	-----	0.5 Z (as $H_2O$ )	Z (as $H_2O$ )

X = mol dry flue gas

Y = mol dry air

Z = mol flue gas moisture

**TABLE 4**  
Theoretical Oxygen Calculations on a Basis of 100 mol Fuel Gas

COMPONENT	AMOUNT (mol)	COMPLETE COMBUSTION EQUATION	THEORETICAL O <sub>2</sub> (mol)
CH <sub>4</sub>	22.0	CH <sub>4</sub> + 2O <sub>2</sub> → CO <sub>2</sub> + 2H <sub>2</sub> O	44.0
CO	18.0	CO + 1/2 O <sub>2</sub> → CO <sub>2</sub>	9.0
H <sub>2</sub>	49.4	H <sub>2</sub> + 1/2 O <sub>2</sub> → H <sub>2</sub> O	24.7
O <sub>2</sub>	0.4	-	-0.4
			77.3

which corresponds to a theoretical air value of 368.1 mol. From part (a), the actual dry air supplied is 431.5 mol. The calculated value of 17.2% excess air agrees with the estimate given in the problem statement.

The amounts previously determined for the dry flue gas (407.4 mol) and flue gas moisture (112.3 mol) indicate a moisture content of approximately 22% in the flue gas. Clearly this does not agree with the measured value of 38%; one explanation is that the measurement is incorrect [2]. As shown in the following analysis, however, there is a more likely explanation.

The fuel firing rate is calculated as 58.8 mol/s by dividing the boiler thermal input by the higher heating value of the fuel gas, correcting to STP, and assuming ideal gas behavior. Since the basis previously used was 100 mol of fuel gas, the scale factor for the process is 0.588 mols/s/mol.

Using 407.4 mol dry flue gas from part (a) and a flue gas moisture content of 38%, the amount of moisture in the flue gas is determined to be 249.7 mol. This gives a value of 657.1 mol for the total amount of flue gas, which, when multiplied by the scale factor, becomes a molar flowrate of 386.4 mol/s. Correcting from STP to 325°C and assuming ideal gas behavior, the volumetric flowrate of the flue gas is 19.0 m<sup>3</sup>/s. Dividing this by the cross-sectional area of the chimney, a stack gas velocity of 5.70 m/s is obtained. This compares favourably with the given value of 5.75 m/s.

It is unlikely that the measurements of both flue gas moisture content and stack gas velocity are wrong. The data, therefore, indicate that more water is leaving the system than is entering. A plausible explanation is the existence of a leak in a water tube inside the boiler.

## CONCLUSION

Although the solution has been presented here in a straightforward manner, the open-ended nature of the problem can create difficulties for some students. In particular, part (b) requires analysis and judgement skills in addition to the knowledge of how to perform a mass balance. For this reason we have found it best to offer exposure to problems of this type in class tutorials and home assignments before using them on tests and exams. This approach generally results in a favourable student response, in addition to illustrating the power and usefulness of the mass balance technique.

## REFERENCES

1. Lewis, W. K., A. H. Radasch, and H. C. Lewis, *Industrial Stoichiometry: Chemical Calculations of Manufacturing Processes*, second edition, McGraw-Hill, New York; pp 114-118 (1954)
2. Felder, R. M., and R. W. Rousseau, *Elementary Principles of Chemical Processes*, second edition, John Wiley & Sons, New York; pg 85 (1986) □

## DEPARTMENT: New Jersey Institute

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and have a number of interesting projects that have been on the back burner for the lack of such students.

## DEPARTMENTAL ADMINISTRATION

Because of the size of the department and the number of degrees it awards (we also administer the freshman chemistry program required of all engineering undergraduates), the chairman is assisted by five associate chairmen. Barbara Kebbekus acts as administrative officer for the chemistry division, and Reginald Tomkins is responsible for recruiting and advising all of our undergraduate students and handles industrial liaison. Richard Trattner administers the environmental science program. Arthur Greenberg advises graduate students in the applied chemistry program, and Basil Baltzis is responsible for recruiting and advising chemical engineering graduate students.

Departmental staff includes two administrative assistants, two secretaries, a machine shop supervisor, a laboratory supervisor, and two lab assistants.

## REFERENCES

1. National Action Council for Minorities in Engineering, *NACME News*, p 6 (August, 1988)
2. "Frontiers in Chemical Engineering Education: Research Needs and Opportunities," National Research Council, National Academy Press, Washington, DC (1988) □

## Random Thoughts . . .

# THE VIEW THROUGH THE DOORS

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One of my favorite leisure-time activities is to walk down the hall and listen to classes in progress, hoping to get some teaching tips. I've got some time this morning—come along with me and let's see what we can pick up.

There's Professor Frobish—he's got the junior fluids course this semester.

\* \* \* \* \*

**Frobish:** "...and on Monday we saw that if you write the coupled partial differential equations of change for this pseudoplastic fluid flowing in a cloverleaf-shaped channel and impose the usual singular perturbation theory boundary conditions you can easily prove that the liquid will emerge at the outlet as long as the pipe is tilted downward."

**Student:** "Professor Frobish."

**Frobish:** "That result by itself is of course only mildly interesting but Monday was the first day of class and I wanted to start slowly. Now today we'll see what happens if we relax some of those simplifying assumptions. Suppose, for example, we say that instead of a pseudoplastic fluid we have a virial gas moving at sonic velocity and the channel is made of expandable rubber and is mounted on a satellite in a decaying orbit. Now if we invoke a six-dimensional stress tensor we can easily see that..."

**Student:** "Professor Frobish!"

**Frobish:** "What is it already?"

**Student:** "You never finished the proof you were doing Monday and I didn't understand any of it as far as you got."

**Frobish:** "Finishing it was an exercise for the class...the mathematics is completely straightforward...but if you need help you'll find something simi-

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lar in that paper by Lundquist I cited."

**Student** (a trace of hysteria entering his voice): "But I can't read Swedish."

\* \* \* \* \*

Oh well, that will probably go on for awhile, so let's move on. Good man, Frobish, although some of the faculty feel that he's too applied—they want more fundamentals in the curriculum. Look in there now...see that guy with the mustache and the tee shirt that says "Chemical Engineers Do It In Fluidized Beds"? That's Greg Furze—he teaches kinetics and gets consistently high ratings. Seems to be some action in there—let's check it out.

\* \* \* \* \*

**Furze:** "Ok, guys...get the chairs in a circle and let's get down to it. You people there are A molecules, got it, and you over there are B's. A's—put on your little hats so we'll all know which species you are. Good. Now, when I yell STARTUP you all get going, ok, and Angie there will keep count."

**Student:** "Hey, Greg, I forget what we're supposed to do."

**Furze:** "No sweat, Joe...this is tough stuff—I don't expect you to get it right away. When I yell you all start milling around inside the chairs...move in straight lines until you bump into someone else. If it's your

species, you just bounce off and keep going. If it's the opposite species you roll a die,, and if you throw a 1 then you yell out REACTION and sit down. Got it?"

**Student:** "Why are we doing this again?"

**Furze:** "Great question, Amy. We're demonstrating the kinetics of...what, gang? Right, a second-order reaction in a well-mixed batch reactor. Now, after this run, just for fun we're going to say that Pete over there is a catalyst and unknown to him there's a trace amount of sulfur in the reactor, which he's deathly allergic to. Pete, as the reaction proceeds you'll start gasping and clutching your throat, and the rest of you..."

\*\*\*\*\*

Interesting fellow, Furze—students like him, but for some reason I've never understood, Frobish doesn't...ah, we've got a treat coming up now. There's Professor Snavely—he's teaching the sophomores this semester and always keeps them laughing.

\*\*\*\*\*

**Snavely:** "...and that's the flow chart. You people understand?...Wonderful! Now, what do we do next...let's see what our old friend Miss Albright has to say. Miss Albright—give us the benefit of your wisdom."

**Student:** "Um...I'm not sure what you're asking, Dr. Snavely."

**Snavely:** "Oh, really? Well, I'll try again, more slowly. Miss Albright. What...do...we...do...next? Got it that time?"

**Student:** "Uh...I guess we need to find the amount of CO<sub>2</sub> in the product."

**Snavely:** "The amount of CO<sub>2</sub> in the product. Miss Albright, have you ever had a chemistry course? Yes? Were you awake during the part of it when they talked about such esoteric concepts as mole fractions? You were? Amazing...hey, you there, the girl with the glasses. If you think you can teach this stuff better than I can why don't you come up and do that talking from up here. No? All right, then...suppose you tell Miss Albright here how she could determine the mole fraction of CO<sub>2</sub> once she learns what it's called."

**Student:** "Uh...I don't know."

**Snavely:** "You don't know? You don't know? Oh, I'm sorry—this is CHE 247...you must have been looking for the medieval history class down the hall and wandered in here by mistake. Why don't you just..."

\*\*\*\*\*

Lot of fun, isn't he? He's on a fast track here—brought in two million dollars in grants last year

and is a shoo-in for tenure. He has terrible luck, though—three or four times a year his car turns up with flat tires in the parking lot...you'd almost think someone was...say, there's lovable old Professor Wombat, teaching his course in process design. Believe it or not, he's taught that course since 1937 without missing a year.

\*\*\*\*\*

**Wombat:** "...and that's the Chamber process, used to make most of the sulfuric acid we use today. Now I'm going to write a ten-year discounted cash flow rate of return on investment table for a typical plant...copy it carefully, since you will be responsible for it on the next test. After that I'll move on to the important reaction between steam and coke that gives us...watery coke...ha ha ha, a little humor there, class...actually it gives us water gas or blue gas, used as the fuel for many of the lights that illuminate our streets today. Now, the table...pay special attention to the interesting way they treat depreciation in Row 18..."

\*\*\*\*\*

Look how the students are gently nodding their heads as they soak up the wealth of real-world information they're getting. Well, I think it's time to get back to...wait, there's Professor Buffo finishing up today's thermo lecture...looks like another 3-piece-of-chalk day from here.

\*\*\*\*\*

**Buffo:** "...and the last problem is even more trivial. Look." (Writes on board)

$$\begin{aligned} dA &= -PdV - SdT \Rightarrow dA = (\partial A/\partial V)_T dV + (\partial A/\partial T)_V dT & dG &= VdP - SdT \Rightarrow dG = (\partial G/\partial P)_T dP + (\partial G/\partial T)_P dT & dH &= (\partial H/\partial S)_P dS + (\partial H/\partial P)_S dP \Rightarrow V = (\partial H/\partial P)_S = (\partial G/\partial P)_T \text{ so} \\ -S &= (\partial A/\partial T)_V = (\partial G/\partial T)_P & \text{ \& } (\partial P/\partial T)_V &= (\partial S/\partial V)_T \Rightarrow (\partial S/\partial P)_T & &= -\beta V = -R/P \end{aligned}$$

**Buffo:** "...but only for an ideal gas, and the rest obviously follows. Is that clear? Good. Ok, next period we'll learn about some fascinating relationships between  $m$ ,  $f$ ,  $\phi$ , and if we have time for it,  $G$  and  $G^P$ . Class dismissed—don't forget the closed book exam on Friday."

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Well, I'd better get back to the office. I'm just completing the report for our upcoming accreditation visit and I've got to establish that half of our curriculum is really engineering design—should be a piece of cake. □

# GENERALIZED SATURATION PROPERTIES OF PURE FLUIDS VIA CUBIC EQUATIONS OF STATE

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**T**HE MAXWELL CRITERIA require that each cubic equation of state (EOS) has unique, reduced saturation properties when its constants are fixed by the usual critical constraints. For example, a numerical reduced vapor pressure curve results as a function of reduced temperature. Use of independent, empirical EOS and vapor pressure equations has caused thermodynamic inconsistencies in previous correlations.

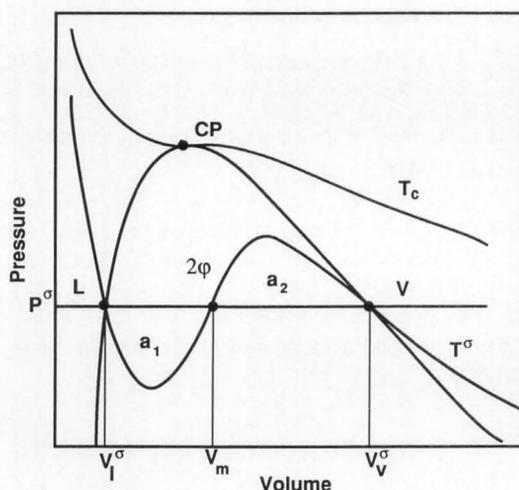
First, this work shows that some simplifications result when the reduced densities of the saturated liquid and vapor are replaced by their sum

$$s \equiv (\rho_{r,l} + \rho_{r,v})$$

and their difference

$$w \equiv (\rho_{r,l} - \rho_{r,v})$$

Second, we tabulated a complete set of saturation properties calculated from the van der Waals EOS.



**FIGURE 1.** A qualitative pressure-volume diagram for a pure substance indicating the coexistence curve with the Maxwell equal area constraint.

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These properties include reduced vapor pressure

$$P_r^\sigma, \quad (dP_r^\sigma/dT_r), \quad \rho_{r,l}, \quad \rho_{r,v}$$

reduced heats of vaporization

$$(\lambda/RT_c), \quad \Delta_J C_{v,v}$$

or the jump in the heat capacity from the single to the two-phase side of the vapor pressure curve,

$$\Delta_J C_{v,l}$$

all as functions of  $T_r$  ( $T_r$  from 0.4 to 0.8 at 0.04 intervals and  $T_r$  from 0.8 to unity at 0.02 intervals).

For other cubic EOS such as Redlich-Kwong (RK), Soave-Redlich-Kwong (SRK), and Peng-Robinson (PR), we provided the same set of saturation properties as for the van de Waals case, although for a single reduced temperature of  $T_r = 0.8$ . For these last three equations we also give the

$$(C_{v,\alpha}^{(1)} - C_v^*)/R$$

or isochoric heat capacity of the saturated vapor or liquid ( $\alpha = v$  or  $l$ ) from the single-phase side w.r.t. the perfect gas value  $C_v^*$  at the same temperature. For SRK and PR equations we used accentric factors

$\omega = 0.0, 0.2, 0.4,$  and  $0.6$ .

Finally, graphs of these results are presented for comparison with experimental results for a number of common compounds ranging from argon to water. The successes and failures of the various cubic EOS are shown clearly for a variety of compounds ranging from spherical molecules to highly-polar, hydrogen-bonding species.

## INTRODUCTION

Vapor-liquid equilibrium (VLE) calculations of a pure substance through an EOS are usually made by the same trial and error procedures used to calculate VLE for mixtures. The iteration variables are usually pressure (P), (when the temperature (T) is provided), or T when the pressure is known. A pressure (or T) is continuously updated in order to satisfy the equal fugacity criteria at equilibrium. For each attempted P (or T), one must evaluate liquid and vapor densities which in turn are used in the evaluation of fugacities.

Any empirical EOS which is fitting both liquid and vapor densities will exhibit van der Waals loops in the two-phase region. The isothermal form of a polynomial EOS must be of odd order in P(V) in order to satisfy mechanical stability criteria for both phases (*i.e.*,  $(\partial P/\partial V)_T < 0$ , as can be observed in Figure 1). Figure 1 shows qualitatively the Maxwell equal-area constraint (or equality of the liquid and vapor fugacities) for cubic EOS. The two "humps" in the two-phase region are characteristics of a cubic equation constrained at the critical point; they are called the van der Waals loops in honor of the first cubic EOS. A fifth degree polynomial would present four of these "humps," a seventh degree six, and so forth.

The total derivative of the Gibbs' free energy for a pure substance is

$$dG = -SdT + VdP \quad (1)$$

A phase change, such as vaporization or melting, for a pure substance occurs at constant temperature and pressure. The specific properties of the thermodynamic functions (A, H, S, *etc.*) will be different for the two equilibrium phases except for the Gibbs' free energy, as can be observed by applying the above equation at constant T and P. This is equivalent to the equilibrium criterium of equality of fugacities since

$$dG = RTd \ln f \quad (2)$$

The Gibbs free energy can be expressed in terms of the thermodynamic functions as

$$G = A + PV \quad (3)$$

where A is the Helmholtz function and V is the specific or molar volume. Differentiation of this equation at constant pressure and temperature gives

$$[dG = dA + PdV]_{T,P} = 0 \quad (4)$$

Integration between the equilibrium vapor and liquid phases provides

$$\int_{A_v}^{A_l} dA = - \int_{V_{r,v}}^{V_{r,l}} PdV = P^\sigma (V_{r,v}^\sigma - V_{r,l}^\sigma) \quad (5)$$

Because the right-hand side of this equation is the area of a rectangle,  $a_1 = a_2$  as in Figure 1.

Cubic EOS are the simplest polynomials that can satisfy Maxwell's criteria. The capabilities of the available cubic EOS vary from equation to equation, particularly in the calculation of liquid densities. The purpose of this study is to evaluate some of the most popular EOS of the van der Waals type with regard to their VLE predictions. The studied equations were

TABLE 1: Generalized Cubic Equations of State (EOS)

$$P = \frac{RT}{(V - b_1)} - \frac{a_c [\alpha(T_r, \omega)]^2}{(V - b_2)(V - b_3)}$$

EOS	$b_1$	$b_2$	$b_3$	$a_c$	$\alpha(T_r, \omega)$	$Z_c$
VdW	$.12500 RT_c/P_c$	0	0	$.42188 R^2 T_c^2 / P_c$	1	3/8
RK	$.08664 RT_c/P_c$	$-b_1$	0	$.42748 R^2 T_c^2 / P_c$	$T_r^{-1/4}$	1/3
SRK	$.08664 RT_c/P_c$	$-b_1$	0	$.42748 R^2 T_c^2 / P_c$	$1 + f_s(\omega)(1 - \sqrt{T_r})$	1/3
PR	$.07780 RT_c/P_c$	$-b_1 \pm \sqrt{2} b_1$	$-b_1 \pm \sqrt{2} b_1$	$.45724 R^2 T_c^2 / P_c$	$1 + f_p(\omega)(1 - \sqrt{T_r})$	.307

$$f_s(\omega) = 0.480 + 1.574 \omega - 0.176 \omega^2$$

$$f_p(\omega) = 0.37464 + 1.54226 \omega - 0.26992 \omega^2$$

van der Waals (VdW), Redlich-Kwong (RK), Soave-Redlich-Kwong (SRK) and Peng-Robinson (PR). Because we forced these equations to satisfy the critical constraints they can be written in a generic way using characteristic parameters in terms of the critical constants as indicated in Table 1.

### PROCEDURE

In this work, we show an alternative way of solving the classical VLE problem which is much simpler and faster. The saturation properties are presented in a reduced form, which allows the reader to compare their performance with any number of compounds by merely scaling these properties by the critical parameters of the substance in question.

The reduced densities of the vapor and the liquid phases are replaced by two new variables:

the sum

$$s \equiv \rho_{r,l} + \rho_{r,v}$$

and the width

$$w \equiv \rho_{r,l} - \rho_{r,v}$$

of the saturation curve on a temperature/density diagram. A simple relation is obtained between  $w$  and  $s$

from the EOS applied to the liquid and the vapor phases, after equating the pressures. For instance, after substituting the two new variables in van der Waals' EOS we obtain

$$w^2 = s^2 - 32 T_r / s + 36 - 12s \quad (6)$$

When this relation is placed into the equation derived from application of the Maxwell equal-area criteria, it provides a function of a single variable which can be zeroed by any numerical technique (*e.g.*, the Newton-Raphson method or bisection algorithms).

For example, from the VdW EOS this single variable function becomes

$$\ln \left[ \frac{s(6-s) - (16 T_r / 3) + sw}{s(6-s) - (16 T_r / 3) - sw} \right] - 3(6-s)w / 8 T_r = 0 \quad (7)$$

with  $w$  from Eq. (6).

An efficient way of calculating VLE using this method is to step down from the critical temperature ( $T_r = 1$ ) for which the value of  $s$  is known ( $s = 2$ ), and use this as an initial estimate for the next temperature. A continuation algorithm may be begun in this way by using only a hand calculator. Linearity of  $s$

**TABLE 2: Predicted Reduced Saturation Properties From Van Der Waals Equation of State**

$T_r^\sigma$	$P_r^\sigma$	$V_{r,v}^\sigma$	$V_{r,\ell}^\sigma$	$\left(\frac{dP_r}{dT_r}\right)^\sigma$	$\frac{\lambda}{RT_c}$	$\left(\frac{dV_{r,v}}{dT_r}\right)^\sigma$	$\left(\frac{dV_{r,\ell}}{dT_r}\right)^\sigma$	$\frac{\Delta_J C_{v,v}}{R}$	$\frac{\Delta_J C_{v,\ell}}{R}$	$\left(\frac{d^2 P_r}{dT_r^2}\right)^\sigma$	$\left(\frac{\partial P_r}{\partial V_{r,v}}\right)_{T_r}^\sigma$	$\left(\frac{\partial P_r}{\partial V_{r,\ell}}\right)_{T_r}^\sigma$
1.00	.10000E+01	.10000E+01	.10000E+01	.40000E+01	.00000E+00	−∞	∞	.45455E+01*	.44554E+00*	.95972E+01*	.00000E+00	.00000E+00
.98	.92191E+00	.13761E+01	.77554E+00	.38091E+01	.84070E+00	−1.2412E+02	.44304E+01	.57100E+01	.36166E+01	.94849E+01	−1.0086E+00	−.50136E+00
.96	.84762E+00	.16118E+01	.70819E+00	.36206E+01	.11778E+01	−1.1510E+02	.26352E+01	.63598E+01	.33139E+01	.93632E+01	−1.3335E+00	−.13256E+01
.94	.77707E+00	.18438E+01	.66369E+00	.34347E+01	.14288E+01	−1.1799E+02	.18970E+01	.69425E+01	.31010E+01	.92344E+01	−1.4148E+00	−.24446E+01
.92	.71021E+00	.20869E+01	.63022E+00	.32513E+01	.16340E+01	−1.2570E+02	.14834E+01	.75050E+01	.29327E+01	.90982E+01	−1.3768E+00	−.38633E+01
.90	.64700E+00	.23488E+01	.60340E+00	.30708E+01	.18090E+01	−1.3676E+02	.12161E+01	.80669E+01	.27922E+01	.89541E+01	−1.2779E+00	−.55945E+01
.88	.58736E+00	.26360E+01	.58106E+00	.28932E+01	.19619E+01	−1.5088E+02	.10282E+01	.86393E+01	.26708E+01	.88015E+01	−1.1500E+00	−.76555E+01
.86	.53125E+00	.29545E+01	.56195E+00	.27188E+01	.20978E+01	−1.6822E+02	.88863E+00	.92302E+01	.25636E+01	.86400E+01	−1.0115E+00	−.10066E+02
.84	.47859E+00	.33113E+01	.54530E+00	.25477E+01	.22197E+01	−1.8919E+02	.78072E+00	.98461E+01	.24673E+01	.84690E+01	−.87331E−01	−.12851E+02
.82	.42932E+00	.37141E+01	.53058E+00	.23801E+01	.23299E+01	−2.1444E+02	.69475E+00	.10493E+02	.23798E+01	.82881E+01	−.74207E−01	−.16034E+02
.80	.38336E+00	.41725E+01	.51741E+00	.22162E+01	.24301E+01	−2.4486E+02	.62465E+00	.11177E+02	.22994E+01	.80966E+01	−.62143E−01	−.19644E+02
.76	.30108E+00	.53041E+01	.49469E+00	.19005E+01	.26050E+01	−3.2622E+02	.51724E+00	.12682E+02	.21560E+01	.76795E+01	−.41814E−01	−.28277E+02
.72	.23108E+00	.68354E+01	.47565E+00	.16025E+01	.27517E+01	−4.4780E+02	.43888E+00	.14417E+02	.20305E+01	.72132E+01	−.26628E−01	−.39043E+02
.68	.17262E+00	.89734E+01	.45933E+00	.13242E+01	.28750E+01	−6.3524E+02	.37930E+00	.16451E+02	.19189E+01	.66933E+01	−.15987E−01	−.52307E+02
.64	.12485E+00	.12066E+02	.44513E+00	.10678E+01	.29782E+01	−9.3577E+02	.33254E+00	.18877E+02	.18184E+01	.61163E+01	−.89822E−02	−.68516E+02
.60	.86869E−01	.16729E+02	.43261E+00	.83568E+00	.30641E+01	−1.4410E+03	.29496E+00	.21821E+02	.17272E+01	.54803E+01	−.46707E−02	−.88236E+02
.56	.57645E−01	.24110E+02	.42145E+00	.63015E+00	.31348E+01	−2.3403E+03	.26414E+00	.25458E+02	.16438E+01	.47871E+01	−.22134E−02	−.11219E+03
.52	.36073E−01	.36517E+02	.41141E+00	.45339E+00	.31921E+01	−4.0569E+03	.23849E+00	.30037E+02	.15673E+01	.40437E+01	−.93591E−03	−.14131E+03
.48	.20967E−01	.58969E+02	.40231E+00	.30713E+00	.32377E+01	−7.6275E+03	.21684E+00	.35923E+02	.14969E+01	.32656E+01	−.34303E−03	−.17686E+03
.44	.11084E−01	.10358E+03	.39402E+00	.19225E+00	.32733E+01	−1.5901E+04	.19840E+00	.43661E+02	.14322E+01	.24802E+01	−.10466E−03	−.22052E+03
.40	.51745E−02	.20363E+03	.38641E+00	.10825E+00	.33003E+01	−3.7906E+04	.18253E+00	.54094E+02	.13727E+01	.17293E+01	−.25098E−04	−.27467E+03

with  $T_r$ , the law of rectilinear diameters, is helpful for sequential temperature calculations. However, cubic EOS do not provide exact compliance with rectilinear diameter except in the immediate critical region.

Knowledge of  $s$  and  $w$  allows back calculation of  $\rho_{r,l}$  and  $\rho_{r,v}$  and the reduced vapor pressure from the EOS itself. This outlined procedure has been followed for all the EOS listed in Table 1. For the SRK and PR equations we calculated equilibrium properties at acentric factors of  $\omega = 0.0, 0.2, 0.4$  and  $0.6$ .

For Redlich-Kwong EOS, the relation between  $s$  and  $w$  is given by a quartic equation. However, because this equation does not have odd terms in  $w$ , it can easily be solved as a quadratic in  $y$  with  $y = w^2$

$$(a)(y^2) + b(T_r, s)(y) + c(T_r, s) = 0 \quad (8)$$

where

$$\begin{aligned} a &= \gamma_1 \gamma_2^3 \\ -b &= 4 T_r^{1.5} \gamma_2^2 - 2 \gamma_1 \gamma_2 (2 + \gamma_2^2 s^2) \\ -c &= s \gamma_1 (2 - \gamma_2 s)^2 (4 + \gamma_2 s) - 4 T_r^{1.5} (2 + \gamma_2 s)^2 \end{aligned} \quad (9)$$

with

$$\gamma_1 = 1.282441, \quad \gamma_2 = 0.259921$$

Once  $w$  is calculated from this expression it is placed in the equation derived from application of the Maxwell equal-area constraint and that nonlinear equation is solved for the single variable  $s$  which for Redlich-Kwong is

$$\begin{aligned} T_r \left( \ln \left[ \frac{2(s-w) - \gamma_2(s^2 - w^2)}{2(s+w) - \gamma_2(s^2 - w^2)} \right] - \frac{4w\gamma_2}{(2 - \gamma_2 s)^2 - (\gamma_2 w)^2} \right) + \\ \frac{\gamma_1}{T_r^{0.5}} \left( \ln \left[ \frac{2 + \gamma_2(s+w)}{2 + \gamma_2(s-w)} \right] + \frac{4w}{(2 + \gamma_2 s)^2 - (\gamma_2 w)^2} \right) = 0 \end{aligned} \quad (10)$$

Table 2 contains a complete set of saturation properties calculated from the Van der Waals EOS. Table 3 contains an example of the saturation properties obtained using the RK, SRK and PR EOS for one re-

**TABLE 3**  
Predicted Reduced Saturation Properties From Classical Cubic EOS at Reduced Temperature  $T_r = 0.8$

REDUCED PROPERTY	REDLICH KWONG	SOAVE-REDLICH- KWONG				PENG-ROBINSON			
		$\omega = 0.0$	$\omega = 0.2$	$\omega = 0.4$	$\omega = 0.6$	$\omega = 0.0$	$\omega = 0.2$	$\omega = 0.4$	$\omega = 0.6$
$P_r^\sigma$	.24594E+00	.25893E+00	.20117E+00	.15707E+00	.12333E+00	.25789E+00	.19878E+00	.15521E+00	.12289E+00
$V_{r,v}^\sigma$	.79603E+01	.74502E+01	.10029E+02	.13288E+02	.17371E+02	.80567E+01	.10981E+02	.14578E+02	.18910E+02
$V_{r,\ell}^\sigma$	.41194E+00	.41443E+00	.39516E+00	.38057E+00	.36914E+00	.39904E+00	.37983E+00	.36587E+00	.35533E+00
$\left(\frac{dP_r}{dT_r}\right)^\sigma$	.21862E+01	.21592E+01	.20216E+01	.18490E+01	.16646E+01	.21355E+01	.19912E+01	.18180E+01	.16411E+01
$\frac{\lambda}{RT_c}$	.44006E+01	.40698E+01	.52176E+01	.63934E+01	.75818E+01	.40162E+01	.51844E+01	.63456E+01	.74784E+01
$-\left(\frac{dV_{r,v}}{dT_r}\right)^\sigma$	.72483E+02	.63550E+02	.10192E+03	.15671E+03	.23318E+03	.68997E+02	.11209E+03	.17203E+03	.25225E+03
$\left(\frac{dV_{r,\ell}}{dT_r}\right)^\sigma$	.63407E+00	.62219E+00	.58449E+00	.55127E+00	.52218E+00	.60137E+00	.55864E+00	.52310E+00	.49355E+00
$-\left(\frac{C_{v,v}^{(1)} - C_v^*}{R}\right)$	-.16617E+00	.24828E-01	.28603E-01	.27945E-01	.25326E-01	.21050E-01	.26367E-01	.26618E-01	.24722E-01
$-\left(\frac{C_{v,\ell}^{(1)} - C_v^*}{R}\right)$	-.25298E+00	.35279E+00	.56557E+00	.75167E+00	.90986E+00	.30114E+00	.53008E+00	.72745E+00	.89315E+00
$\frac{\Delta_j C_{v,v}}{R}$	.33933E+02	.29054E+02	.45892E+02	.66805E+02	.91731E+02	.28595E+02	.45605E+02	.66117E+02	.89610E+02
$\frac{\Delta_j C_{v,\ell}}{R}$	.46097E+01	.41213E+01	.53144E+01	.64638E+01	.75550E+01	.40378E+01	.52281E+01	.63382E+01	.73565E+01
$\left(\frac{d^2 P_r}{dT_r^2}\right)^\sigma$	.13393E+02	.13402E+02	.15930E+02	.17660E+02	.18676E+02	.13206E+02	.15701E+02	.17327E+02	.18240E+02
$-\left(\frac{\partial P_r}{\partial V_{r,v}}\right)_{T_r}^\sigma$	.24220E-01	.26854E-01	.16490E-01	.10154E-01	.62976E-02	.24456E-01	.14779E-01	.90961E-02	.57342E-02
$-\left(\frac{\partial P_r}{\partial V_{r,\ell}}\right)_{T_r}^\sigma$	.42996E+02	.39739E+02	.58069E+02	.79396E+02	.10343E+03	.45461E+02	.68210E+02	.94312E+02	.12297E+03

duced temperature ( $T_r = 0.8$ ). For PR and SRK, we used acentric factors of ( $\omega$ ) 0.0, 0.2, 0.4, and 0.6. The interested reader, however, may obtain from us an unabridged version of Table 3 with a finer grid of  $\omega$  and a complete range of  $T_r$ .

We compared the saturation properties for a number of substances ranging from spherical to highly-polar, hydrogen-bonding species. The critical properties were taken from Ambrose [1, 2]. The sources for the experimental data of water were taken from Haar, *et al.* [3]. Argon, CO<sub>2</sub> and methane were taken from the IUPAC international tables [4], [5], and [6], respectively. For pentane and neopentane, we took the correlated values of [7] and [8], respectively.

Figure 2 is a plot of reduced temperature against reduced density obtained from the VdW, RK, SRK and PR EOS—the last two equations of state with zero acentric factors; this diagram emphasizes the liquid-phase predictions, which are generally poor, particularly for CO<sub>2</sub> and water. Use of the acentric factor in the VLE calculations of SRK and PR EOS slightly improves the liquid-phase predictions. We encourage the reader to compare the performance of all the equations at  $T_r = 0.8$  and at different values of the acentric factor  $\omega$  where applicable.

The difficulties with all the EOS for the vapor side predictions are enhanced in Figure 3, which shows  $T_r$  against  $Z_r$  (the reduced compressibility factor). This

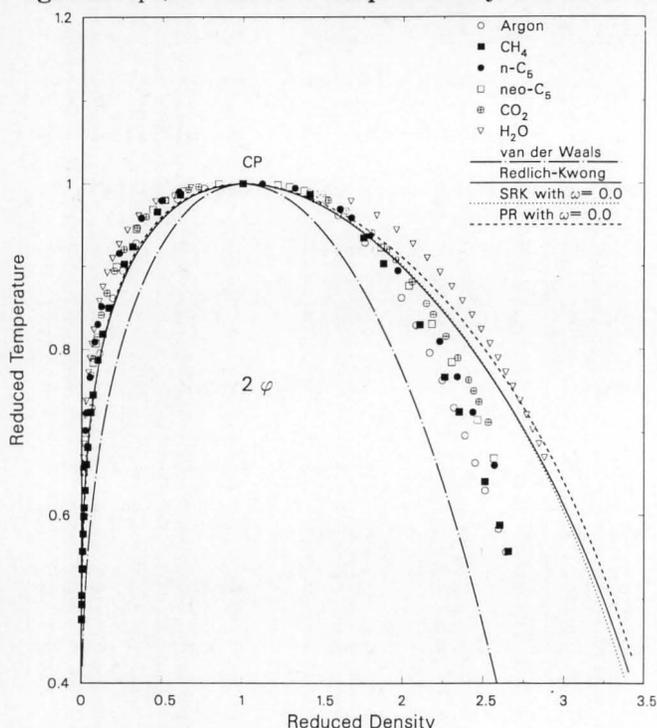


FIGURE 2. Comparison of reduced temperature vs. reduced densities in the coexistence curve.

plot emphasizes the difficulties that cubic EOS, constrained at the CP, have in the prediction of saturation properties. The non-universality of the critical compressibility factor ( $Z_c$ ) is clearly seen by comparing the spread of the data points as the perfect gas value is approached ( $T_r < 0.6$ ). All the EOS tested produce a unique limiting value which is the inverse of their predicted  $Z_c$ .

Once the basic properties

$$\rho_{r,l}, \quad \rho_{r,v}, \quad P_r^\sigma$$

are obtained from the Maxwell minimization technique, the rest of reduced saturation properties are obtained sequentially upon application of the Clapeyron equation and standard thermodynamic relations as follows.

#### ADDITIONAL SATURATION PROPERTIES

The dimensionless heat of vaporization,  $\lambda/RT_c$ , can be calculated using density residual properties:

$$\frac{\lambda}{RT_c} = \frac{H_i^v - H_i^l}{RT_c} = \frac{(H_i^r)_v - (H_i^r)_l}{RT_c} \quad (11)$$

Where  $H_i^r$  is the residual enthalpy defined as the actual enthalpy minus that of the ideal gas [9]:

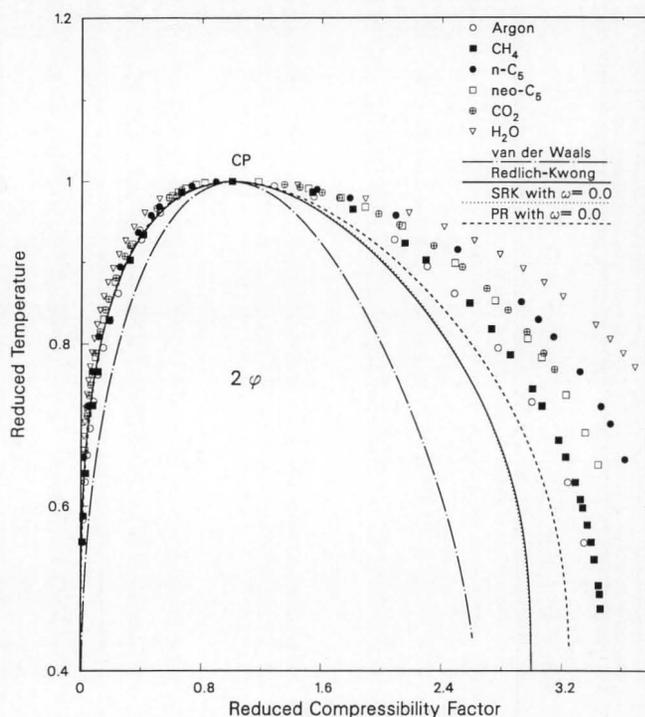


FIGURE 3. Comparison of reduced temperature vs. reduced compressibility factors in the coexistence curve.

$$\left( H_i^r \right)_v = H_i^v - H_i^* \quad (12)$$

The residual enthalpies are evaluated from

$$\frac{\lambda}{RT_c} = T_r \int_{\rho_{r,l}}^{\rho_{r,v}} \left[ \left( \frac{\partial Z_r}{\partial T_r} \right)_{\rho_r} \frac{d\rho_r}{\rho_r} \right] + (Z_{r,v} - Z_{r,l}) \quad (13)$$

This integral is easily evaluated from any of the EOS listed in Table 1 with the limits from the VLE calculations. Upon use of the Clapeyron equation, the dimensionless vapor pressure slope then becomes

$$\left( \frac{dP_r}{dT_r} \right)^\sigma = \left( \frac{\lambda}{RT_c} \right) \left( \frac{1}{Z_c T_r (V_{r,v}^\sigma - V_{r,l}^\sigma)} \right) \quad (14)$$

The slopes of the saturated liquid and vapor volumes are calculated as

$$\left( \frac{dV_{r,\alpha}}{dT_r} \right)^\sigma = \left[ \left( \frac{dP_r}{dT_r} \right)^\sigma - \left( \frac{\partial P_r}{\partial T_r} \right)_{V_r}^\sigma \right] \left[ \left( \frac{\partial V_{r,\alpha}}{\partial P_r} \right)_{T_r}^\sigma \right]^{-1} \quad (15)$$

The dimensionless isochoric heat capacity of the vapor evaluated from the single phase side is calculated from

$$\left( \frac{C_{v,v}^{(1)} - C_v^*}{R} \right) = - \int_0^{\rho_{r,\alpha}} \left[ \left( \frac{T_r}{\rho_r^2} \right) \left( \frac{\partial^2 P_r}{\partial T_r^2} \right)_{\rho_r} \right] d\rho_r \quad (16)$$

Since the equation of Van der Waals provides straight isochores

$$\left( \frac{\partial^2 P_r}{\partial T_r^2} \right)_{\rho_r} = 0$$

the isochoric heat capacity coincides with the ideal gas heat capacity  $C_v^*$ . The jumps in the heat capacities are evaluated as

$$\frac{\Delta_J C_{v,\alpha}}{R} = Z_c T_c \left( \frac{dV_{r,\alpha}}{dT_r} \right)^\sigma \left[ \left( \frac{\partial P_r}{\partial T_r} \right)_{V_r}^\sigma - \left( \frac{dP_r}{dT_r} \right)^\sigma \right] \quad (17)$$

In Eq. (12),  $\alpha$  indicates that the quantity can be evaluated either for the liquid or for the vapor side.

The isochoric heat capacity for the vapor phase evaluated from the two phase side is not reported in Table 2, but can be calculated as follows:

$$\left( \frac{C_{v,v}^{(2)} - C_v^*}{R} \right) = \frac{\Delta_J C_{v,v}}{R} + \left( \frac{C_{v,v}^{(1)} - C_v^*}{R} \right) \quad (18)$$

with an equivalent expression for the isochoric liquid heat capacity.

## A CLASSROOM APPLICATION

This example could be used as a part of a test or a graduate qualification exam. Assuming that the properties of iso-octane can be represented by the Redlich-Kwong EOS, the student is asked to use the generalized saturation properties given in Table 3 to estimate the following quantities at  $T_r = 0.8$ .

- [1] The vapor pressure (in bars), as well as the saturation volumes for the liquid and the vapor phase in ( $\text{cm}^3/\text{mol}$ ).
- [2] How could he/she verify the consistency of the heat of vaporization  $\lambda$ , given in the table with the corresponding values of the vapor pressure and the saturation volumes?
- [3] Using the Redlich-Kwong, derive an expression for the residual isochoric heat capacity ( $C_v - C_v^*$ ), as a function of pressure (or volume) along an isotherm in the gas phase, and calculate the value of  $C_v$  for saturated iso-octane vapor at  $T_r = 0.8$  as taken from the two-phase side using their derived equation. (Note  $C_v^* = 21 \text{ J/mol-K}$ ).

## DISCUSSION

The limiting values of the saturation properties at the critical point were evaluated analytically or numerically (the starred values). The slope of the vapor pressure curve evaluated at the critical point is collinear to the isochoric slope

$$\left( \frac{\partial P_r}{\partial T_r} \right)_{V_r}^\sigma \Big|_{\text{CP}}$$

taken from the single phase side. Even though the analytical expression resulting from Clapeyron equation (Eq. (11)) diverges at the CP, this divergence is removed upon application of L'Hopital's rule taking the limit when the reduced densities approach to unity.

The "critical" values for

$$\frac{\Delta_J C_{v,\alpha}}{R} \quad \text{and for} \quad \left( \frac{d^2 P_r}{dT_r^2} \right)^\sigma$$

were evaluated at a reduced temperature of  $T_r = 0.9999$  which for most practical applications is sufficiently close to the critical point.

It is well known that the curvature of the isochores

$$\left( \frac{\partial^2 P_r}{\partial T_r^2} \right)_{\rho_r}$$

is negative for gas densities, increases with density becoming zero near the critical density, and then posi-

tive for liquid densities. None of the cubic EOS tested is able to reproduce this feature which is reflected in

$$\left( \frac{C_{v,v}^{(1)} - C_v^*}{R} \right)$$

(since  $C_v^*$  is smaller than  $(C_v^{1,2})_{l,v}$ )

VdW provides straight isochores everywhere. For the other EOS analyzed, the sign of the curvature is either fixed and negative as in the RK EOS, or temperature dependent as in the PR and SRK EOS. In either case, for a given temperature the sign remains regardless of the density (vapor or liquid). For example, RK provides the right physics for the curvature of vapor densities but fails for the liquid.

The Soave-Redlich-Kwong and Peng-Robinson EOS were designed to give a better representation of the liquid phase behavior. This they do so even with the isochoric curvature

$$\left( \frac{\partial^2 P_r}{\partial T_r^2} \right)_{\rho_r}$$

although not in the full temperature range and at the expense of misrepresenting the vapor curvature. Along any isochore the curvature will be negative for all temperatures above the "switching" temperature, zero itself at this temperature, and positive below. This switching temperature depends upon the acentric factor. Table 4 contains these temperatures for SRK and PR EOS as a function of  $\omega$ .

### CONCLUSIONS

We believe that Table 2 constitutes a most complete "thermodynamic dictionary of reduced saturated properties." Further, we can provide the reader with the unabridged version of Table 3 which shows the

**TABLE 4**  
Reduced Switching Temperature in SRK  
and PR EOS as a Function of  $\omega$

$\omega$	Soave-Redlich-Kwong		Peng-Robinson	
	$f_s(\omega)$	$T_r^s$	$f_p(\omega)$	$T_r^s$
0.0	0.48000	0.56035	0.37464	0.54858
0.2	0.78776	0.59106	0.67229	0.58012
0.4	1.08144	0.61625	0.94836	0.60527
0.6	1.36104	0.63727	1.20285	0.62569

$$f_s(\omega) = 0.480 + 1.574(\omega - 0.176)(\omega^2)$$

$$f_p(\omega) = 0.37464 + 1.54226(\omega - 0.26992)(\omega^2)$$

real goodness (or weakness) of the most popular equations of state. Our procedures are different and somewhat more general than those of Adachi [10], and Soave [11, 12].

These reduced properties may have multiple uses either as reference values for experimental designs or as valuable information (initial guesses, initiation algorithms) in multicomponent VLE calculations. We have also given the basis for calculating VLE in terms of convenient variables (s and w) that allow the calculations in a much faster and convenient way.

### ACKNOWLEDGMENTS

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### NOMENCLATURE

A	= Helmholtz free energy function.
$C_{v,v}$	= Isochoric heat capacity of the vapor
$C_{v,l}$	= Isochoric heat capacity of the liquid
EOS	= Equation of State
$H_i$	= Molar Enthalpy of component i
P, V, T	= Pressure, Volume, Temperature
R	= Universal Gas Constant
VLE	= Vapor Liquid Equilibria
Z	= Compressibility factor

### Greek Letters

$\Delta_j C_{v,\alpha}/R$	= jump in $C_v$ single minus two-phase side
$\lambda/RT_c$	= reduced heat of vaporization
$\omega$	= acentric factor
$\rho$	= density
$\sigma$	= property at saturation

### Subscripts

c	= critical property
i	= component i
l	= liquid value
r	= reduced property with respect to critical parameters
v	= vapor value

### Superscripts

$\sigma$	= property at saturation
*	= ideal gas value, or extrapolated value in Table 2.
(1,2)	= single—two phase value
l	= liquid
v	= vapor

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authors could obtain new equipment like a laser printer, or at least a new ribbon. There are quite a few minor typographical errors that might have been eliminated by better proofreading by the authors. Neither the editors nor the publisher are responsible for this.

It was not clear if any of the discussion (not included) at the meeting was incorporated into the papers as they appeared. There is a brief note included that was an outgrowth of a discussion that arose at the meeting.

The editors grouped the contributions into nine sections: fundamentals (5 papers), coherent structures (10), wall shear flow (7), free shear flow (7), scalar and buoyant transport (5), modeling and prediction of turbulent transport (9), numerical simulations of turbulence (4), measurement techniques (6), and turbulent transport in applications (4).

The eight keynote papers are all noteworthy and are:

- 1) Coherent Structures Associated with Turbulent Transport, by Blackwelder,
- 2) The Organized Motion and Its Contribution to Transport in Shear Flows, by Antonia,
- 3) Turbulence Management in Free Shear Flows by Control of Coherent Structures, by Husian, Bridges, and Hussain,
- 4) Turbulent Transfer to a Wall at Larger Schmidt Numbers, by Hanratty and Vassiliadou,
- 5) Natural Convection Mass Transfer in an Inclined Enclosure at High Rayleigh Number, by Goldstein, Chiang, and Sayer,
- 6) Recent Results in the Prediction of Turbulent Separated Flows, by Pletcher,
- 7) Advances in Turbulent Transport Modeling Based on Direct Simulations of Turbulence, by Reynolds, Rogers, and Sandham, and
- 8) Investigation of Heat and Momentum Transport in Turbulent Flows Via Numerical Simulations, by Kim.

The topics cover the broad areas of turbulent transport research and thus will find limited use by any one individual. Certainly, institutions that have research interests and programs in the areas will want the volume for library use. About 20% of the contributions are on a variety of fundamentals and the remainder on a wide range of applied problems that involve coupled phenomena and/or a complex geometry. There is a clear increase in the use of computers in experimental and numerical investigations of turbulent flows. The use of large data bases generated on supercomputers is evident.

In the time and space available for this review it was impossible to read all the contributions in detail. Thus, I have concentrated on the keynote lectures and those contributions in the fields that I have worked in. The more senior and well-known authors did speculate on ideas that are neither proven nor necessarily shared by others. They did this honestly, and their efforts are appreciated by this reviewer. Many of the contributions are complete to a degree that they could be considered for publication in the best peer-reviewed journals. There are also papers that are incomplete in their background review and in their understanding of principles. These would not receive consideration for journal publication in their present state.

*Continued on page 181.*

## ChE book reviews

### TRANSPORT PHENOMENA IN TURBULENT FLOWS: Theory, Experiment, and Numerical Simulation

M. Hirata, N. Kasagi, Editors

Hemisphere Publishing Corp., New York; 921 pages, \$150 (1988)

Reviewed by

Robert S. Brodkey

Ohio State University

About one hundred fifty authors have contributed fifty-six general papers and eight keynote addresses to the 2nd International Symposium on Transport Phenomena in Turbulent Flows, held at the University of Tokyo in October, 1987. Over one hundred ten extended abstracts were submitted; thus the volume represents a selection of half of those submitted. The volume (921 pages) was delivered to me for review in less than a year from the date of the symposium; a positive note for the editors, Hirata and Kasagi, and for the publisher, Hemisphere. The copy-ready text varies from papers that are as good as a press-printed journal article to those of poor quality that require the reader to guess at what was intended. One would hope that in the future these few

# TRIANGULAR DIAGRAMS TEACH STEADY AND DYNAMIC BEHAVIOUR OF CATALYTIC REACTIONS

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**B**Y THE TIME students take their first reaction engineering course, they have usually become very familiar with triangular diagrams. These are often introduced in the first or second year stoichiometry courses and are a part of physical chemistry and most engineering thermodynamics courses.

Triangular diagrams turn out to be quite useful in illustrating the dynamic behaviour of heterogeneous catalytic reactors. Thus, there is a good case for introducing them into an undergraduate chemical reaction engineering course.

The purpose of this article is to illustrate how the triangular diagram can aid in presenting some of the rather complex transient interactions that occur among gas and surface species during heterogeneous catalytic reactions. To avoid undue complexity, we assume a catalyst bed in which there are no limitations of transport either in or around the catalyst particles. Both CSTR's and differential reactors are described by identical equations for a gradientless system in the following derivation so what follows applies to both reactor types.

In chemical reaction engineering, triangular diagrams are used to represent selectivity in complex reactions. Wei and Prater [1] seem to have pioneered their use to illustrate the course of a complex homogeneous reaction sequence. States of the system rather than time appear in triangular diagrams. Occasionally, these diagrams have appeared in textbooks [2, 3], but usually in conjunction with an example. We have not seen their use for heterogeneous catalytic reactions, the subject of this article.

The triangular diagram is helpful for showing the

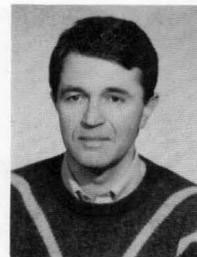
progress of the reaction both in the gas phase and on the catalyst surface. It provides a wealth of information that is hard to present otherwise.

## BASIC EQUATIONS

Figure 1 is a schematic diagram of a reactor with an ideally mixed gas phase. Let us suppose that in the reactor  $k$  gaseous components  $A_i$  ( $i = 1, \dots, k$ ) are present with molar concentrations  $c_i^0$  (mol/mL) at the reactor inlet and  $c_i$  at the reactor outlet (equal to the concentrations inside the reactor). Components  $A_j$  ( $j = k + 1, \dots, n$ ) are adsorbed on the catalyst surface with molar concentrations  $c_j$  (mol/g<sub>cat</sub>).

The reactor has a gas phase volume  $V$  (mL) and

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**Bob Hudgins** is a professor of chemical engineering at the University of Waterloo, Canada, and holds degrees from the University of Toronto and Princeton University. He teaches reaction engineering, staged operations, and laboratories that go with them. His research interests lie in periodic operation of catalytic reactors and in the improvement of gravity clarifiers.



**P. L. Silveston** has been at the University of Waterloo since 1963. Originally from the U.S. he was educated at M.I.T. and the Technical University of Munich (West Germany). His teaching activities have been in reactor engineering, thermodynamics, engineering economics, process design, and entrepreneurship. Research interests are in the cyclic forcing of chemical reactor and coal carbonization and gasification.



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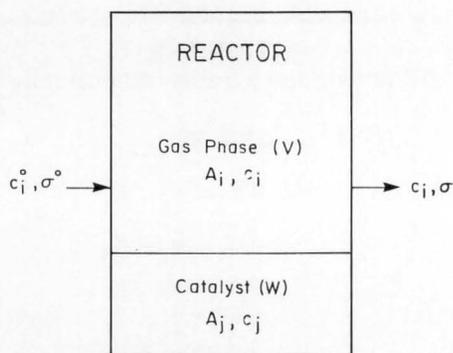


FIGURE 1. Reactor scheme

contains a stationary catalyst bed of weight  $W$  (g), the whole reactor system being maintained at constant temperature and pressure. The reaction mixture is introduced into the reactor with the inlet space velocity  $\sigma^0$  ( $s^{-1}$ ), defined as the ratio of the volumetric flow rate and reactor volume, and leaves the reactor with the outlet space velocity  $\sigma$ . Generally  $\sigma \neq \sigma^0$  because the total number of moles may be changed by the reaction and, in unsteady operation, because of adsorption and/or desorption processes. Mass balances on the reaction components in the fluid phase of the reactor give  $k$  differential equations

$$\left(\frac{dc_i}{dt}\right) = \sigma^0 c_i^0 - \sigma c_i + \left(\frac{W}{V}\right)R_i; \quad i = 1, \dots, k \quad (1)$$

where  $R_i$  (mol/g<sub>cat</sub>·s) is the rate of formation of any gaseous component  $A_i$  ( $i = 1, \dots, k$ ) and  $t$ (s) is time. Similarly, for the components on the catalyst surface, we have

$$\left(\frac{dc_j}{dt}\right) = R_j; \quad j = k + 1, \dots, n \quad (2)$$

Concentrations in the reactor fluid phase sum to the total molar concentration,  $c_T$  (mol/mL), while those on the surface and any free sites sum to the total concentration of the active sites (assumed constant here) on the catalyst surface,  $c_L$  (mol/g<sub>cat</sub>). The set of  $n$  balance Eqs. (1) and (2) is complemented by the initial conditions, for the  $n$  species. The mass balance equations may be recast in dimensionless form as follows

$$\left(\frac{da_i}{d\tau}\right) = a_i - \left(\frac{\sigma}{\sigma^0}\right)a_i + \phi \rho_i; \quad i = 1, \dots, k \quad (3)$$

and

$$\left(\frac{da_j}{d\tau}\right) = \rho_j; \quad j = k + 1, \dots, n \quad (4)$$

Dimensionless variables used in Eqs. (3) and (4) are

Triangular diagrams turn out to be quite useful in illustrating the dynamic behaviour of heterogeneous catalytic reactors. Thus, there is a good case for introducing them into an undergraduate chemical reaction engineering course.

TABLE 1  
Dimensionless Variables

Variable	Definition
dimensionless bulk concentration at the reactor inlet	$a_i^0 = c_i^0/c_T; \quad i = 1, \dots, k$
dimensionless bulk concentration in the reactor	$a_i = c_i/c_T; \quad i = 1, \dots, k$
dimensionless concentration on the catalyst surface	$a_j = c_j/c_L; \quad j = k+1, \dots, n$
dimensionless time	$\tau = t\sigma^0$
dimensionless rate of formation of gaseous component $A_i$	$\rho_i = R_i/(c_L\sigma^0); \quad i = 1, \dots, k$
dimensionless rate of formation of surface component $A_j$	$\rho_j = R_j/(c_L\sigma^0); \quad j = k+1, \dots, n$
capacity factor	$\phi = W_{cL}/(V_{cT})$ (molar capacity of catalyst surface/molar capacity of fluid phase)

summarized in Table 1. The material balances, Eq. (3), contain the space velocity at the reactor outlet,  $\sigma$ , which can be determined only with difficulty. This quantity can be expressed as the function of the space velocity at the reactor inlet,  $\sigma^0$ , by summing the  $k$  equations [Eq. (3)] and noting that the summation of derivatives must equal to zero. After rearrangement

$$\sigma = \sigma^0 \left[ 1 + \phi \sum_{i=1}^k \rho_i \right] \quad (5)$$

The solution of the model for initial conditions gives the time profiles of concentrations in the reactor gas phase as well as on the catalyst surface either for steady state or during transient operation of the reactor. What triangular diagrams show may be seen from the following example.

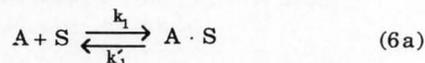
## NUMERICAL EXAMPLE

### Kinetic model

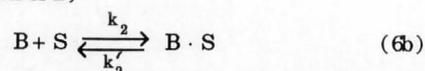
Consider a simple irreversible heterogeneous catalytic reaction between gaseous components A and

B forming gaseous product C proceeding via the following elementary steps

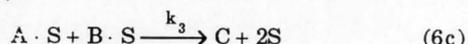
(adsorption/desorption of A)



(adsorption/desorption of B)



(surface reaction)



Forward and reverse reaction rate constants are denoted as  $k_i$  and  $k'_i$ , respectively. Gaseous components are represented as

$$A \equiv A_1; \quad B \equiv A_2; \quad C \equiv A_3$$

and for components on the catalyst surface

$$A \cdot S \equiv A_4; \quad B \cdot S \equiv A_5; \quad S \equiv A_6$$

The dimensionless rates of formation of individual components are given in Table 2, while the dimensionless rate constants with numerical values are shown in Table 3.

Defining the normalized rate of product formation,  $\rho$ , as the ratio of actual to maximum possible rates,  $\rho_3$ , where the maximum possible rate of product formation,  $\rho_{3,\max}$ , is attained for  $a_4 = a_5 = 0.5$ ,

$$\rho = \frac{a_4 a_5}{(a_4 a_5)_{\max}} = \frac{a_4 a_5}{(0.5)(0.5)} = 4 a_4 a_5 \quad (7)$$

The material balance [Eqs. (3) and (4)] for  $k = 3$  and  $n = 6$  can then be used to simulate steady-state and transient behaviour of the  $A + B \rightarrow C$  catalytic reaction in a CSTR. The values of the parameters used for numerical calculations are as follows:  $W = 5$  g,  $V = 10$  mL,  $c_T = 2.437 \times 10^{-5}$  mol/mL,  $c_L = 1.0 \times 10^{-4}$  mol/g. The dimensionless rate constants  $K_i$  ( $i = 1, 2, 3$ ) and  $K'_j$  ( $j = 1, 2$ ) are dependent on the space velocity  $\sigma^0$  (see Table 3). Thus, numerical values of rate constants in Table 3 correspond to the space velocity,  $\sigma^0 = 1.0$  s $^{-1}$ . The value of the total molar concentration,  $c_T$ , follows from its definition,  $c_T = P/(RT)$ , for  $P = 101.3$  kPa and  $T = 500$  K.

#### Steady-state reactor behaviour

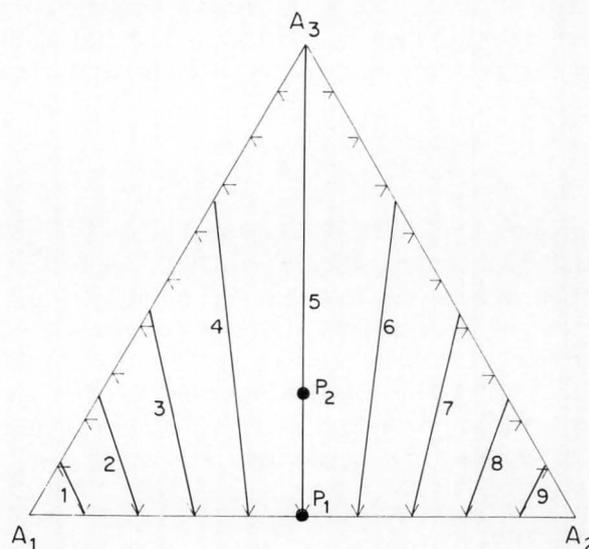
At steady-state, the derivatives (accumulation terms) on the left side of Eqs. (3) and (4) are equal to zero, reducing the set of coupled differential equations

**TABLE 2**  
Dimensionless rates of Formation

Rate	Definition
$\rho_1$	$-K_1 a_1 a_6 + K'_1 a_4$
$\rho_2$	$-K_2 a_2 a_6 + K'_2 a_5$
$\rho_3$	$K_3 a_4 a_5$
$\rho_4$	$-(\rho_1 + \rho_3)$
$\rho_5$	$-(\rho_2 + \rho_3)$
$\rho_6$	$-(\rho_4 + \rho_5)$

**TABLE 3**  
Dimensionless Rate Constants

Constant	Definition	Numerical Value
$K_1$	$(c_T/\sigma^0)k_1$	1.00
$K'_1$	$(1/\sigma^0)k'_1$	0.05
$K_2$	$(c_T/\sigma^0)k_2$	0.30
$K'_2$	$(1/\sigma^0)k'_2$	0.10
$K_3$	$(c_L/\sigma^0)k_3$	0.10



**FIGURE 2.** Steady-state gas concentrations in the reactor for different feed compositions,  $a_1^0 / a_2^0$

(1) 0.9/0.1	(2) 0.8/0.2	(3) 0.7/0.3
(4) 0.6/0.4	(5) 0.5/0.5	(6) 0.4/0.6
(7) 0.3/0.7	(8) 0.2/0.8	(9) 0.1/0.9

to algebraic ones. Because of the nonlinearity resulting from the reaction rate expressions the system has to be solved numerically (see for example, Ralston [4]).

Figure 2 shows typical results for the bulk phase of the reactor for different feed composition ratios  $a_1^0/a_2^0$ . For example, let us suppose that the reaction mixture at the reactor inlet has the stoichiometric composition  $a_1^0 = a_2^0 = 0.5$  (no product  $A_3$  is present). This composition corresponds to the point  $P_1$  on the diagram. Depending on the space velocity,  $\sigma^0$ , used, the composition of the gaseous phase in the reactor will move along the line  $P_1A_3$ . For example, for  $\sigma^0 = 0.03 \text{ s}^{-1}$ , the steady-state composition of the reactor gas phase is given by the point  $P_2$  ( $a_1 = 0.22$ ,  $a_2 = 0.22$ ,  $a_3 = 0.56$ ).

The smaller  $\sigma^0$  is the closer to the point  $A_3$  the resulting composition will be. For infinitesimal  $\sigma^0$ , full conversion of reaction components will be attained and only pure product  $A_3$  will be present in the reactor. For non-stoichiometric inlet compositions, the resulting reaction mixture will always contain unreacted components  $A_1$  and/or  $A_2$  as is shown in Figure 2. The location of the composition point will again depend on the space velocity used.

Figure 3 gives the catalyst surface concentrations corresponding to the gas-phase concentrations in Figure 2. The asymmetry of Figure 3 is striking and is a direct result of the fact that  $A_1$  is more strongly ad-

sorbed on the catalyst than  $A_2$  (cf. values of rate constants in Table 3).

As in Figure 2 the steady-state combination of the surface concentrations depends on the space velocity. The origins of the surface concentration lines have been calculated for a very high space velocity ( $\sigma^0 = 1 \times 10^6 \text{ s}^{-1}$ ) for which the composition of the reaction mixture leaving the reactor is essentially the feed composition (zero conversion). The feed composition ratios lying along axis  $A_1A_2$  in Figure 2 do not correspond to the axis  $A_4A_5$  in Figure 3. Instead, they correspond to surface concentrations along a curve formed by joining the lowest points in lines 1 to 9. This curve then accounts for the number of unoccupied catalyst sites ( $A_6$ ) which varies with the feed composition. For example, the surface concentrations for the fluid-phase composition, given by the point  $P_1$  ( $a_1^0 = a_2^0 = a_1 = a_2 = 0.5$ ) in Figure 2, is denoted as  $P'_1$  in Figure 3 ( $a_4 = 0.82$ ,  $a_5 = 0.08$ ). The gas phase concentration given by the point  $P_2$  in Figure 2 corresponds to point  $P'_2$  in Figure 3. For stoichiometric feed, the composition on the catalyst surface will follow line 5 in Figure 3, finally attaining the vertex  $A_6$ . This point corresponds to the total conversion of both reaction components  $A_1$  and  $A_2$  (product  $A_3$  is not adsorbed).

The normalized steady-state rate  $\rho$  (Eq. 7) is proportional to the product of surface concentrations  $a_4$  and  $a_5$ . The dashed curves in Figure 3 are lines of normalized rate  $\rho = 4a_4a_5$ . The highest value of  $\rho$  occurs at point B ( $a_4 = a_5 = 0.5$ ;  $\rho = 1$ ); and  $\rho$  decreases with increasing distance from B (i.e., with increasing space velocity). The curves depicted in Figure 4 for two different feed compositions are typical of the steady-state rate surface.

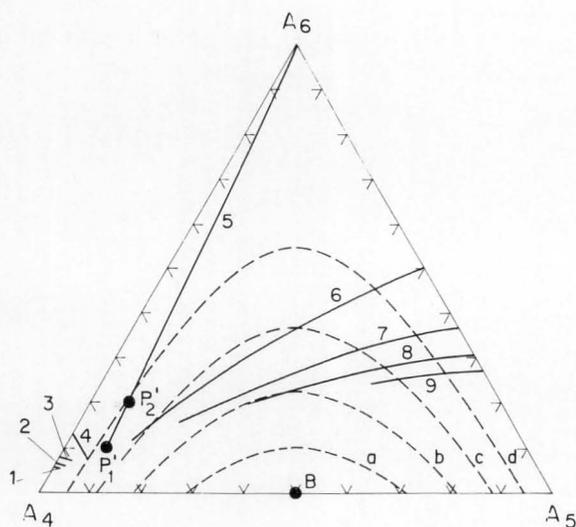


FIGURE 3. Steady-state surface concentration for different feed compositions,  $a_1^0/a_2^0$

(1) 0.9/0.1	(2) 0.8/0.2	(3) 0.7/0.3
(4) 0.6/0.4	(5) 0.5/0.5	(6) 0.4/0.6
(7) 0.3/0.7	(8) 0.2/0.8	(9) 0.1/0.9

Lines of constant normalized rate,  $\rho$  (dashed lines):

(a) $\rho = 0.8$	(b) $\rho = 0.6$	(c) $\rho = 0.4$	(d) $\rho = 0.2$
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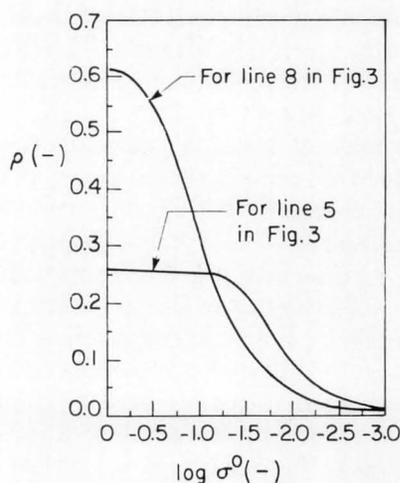


FIGURE 4. Steady-state normalized rates,  $\rho$ , for different space velocities,  $\sigma^0$  and two feed compositions,  $a_1^0/a_2^0$ , corresponding to line 5 in Figure 3 and line 8 in Figure 3.

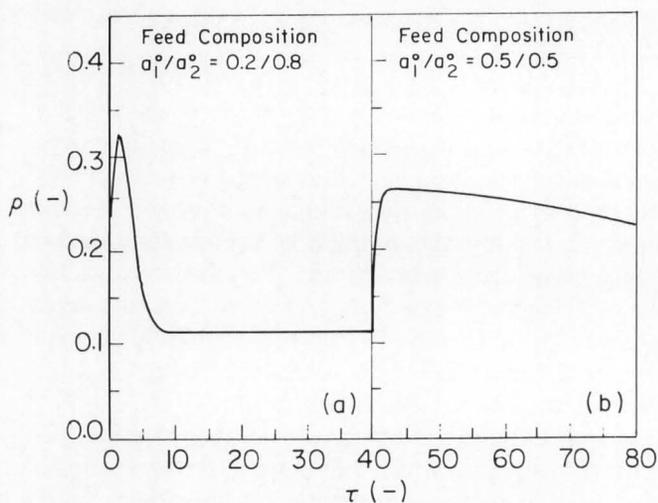


FIGURE 5. Transient of normalized rate,  $\rho$ , after step-change of feed composition  $a_1^0/a_2^0$

- (a)  $a_1^0/a_2^0 = 0.5/0.5$  —step-change— $\rightarrow a_1^0/a_2^0 = 0.2/0.8$   
 (b)  $a_1^0/a_2^0 = 0.2/0.8$  —step-change— $\rightarrow a_1^0/a_2^0 = 0.5/0.5$

### Transient Reactor Behaviour

In general, a catalytic reactor seldom operates under ideal steady-state conditions. Small random fluctuations of the system variables (*e.g.*, temperature, pressure, space velocity, and composition) and changes in the catalyst activity are common. Another kind of transient reactor behaviour occurs after the forced change of either feed composition or reactor temperature. Analysis of forced transient reactor behaviour can furnish mechanistic information (such as the surface populations during reaction) that cannot be obtained from steady-state data.

In the following example, a step-change of the feed composition is used. The dynamic operation of the reactor can be predicted by the numerical integration of balance Eqs. (3) and (4).

The normalized transient rate,  $\rho$ , after a step-change in the feed composition is shown in Figures 5a and 5b. The reactor is initially at steady-state with feed composition  $a_1^0 = a_2^0 = 0.5$ , and space velocity  $\sigma^0 = 0.03 \text{ s}^{-1}$ . At time zero, the feed composition is stepped to  $a_1^0 = 0.2$ ,  $a_2^0 = 0.8$  while  $\sigma^0$  remains unchanged. After the period  $\tau = 40$ , the original feed composition ( $a_1^0 = a_2^0 = 0.5$ ) is restored. The effect of switching the feed composition can be seen in Figure 5a. An overshoot in  $\rho$  occurs immediately after the step-change of input. The maximum is reached at  $\tau = 2$ . Figure 6 illustrates the changes occurring on the catalyst surface for the cycle given in Figure 5, and explains the overshoot. The value of  $\rho$  is proportional to  $a_4 \times a_5$ . The starting point  $P_1'$ , being low in compo-

nent  $A_5$  on the catalyst surface, is not conducive to a high rate of product  $A_3$  formation. Immediately after the feed step-change, the value of  $a_4$  suddenly decreases as a result of the low concentration of  $A_1$  in the feed ( $a_1^0 = 0.2$ ). Thus the surface concentration of  $A_5$  increases and moves towards the region of higher  $\rho$ . The direction of the movement of the surface concentration is illustrated by the arrows in Figure 6. These surface changes lead immediately to a reduced surface coverage ( $A_6 = \text{free centers}$ ) and a higher value of the rate ( $\rho = a_4 a_5$ ). For dimensionless time  $\tau > 2$ , the surface concentration  $a_4$  becomes small and the rate  $\rho$  decreases. At  $\tau = 40$ , the catalyst reactor reaches a new steady-state (point  $P_3'$ ) and at this time the feed composition is stepped back to the original value ( $a_1^0 = a_2^0 = 0.5$ ). The processes on the catalyst surface are represented by the closed trajectory returning from point  $P_3'$  to  $P_1'$ . At time  $\tau = 80$ , the system resumes its original steady-state (point  $P_1'$ ).

Figure 6 thus illustrates that the surface, passing between two separate steady states, does not follow the same path. Instead, the path depends on the direction of the change in feed composition.

### CLASSROOM USE

Figures 2 and 3 illustrate the importance of the adsorption equilibrium coefficient. For the parameters used it can be seen that the compositions of the adsorbate phase and the fluid phase are very different. In a similar fashion, as the composition of the feed varies from  $A_1$  to  $A_2$  in Figure 2, the surface composition does not move along the axis  $A_4A_5$  in

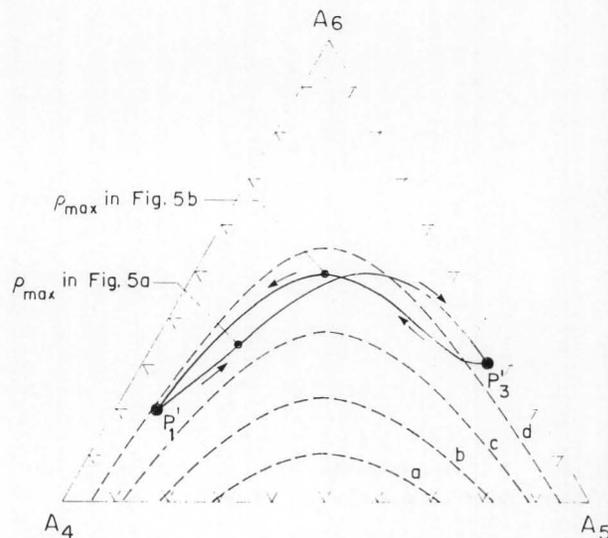


FIGURE 6. Transient of surface concentrations after step-change of feed composition as in Figure 5. Lines of constant normalized rate,  $\rho$  (dashed lines);

- (a)  $\rho = 0.8$  (b)  $\rho = 0.6$  (c)  $\rho = 0.4$  (d)  $\rho = 0.2$

Figure 3; instead, it follows a curved path given by the locus of the lowest points of the numbered lines in Figure 3 as discussed above.

Normally students conceive of reactions in terms of the microreversibility theorem and would assume that the reverse path following a reversal of the step-change would be the same as the forward path. Figures 5 and 6 show that this is not the case. Thus, microreversibility is inappropriate for describing surface concentrations in this and similar systems.

An exercise that students will find interesting is to calculate the surface composition for a non-reaction system and a reacting one even if the rate constants are very small. Will these compositions be identical?

## CONCLUSIONS

Triangular diagrams are useful for teaching steady-state and transient reactor behaviour of catalytic reaction models. Concentrations of surface species, not normally measurable, are particularly easy to reveal and to use to suggest interpretations of transient operation. Similar calculations can, of course, be performed for catalytic reactions with arbitrary mechanisms. In the example presented, the transient reactor behaviour was excited by the step-change of feed composition. Other types of steady-state feed disturbances (*e.g.*, sine, ramp, *etc.*) can be used after proper formulation of the initial conditions.

For systems having more than three components, appropriate subsystems of variables may be chosen. The main advantage of the triangular diagram lies in its power to compress into understandable form a great deal of information about the progress of gas and surface species in catalytic reaction. The FORTRAN programs used in this study are available from the authors.

## ACKNOWLEDGEMENTS

The authors are grateful for support through the Natural Sciences and Engineering Research Council of Canada in the form of an International Scientific Exchange Award (to K.K.) and an operating grant (to R.R.H.).

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## REVIEW: Transport Phenomena

Continued from page 175.

I would like to single out a few papers that are worth extended attention. The keynote lectures all fall into this class, although their coverage varies considerably. They do provide the reader a wealth of information gathered by the authors. In addition, on coherent structures, Blackwelder's short post-conference note is noteworthy. Criminale's contribution offers new insight. Other noteworthy contributions are by Walker and Herzog, and Nishino, *et al.* On wall shear flows, the contributions by Nagano and Tagawa, Usui and Sano, and Ueda *et al.*, should receive more than casual consideration. On free shear flows, I enjoyed reading contributions by Tabatabai *et al.*, Stapountzis, and Kobayashi *et al.* Since I have a special interest in scalar transport, I read all of these. My knowledge of modeling details is more limited; these papers appear to be of interest to one involved in transport modeling, a necessity in our modern engineering society. The numerical simulations of turbulence and transport is a new and budding field; thus contributions rapidly become dated. The two keynote lectures form a good starting place, and the general contributions add to them. Measuring techniques are varied and should receive the researcher's careful attention. The ideas advanced by Bawirzanski *et al.*, Ciccone *et al.*, Akino *et al.*, and Hardalupas *et al.*, are all worthwhile contributions. □

## BUOYANCY-INDUCED FLOWS AND TRANSPORT

by Benjamin Gebhart, Yogesh Jaluria, Roop L. Mahajan, and Bahgat Sammakia  
Hemisphere Publishing Corp., 79 Madison Ave., New York, NY 10016; 1001 pages, \$95 (cloth); 971 pages, \$49 (paperback); 1988

Reviewed by

J. S. Vrentas

The Pennsylvania State University

With seventeen chapters and more than nine hundred pages, this book deals with a wide range of buoyancy-induced flow problems. The analysis of steady and unsteady laminar external flows driven by both thermal and concentration effects is the focus of the first third of the book. Fluid property variations, turbulence, mixed convection, non-Newtonian effects, and the characteristics of instabilities are considered in subsequent chapters. Buoyancy-driven motions in fluid layers and in enclosures as well as natural convection in porous media are also discussed. Since problems are presented at the end of each chapter, this book can be used not only as a reference source but also as a textbook for a graduate specialty course. A significant part of the book could be covered in a one-semester course at the graduate level.

The authors present their analysis from an engineering perspective.  
Continued on page 193.

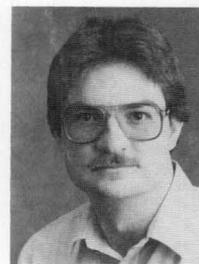
## BIOTECHNOLOGY LABORATORY METHODS

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**T**HE PAST TWO DECADES have seen tremendous growth and interest in biotechnology. As a result of recent advances in molecular biology and genetics, many new pharmaceutical, chemical, and agricultural products of microorganisms and cultured plant, animal, and insect cells are now available, or soon will be. The successful industrial-scale manufacture of these products will, in large part, depend upon new engineering initiatives in the development of high-rate bioreactors, efficient separation and purification techniques for bioproducts, and computer-interfaced instrumentation for optimal bioprocess control. These needs represent a major challenge to chemical engineering education—a challenge to provide students with appropriate training in both engineering and biology.

In order to help meet this challenge, many if not most chemical engineering departments now offer one or more elective courses in biochemical engineering, such as the course described by Bailey and Ollis [1]. In addition, interested students are encouraged to take technical electives from other departments in areas such as biochemistry, microbiology, and molecular biology. However, relatively few opportunities exist for these students to obtain direct laboratory experience in biotechnology methods, most likely because of the cost and effort associated with developing such opportunities. An exception is the biochemical engineering laboratory course described recently by Ng *et al.* [2]. At the University of Colorado, we have developed a course entitled “Biotechnology Labora-

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tory” which introduces the students to a variety of laboratory methods associated with biotechnology and yet which has required only limited resources.

### HISTORY OF THE COURSE

In the spring semester of 1984, our department initiated a lecture course entitled “Recent Advances in Biotechnology” [3]. This course, which is open to seniors and graduate students in both engineering and science, exposes the students to the many facets of biotechnology, including microbiology, molecular biology, biochemistry, biochemical engineering, and industrial applications. Guest lectures are given by faculty members from several disciplines and by local industry representatives. After our initial offering of this course, however, it became apparent that a laboratory component was an important missing ingredient.

In October of 1984, the five officers of our undergraduate Biomedical Engineering Society sent a memo to our then department chairman, Max Peters, stating:

At a recent BMES meeting, we discussed the possibility of the Chemical Engineering Department offering a “hands on” laboratory course for students who are planning careers in the biotechnology area. Although other departments offer

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laboratory courses in the bio area, there are no courses presently given that would fit the needs of an engineering student wishing to pursue a career in biotechnology.

We would like to suggest that the Department of Chemical Engineering offer a one hour credit optional laboratory course for students taking ChE 580, Recent Advances in Biotechnology . . .

In response to this request, Professors Robert Davis and Igor Gamow introduced a one credit hour course, "Biotechnology Laboratory," in the spring semester of 1985. The initial course offering was taken by 20 students—primarily undergraduates—and included experiments in microbiology, fermentation, genetic engineering, and ultrafiltration. With the aid of the latest addition to our faculty, Dhinakar Kompala, the course has been expanded to two credit hours. This expansion has led to a modest but welcome reduction in the class size. Unlike the associated lecture course, this laboratory course has been taken almost exclusively by chemical engineers. It is composed of graduating seniors who plan to attend graduate school or to work as biochemical engineers, and of graduate students who have chosen research projects in the biotechnology area.

#### COURSE CONTENT AND PHILOSOPHY

Experiments in biotechnology often require sophisticated equipment and can be quite expensive to undertake, and yet we were charged by our chairman to spend "a few thousand dollars at most" in developing this new laboratory course. Fortunately, we have been able to develop an effective course with available equipment in our undergraduate laboratory, borrowing of speciality items from our research laboratories, government surplus equipment, and a minimum of new purchases.

During the last few years, several new experiments have been introduced, and the original experi-

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ments have evolved with time. Our current repertoire of seven experiments is given in Table 1. Each year, typically four or five of these experiments are offered. Our philosophy is to choose the experiments to cover a spectrum of the subfields of biotechnology: microbiology, molecular biology, enzymology, microbial kinetics, biochemical reactor design, and bioseparations. A specific goal is to introduce the students to important laboratory methods such as sterile techniques, phenotype identification, fermentation, culture monitoring, electrophoresis, chromatography, ultrafiltration and microfiltration.

In order to maintain our original objective of providing each student with hands on experience in biotechnology, the experiments are performed by teams limited to four or five students. Since most of the tasks, such as plating cultures and taking and analyzing samples, are repeated many times during the course of an experiment, this requires that all of the students participate fully. The students receive grades based upon their participation and the brief reports which they prepare on the experiments.

Because of the diversity of experiments and methods involved, we have drawn on expertise outside of our department to assist with the experiments. Ray Fall from the Chemistry and Biochemistry Department at the University of Colorado has assisted with the recombinant DNA and molecular cloning experiments, Dale Gyure from Coors Biotech Products Company has assisted with the mass transfer and filtration experiments, and Geoff Slaff from Synergen has assisted with the chromatography experiments.

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**TABLE 1**  
**List of Experiments**

#### MICROBIOLOGY AND MOLECULAR BIOLOGY

- Recombinant Bacterial Growth and Instability
- Recombinant DNA and Molecular Cloning

#### KINETICS AND FERMENTATION

- Enzyme Kinetic Measurements
- Mass Transfer Coefficients in a Stirred Fermentor
- Yeast Growth Kinetics and Fermentation

#### DOWNSTREAM PROCESSING—BIOSEPARATIONS

- Microfiltration and Ultrafiltration
  - Column Chromatography
- 

#### EXPERIMENT SUMMARIES

##### Recombinant Bacterial Growth and Instability

The excitement and interest in modern biotechnology are primarily generated by the ability to produce foreign proteins through recombinant DNA technology. To familiarize our students with some characteristics associated with the cultures of recombinant organisms, we have designed this experiment involving simple shake flask batch cultures of recombinant bacteria *E. coli* (RR1/pBR322). The equipment items required are a spectrometer (visible range) and a

water bath shaker (see Table 2 for a list of our source and estimated new purchase price for each item). The materials required include shake flasks, petri dishes, media, culture stocks, pipets, and antibiotics (total estimated cost of \$50 per experiment).

Three shake flasks are prepared with appropriate media to culture the following: (i) plasmid-free host cells in M9 minimal medium (see Maniatis *et al.* [4] for media recipes); (ii) plasmid-bearing cells in M9 medium plus tetracycline, and (iii) plasmid-bearing cells in M9 medium with no antibiotics. By measuring optical density at regular intervals and plotting it versus time on a semi-log graph for the first two cultures, we determine  $\mu^-$  and  $\mu^+$ , the specific growth rates of plasmid-free and plasmid-bearing cells, respectively. For the third flask containing recombinant cells with no antibiotics, the fraction of cells containing the plasmids is also determined at two and five hours by plating the cells, after serial dilutions, on a petri dish containing a rich medium such as LB, and then replicating the grown colonies onto a dish with LB medium plus ampicillin, using a sterile nylon pad. The phenomenon of 'segregational instability' becomes obvious as the fraction of plasmid-carrying cells drops dramatically. Further, with all the measurements made here, plus the simple mathematic model proposed by Imanaka and Aiba [5] for the dynamics of these cultures, it is possible to estimate the average plasmid copy number for this host/plasmid system.

### Recombinant DNA and Molecular Cloning

This experiment is designed to familiarize the students with some of the basic recombinant DNA methods such as bacterial transformation with extra-chromosomal DNA, testing for gene expression, and restriction enzyme analysis. The equipment items required are a microcentrifuge, a small refrigerator, an incubator oven, and an electrophoresis unit. The materials required include culture stocks, media, plasmid stocks, petri dishes, restriction enzymes, pipets, antibiotics, microfuge tubes, and molecular weight markers (total estimated cost of \$75 per experiment).

In the first part of the experiment, *E. coli* HB101 cells are grown in a rich liquid medium, centrifuged, chilled, and subjected to calcium chloride shock, according to the detailed protocol by Maniatis *et al.* [4], to make them 'competent' for taking up plasmid DNA. About 5  $\mu$ L of pBR322 plasmid DNA at a concentration of 0.1 g/l is added to cold culture tubes containing 100  $\mu$ L of competent cells. After incubating for 30 min at 4°C, the tubes are kept at 42°C for 2 min and then incubated at 37°C for 30 min with addition of 1 ml of

**TABLE 2**  
**Major Equipment Needed**

ITEM	SOURCE	EST. PUR. PRICE
1. Spectrometer	Undergraduate Lab	\$ 800
2. Water Bath Shaker	Government Surplus	800
3. Microcentrifuge	Research Lab	1,300
4. Electrophoresis Unit	Research Lab	800
5. Refrigerator	Purchased	200
6. Incubator Oven	Government Surplus	200
7. Fermentor	Undergraduate Lab	12,000
8. Oxygen Electrode	Homemade	300
9. Chart Recorder	Undergraduate Lab	800
10. Microscope	Government Surplus	500
11. Plate-and-Frame Filter	Manufacturer Demo	1,500
12. Hollow-Fiber Filter	Purchased	600
13. Peristaltic Pump	Research Lab	400
14. Ultrafiltration Cell	Homemade	150
15. Magnetic Stirrer	Government Surplus	150
16. UV-vis Spectrophotometer	Research Lab	7,000
17. Chromatography Col.	Purchased	200

LB medium. Finally, these cells are plated on culture plates with and without ampicillin or tetracycline to determine the transformation efficiency, since the pBR322 plasmid contains genes that render the transformed cells resistant to these antibiotics.

In the second part of this experiment, two plasmids, pBR322 and pSY426, a poorly characterized recombinant plasmid derived from pBR322 and containing an extra piece of DNA encoding for  $\beta$ -glucosidase, are digested with the restriction endonucleases Eco RI, Sal I and Bam HI in single, double, and triple digests. These digests are loaded and run on agarose gel electrophoresis units, along with known molecular weight markers. From the size of fragments on the gel and the known map of pBR322, a partial restriction map of pSY426 is then constructed.

### Enzyme Kinetic Measurements

This experiment is designed to study the effects of competitive and non-competitive inhibitions, substrate and enzyme concentrations, thermal denaturation and pH on enzyme activity. The enzymes used are urease and amylase. These enzymes, their substrates, buffers, and other supplies may be obtained as an experimental enzymology kit from Carolina Biological Supply Company (estimated cost of \$50 per experiment). A detailed laboratory procedure manual

is supplied along with these materials, which we modified slightly to provide a more quantitative study of each effect.

Urease is used to study the effect of inhibitions and concentrations. Mixtures of urea and thiourea at four different relative concentrations are used to measure the effect of competitive inhibition. Potassium iodide is used to demonstrate non-competitive inhibition. The enzymatic reaction is conducted in one-half of a divided circular dish, supplied by the vendor. Gaseous ammonia produced by the reaction diffuses to the other half of the dish and changes an acidic dye solution to a basic solution with a change in color. The same reaction may also be conducted in the presence of the dye solution in either a test tube or a small shake flask. The time of reaction before the color change is noted and used as a quick measure of the inverse of enzymatic activity. Similarly, the enzymatic activity for different substrate and enzyme concentrations are measured. The effects of pH and thermal denaturation are measured on the amylase activity using iodine-potassium iodide drops to indicate the complete degradation of amylase.

#### Mass Transfer in a Stirred Fermentor

One of the most important control variables in an aerobic fermentation is the dissolved oxygen concentration. The purpose of this experiment is to determine the effects of aeration and agitation on the rate of oxygen mass transfer from air bubbles to the fermentation medium, as quantified by the so-called  $k_L a$  value [5]. The required equipment items for this exercise are a stirred vessel with an air supply (we used the fermentor described in the next experiment, although a homemade replacement could be made using a gallon jar and a motorized stirrer for about \$200), a rotameter for gas flowrate, a dissolved oxygen electrode, and a strip chart recorder. In addition, a half-full nitrogen tank with a regulator is required (approximate cost of \$15 per set of experiments).

The experimental procedure involves filling the vessel to its working volume with water or fermentation broth and then saturating the liquid with air. Once a steady electrode response is achieved, the air flow is suddenly replaced by nitrogen flow, which then strips the oxygen out of solution in a transient manner. From the decay characteristics of the voltage response of the probe, the corresponding  $k_L a$  value may be inferred [6]. This procedure is then repeated for each desired stir rate and gas flow rate. Conclusions may then be drawn regarding the relative influence of agitation and aeration in order to provide an adequate

dissolved oxygen supply for an actual fermentation.

#### Yeast Growth Kinetics and Fermentation

The goals of this experiment are to familiarize the students with the various steps involved in a typical fermentation run and to determine the fermentation characteristics of baker's yeast growing on carbohydrates with and without air. For this experiment, we have used an available twenty year old New Brunswick Scientific's Labroferm fermentor, which contains three 7-liter fermentation jars in a water bath. However, the less expensive alternative of three

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1-liter flasks on magnetic stirrers is equally appropriate (estimated cost of \$600). Other equipment items required for this experiment are a water-bath shaker, a spectrometer, and a microscope with a hemacytometer slide. Materials required include shake flasks, test tubes, pipets, media, baker's yeast, and enzyme assay kits (estimated cost of \$30 per experiment).

During the first class period, a rich medium containing yeast extract, malt extract, peptone, and glucose is made in three 250 ml flasks and sterilized in an autoclave. Using sterile techniques near a Bunsen burner or in a laminar flow hood, a previously grown inoculum is transferred into each of these flasks. The flasks are placed in a water bath shaker and allowed to grow overnight. Also using the previously cultured cells at various dilutions, a calibration curve is developed between the optical density measured with a spectrometer and the cell concentration measured with a hemacytometer. The three fermentor jars are filled with rich media and connected with tubing for air inlet, outlet, and culture sampling devices. In one of the jars, the 10 g/l of glucose in the rich medium is substituted with a mixture of glucose and fructose in the ratio of 1:4; in a second jar, the air inlet tube is clamped shut.

During the second class period, usually on a weekend morning, the three fermentors are inoculated with 100 ml of the cultures from the three small flasks freshly grown overnight. Samples are withdrawn every 30 min from each fermentor for measuring optical density. The experiment is continued for about 10-12 hours, until the optical density readings show no further increase. Occasionally, samples are

also collected for determining glucose and ethanol concentrations through enzymatic assay kits. Analysis of the data usually reveals a single growth phase in the fermentor with no air inlet, two growth phases in the fermentor with air and glucose as the only carbohydrate, and three growth phases with careful data collection in the other fermentor. Further analysis of the data, with a semilog graph of cell concentration versus time, will show identical specific growth rates during the first growth phases corresponding to the glucose fermentative pathway. The second and third growth phases will show decreasing growth rates.

### Microfiltration and Ultrafiltration

Downstream processing in order to recover and purify a fermentation product from dilute solution often represents the largest cost in a biotechnology process. This experiment, which is carried out in two separate parts, uses membrane filtration for cell and protein separations. In the first part, the yeast cells from the previous experiment are concentrated using both a hollow-fiber and a plate-and-frame tangential-flow microfilter. This requires the filters and housings, a peristaltic tubing pump, a 4-liter feed jar, a pressure gauge, a graduated cylinder, and a stop watch. The filter is operated in a batch concentration configuration where the permeate is removed and the retentate is recycled to the feed jar. The purpose is to measure the decline in permeate flux due to fouling of the membrane as the cell concentration in the feed increases. Other process variables that may be studied include the pressure drop across the membrane and the flow rate at which the suspension is circulated through the filter.

The second part of the experiment uses an ultrafiltration cell with an internal magnetic stir bar in order to separate two proteins, lysozyme (MW = 14,600) and bovine hemoglobin (MW = 64,000). A polymeric membrane with a specified molecular weight cutoff of 30,000 is used in the ultrafiltration cell. The proteins and disposable membranes cost approximately \$15 per experiment. The ultrafiltration is carried out at a constant transmembrane pressure drop (40 psig), and the permeate flux as a function of time is measured in order to determine the effects of membrane fouling and concentration polarization. Concentrations of the proteins in the initial sample and in the final filtrate and retentate are measured by UV-vis spectrophotometry (hemoglobin absorbs strongly at 400 nm and so may be measured in the visible range, whereas lysozyme requires a measurement at 280 nm in the ultraviolet range). These measurements are then used to determine rejection coeffi-

cients, which are important in scale-up calculations.

### Column Chromatography

Column chromatography is the predominant technique used in industry for purifying biological compounds such as proteins, nucleic acids, and antibiotics. The goal of this experiment is to expose the students to the fundamentals of chromatography, in general, and to the separation of proteins based on their relative sizes using gel filtration chromatography, in particular. Equipment items required for this lab are two plastic columns, a peristaltic tubing pump, and a UV spectrophotometer. The disposable materials include sephadex G-75 resin, two proteins of different molecular weight (we use cytochrome c with MW = 12,400 and ovalbumin with MW = 43,000), and blue dextran as a void volume indicator (estimated cost of \$40 per experiment).

During the lab, the students pack the columns with resin, load the columns with a mixture of the two proteins and the indicator, run the columns to separate the proteins, and collect frequent samples from the eluent streams. Total protein concentration in each sample is estimated by measuring the absorption in the ultraviolet range with the UV spectrophotometer. Two different sized columns are used to familiarize the students with the problems associated with scale-up. From the elution diagrams obtained, the students determine important parameters such as the distribution coefficient for each protein, the standard deviation of each of the elution peaks, and the resolution between the two peaks representing the larger and smaller proteins.

### CONCLUDING REMARKS

The biotechnology laboratory course at the University of Colorado has been maintained, and indeed has flourished, as a cooperative effort. The industry representatives have volunteered their assistance, the faculty members have participated in addition to their normal teaching responsibilities, and the students have elected to take the course above and beyond the normal requirements. Because of time requirements, the experiments have been carried out during evening and weekend hours. Nevertheless, all involved feel that it is a worthwhile effort.

Finally, we have not required a published laboratory manual, although several manuals describing many of the general procedures used are available [4, 7-9]. Instead, we have prepared a handout for each of the experiments. Single copies of a compilation of these handouts may be obtained free of charge from the authors.

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## FACULTY MOTIVATION

Continued from page 137.

tronic media (expert systems, video transmission, etc.) might be used to bring the most up-to-date technology and best practitioners within the reach of all interested engineering faculty.

## CONCLUSION

As Nehari and Bender [22] suggest, it is not just the transmission of information, but the transmission of meaning that is important to vital teaching. Education succeeds when the student becomes intrinsically motivated to acquire the learning, and to look upon the activity as an end in itself. A teacher who sets an excellent role model for the students, both in terms of personal enjoyment and intellectual curiosity, has a good chance to teach the students similar enjoyment.

Before we can consider environments for encouraging faculty, either as teachers or as researchers, we must consider faculty as individual human beings, with human characteristics. At most, this paper may be considered to provide some clues, based on a larger engineering/science faculty sample, concerning the developmental stages and motivation on the formation of an environment to encourage vital teaching.

Faculty see the opportunity and resources to improve their professional skills in somewhat the same light as unused computer availability; if opportunities

are made available in a non-threatening manner, the faculty will naturally seek and use them.

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# CHEMICAL ENGINEERING CURRICULA FOR THE FUTURE

*Synopsis of Proceedings of a U.S.-India Conference, January, 1988*

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**T**HE GOVERNMENT OF India is committed to rapid industrial growth in which new technologies hold a prominent role, and it shares common concerns at the educational level and on curricular matters with chemical engineers from the United States. A seminar was held at Bangalore, India, in January of 1988, to deliberate curricular changes in undergraduate chemical engineering in view of emerging technologies. The International Division of the National Science Foundation provided grants which enabled several American delegates from chemical industries and academia to attend the seminar, which was also attended by Indian delegates from both industry and academia.

The seminar approached the issue of chemical engineering education by organizing a first session of presentations by industrial and academic personnel on specific areas of technology. In a second session, delegates debated various aspects of the undergraduate curriculum, including basic science and core courses, chemical engineering courses, and electives. After completion of the formal presentations and the discussions, individual committees deliberated on each of the foregoing curriculum components to arrive at a consensus of specific recommendations for the academic communities in the United States and India. In addition, a panel composed of delegates from industry and academia debated "The Emerging Technologies and the Role of Chemical Engineering in Them" in an open forum.

The proceedings of the seminar have been compiled into a Report to the National Science Founda-

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**The government of India . . . shares common concerns at the educational level and on curricular matters with chemical engineers from the United States.**

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tion. The purpose of this summary is to provide a brief report on its results and recommendations.

## PERSPECTIVES ON EMERGING TECHNOLOGIES

The discussions on emerging areas of technology covered biotechnology, materials for structural, microelectronic, and catalytic applications, and new separations processes. In each of these areas, perspectives were presented by both industrial and academic personnel.

### Biotechnology

Stanley I. Proctor and Walter Bauer (Monsanto) presented the areas of opportunity in biotechnology. Five categories (human health care, animal science, crop science, waste management, and miscellaneous products) were presented as the main areas of opportunity. Dr. Proctor emphasized that most of the unit operations in bioprocesses are the same as those used in classical chemical engineering, but distinctive elements of bioprocessing include special needs for sterile operating conditions for bioreactors, stringent control requirements for maintaining living systems, sophisticated separation techniques for dilute systems, *etc.* Scale-up methods for equipment operated at laboratory scale, such as chromatographic columns (*e.g.*, for the separation of proteins), were emphasized. Dr. Proctor also addressed the special needs of biotechnology and concluded that the training of chemical engineers to work in biotechnology should be handled as an option to the traditional program. He pointed out that although the biotechnology industry is a significant employer, it is not viewed as a major employer.

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He also encouraged joint appointments of life science trained faculty in chemical engineering and life science departments.

George T. Tsao (Purdue University) provided an academic view of opportunities in biotechnology and identified five basic components of biotechnology processing: reactor engineering, separation, genetic engineering, analysis and characterization, and post-treatment. The development of a suitable methodology to deal with each requires a cooperative effort with personnel in biochemistry, molecular genetics, chemistry, and microbiology. Professor Tsao also focused on the variety of products (foodstuffs, health products, specialty substances, bulk chemicals, waste utilization) arising from biotechnology processing and outlined several research areas of interest to chemical engineers. He emphasized the need for more background in general biological sciences, along with elective courses in bioreaction engineering and bioseparation, and outlined some general guidelines for their contents.

#### Material Engineering and Technology

There were five presentations (two by industrial delegates and three by academic delegates), and the topics covered polymers and their processing, ceramics, catalysts, and microelectronic materials. Presentations varied between those focusing on a class of materials for different applications (such as polymers, ceramics, and composites) and those that were geared to specific applications (such as catalysts and microelectronic devices). Robert Laurence (University of Massachusetts) and Sheldon Isakoff (Du Pont) presented surveys of the first type, while Lanny Schmidt (University of Minnesota) addressed catalyst materials specifically, and V. R. Raju (Bell Laboratories) and Tim Anderson (University of Florida) focused on microelectronic materials.

*Polymeric and Ceramic Materials-Composites:* Professor Laurence provided an academic perspective on polymeric materials. He observed that the polymer industry, while maintaining its involvement with traditional commodity polymers such as polyolefins and PVC, has undergone a significant "restructuring" in its emphasis on new and advanced materials. In regard to newer applications he demanded broader understanding of polymer synthesis, electrochemical properties, morphology, and analytical methods. While the curriculum might include some in-depth courses in polymer science and engineering, he concluded that essential concepts of materials and polymers should also be incorporated in other core courses.

Dr. Isakoff focused mainly on structural materials. He covered the applications of various materials (advanced engineering plastics, structural composites, ceramic materials, *etc.*) and outlined the prevailing problems, avenues for their resolution, and areas where chemical engineers play a significant role. He stated that chemical engineers must be able to "speak the language" associated with advanced materials technology and believes this can be accomplished by offering special optional courses and minor specialization at the undergraduate level. He stated that examples from the new materials fields can be used in lectures, laboratories, and homework problems just as effectively as those from more conventional areas.

*Catalysis and Materials:* Professor Schmidt observed that the traditional scenario of "sequential" development of product-process combination in stages has given way to a situation requiring joint consideration of the entire process (reactor, catalyst, separations, feedstocks, by-products, and markets). A fundamental understanding of solid materials is necessary. He suggested that in order to understand the principles of crystal structure, phase behavior, electronic structure, and defects (all essential prerequisites to, and understanding of, catalysts), an introductory course in materials characterization techniques, such as X-ray diffraction, is necessary, and he pointed out that in pursuing the material aspects of catalysis one is concerned with issues very similar to those involved in processing procedures for microelectronic and ceramic materials.

*Microelectronic Materials:* Dr. Raju recounted chemical engineering principles encountered in the fabrication of optical fibers and integrated circuits, with special emphasis on the preparation of ultrapure glass preforms using the modified chemical vapor deposition process. He pointed out that the electronics industry uses a wide variety of processes (deposition, etching, diffusion, implantation, *etc.*) in which different types of chemical reactors are employed to carry out both homogeneous and heterogeneous reactions under precisely controlled conditions and that the necessary chemical engineering background has not been brought to bear on the optimal design of such chemical reactors. He also pointed to the need for an understanding of interfacial phenomena on a molecular level in developing processing techniques for manufacturing devices in which minute components are put together. Interfacial effects are extremely important in "thin film" deposition, controlled etching of microstructures, adhesive bonding, and in the realization of high performance organic materials as dielectrics in integrated circuits.

Tim Anderson presented an academic perspective of the opportunities for chemical engineers in electronic materials processing industries. He pointed out that these industries present many fundamental chemical engineering processes, with the major distinction between traditional chemical processing and EMP being the smallness of the scale of operation characterizing the latter. He outlined the various problems which can be tackled by chemical engineers, stressing that it is the unique coupling of process engineering with process chemistry that makes chemical engineering an integral part of electronic device manufacturing. He presented three different approaches for introducing electronic materials processing concepts to the undergraduate student and recounted in detail his experience with a specific senior elective course at the University of Florida.

#### **New Separations Processes**

E. N. Lightfoot (speaker) and M. C. M. Cockrem (both of the University of Wisconsin) presented an academic perspective on new separations processes. Using recovery from dilute solutions as an example, Professor Lightfoot illustrated the power of careful problem definition and application of transport phenomena in separations processes and equipment design. He pointed out that examination of crude economic data suggests that recovery of potentially valuable solutes from dilute solutions is dominated by the cost of processing large masses of unwanted material. This suggestion is confirmed by examination of the most widely used current processing techniques. He suggested a general strategy for reducing recovery costs.

Shivaji Sircar (Air Products and Chemicals, Inc.) concentrated on bulk separation of gas and liquid mixtures by adsorption and membrane technologies. He briefly described the process principles and their recent applications in the bulk separation of gas and liquid mixtures. In identifying research needs, Dr. Sircar pointed out that fundamental work towards understanding single and multicomponent fluid-solid adsorption interactions, both in terms of thermodynamic equilibria and interactive mass transport, was inadequate, and he added that some other areas in which fundamental work is needed include the transport of a fluid through solid membranes, durability of membranes under mechanical and thermal stresses, *etc.* He feels that the coverage of adsorption and membrane science technologies in texts on unit operations is inadequate and needs updating.

The foregoing presentations concluded the session in which specific technologies were discussed. Of par-

ticular interest in regard to education was the emphasis placed by several speakers on retaining the strong fundamental base of chemical engineering—some speakers warning against neglect of traditional areas and others warning against excessive introduction of technology at the expense of basic issues. The message came through that the problem is how to *enhance* the fundamental base of chemical engineering so that students will become literate in different areas of technology and be able to function efficiently in a multidisciplinary team of scientists and engineers.

#### **EVALUATION OF CURRENT CURRICULA**

In addressing the chemical engineering curriculum, four categories were identified: basic science courses, core courses, chemical engineering courses, and electives. Delegates from both sessions were present for the discussion, although the speakers in this session were entirely from academia.

##### **Basic Science Courses**

H. Ted Davis (University of Minnesota), J. M. Caruthers (Purdue University), and G. Padmanaban (Indian Institute of Science) covered different components of basic science requirements which are generally not covered in the present curricula.

Professor Davis made a strong plea for background in interface science and interfacial engineering, observing that the traditional background provided very little training in this area of increasing importance. He pointed out that interfacial processes impact a substantial part of a \$150 billion U.S. industry because of its concern with products affected by interfacial engineering. The mixing of water, oil, and surfactants under suitable conditions produces applications of interfacial engineering in biotechnology, microelectronic and ceramic materials processing, *etc.* Professor Davis strongly recommended an elective course on the fundamentals of colloid and interface science which could also be taken by graduate students seeking specialization in this area.

Professor Caruthers pointed out that chemical engineers have a special role to play in advanced materials where the molecular/microscopic structure, manufacturing process, and ultimate product performance are intimately related. He feels that all chemical engineering students must have some familiarity with the solid state, but he ruled out the elective approach and instead proposed a required course in materials science taught (say) in the sophomore year. He presented topics that could be covered in the course, placing emphasis away from metals.

**In addressing curricular changes, the diversity of existing curricula makes a universal formula impossible. The seminar was designed as an intellectual discourse on curricular changes in the hope of evolving some general guidelines.**

Professor Padmanaban addressed the issue of a life science background for chemical engineers and warned against adherence to engineering methodology without sensitivity to biological complexities. He proposed a life science package of twenty-five credits in biology courses in a four-year bachelor's degree program in biochemical engineering. Since this requirement (which he believes is essential for good biochemical engineers) may be oversized, he suggested pruning the requirement down to 8-10 credits in the BS program, deferring the rest to a master's degree in biochemical engineering. He feels that not all chemical engineering institutions need to offer such a program. He also argued for biology courses to be taught by biologists, with special books to be written to suit chemical engineers.

#### **Chemical Engineering Courses**

The chemical engineering courses that were discussed were: thermodynamics, transport processes, chemical reaction engineering, process design, and process control. Discussion centered around how these courses can be modified in the light of newer requirements.

*Thermodynamics:* M. S. Ananth (Indian Institute of Technology, Madras) discussed thermodynamics as taught to chemical engineers and presented the outline of a course at IIT, Madras, much of which is "conventional" by design. He stated that changes are needed in the type of examples used and cited several examples with applications in biology and biochemistry, and in fuel cells and thermochemical cycles, as new areas of concern. He also emphasized the importance of computers in the teaching of thermodynamics, citing their impact in solving complex problems.

*Transport Processes:* R. A. Brown (Massachusetts Institute of Technology) argued that the need for understanding of transport processes was greater than ever before because in the new areas of application the focus is on fine-scale structural and chemical features of the product, and complex transport processes abound in the processing of the materials. He observed that a transport course must impart an understanding of transport processes and must provide a basic grasp of the key techniques of analysis. He provided arguments that the separation of techniques for analysis from applications was not necessary and pre-

sented an advanced undergraduate/graduate-level course in "Analysis of Transport Processes" in which the major emphasis is on teaching basic concepts in heat, species, and momentum transport and on the techniques for closed-form analysis of these processes. He presented the topics in detail and pointed out that examples from a variety of application areas could be easily incorporated by using the experiences of the lecturer and through text sources from these areas.

*Process Control:* Thomas F. Edgar (University of Texas, Austin) reviewed the developments in process control instruction and presented an outline for revision. He pointed out that in the coming years a process control course should not only cover analog controllers and continuous systems, but should also expose the student to digital control and discrete systems concepts. Hands-on experience in distributed control with industrial grade equipment would be helpful, and the availability of computer-aided instruction software with graphics would greatly enhance teaching effectiveness. Such software could also expose the student to plantwide control concepts as opposed to analyzing only single loop systems.

Professor Edgar feels that a lack of fundamental understanding is preventing the development of closed-loop control strategies and mentioned two specific examples—one in solid-state device processing and the other in batch and fed-batch bioreactors. As improved understanding of such processes develops, it would be worthwhile to include examples built around them in the course on process control. Professor Edgar also presented an outline of a futuristic (in the year 2000) course on process control which focuses on discrete control systems concepts.

#### **Chemical Engineering Electives**

In addition to the elective courses discussed below, the course on interfacial science and engineering proposed by Professor Davis during the discussion on science courses, and the course in electronic material processing discussed by Professor Anderson in Session I must also be regarded as recommended electives.

*Biochemical Engineering:* H. C. Lim (University of California, Irvine) feels that the scientific base of chemical engineers must be broadened to include life sciences, and he pointed out that life science concepts can be incorporated into traditional courses (*i.e.*, one

can cover life science examples in a kinetics and reactor design course). He also asked that the undergraduate curriculum be flexible enough to allow specialization through carefully planned elective courses and that students opting for biochemical engineering be advised to take life science courses in their sophomore and junior years. He argued that with a strong life science background, the application-oriented courses can focus more on the engineering aspects of emerging technologies. He also feels the need for flexibility in the rules of accreditation in order to provide for more strength in life sciences and biochemical engineering.

*Polymer Science and Engineering:* S. K. Gupta (Indian Institute of Technology, Kanpur) observed that incorporating polymer background into the chemical engineering curricula has been slow. In discussing an elective course in polymer science and engineering, Professor Gupta asked for integration of the fundamental concepts from the polymer field into the core courses. He illustrated polymer topics that can be absorbed into the basic courses in chemistry (mechanics, thermodynamics, reaction and reactor engineering, transport phenomena, and process control and optimization), and he pointed out the scarcity of textbooks in this vein. He argues that many of the topics currently covered in polymer electives can actually be covered in the core courses, leaving newer material for an elective course. He outlined the contents of such a course, and although the list of topics is application-oriented, the treatment of the topics itself is fundamental. Heavy emphasis is placed on biopolymers, which he believes offer considerable scope for contributions by macromolecular engineers.

*Artificial Intelligence:* Venkat Venkatasubramanian (Purdue University) presented an elective course in artificial intelligence (AI). He argued that AI and knowledge-based systems provide an important framework for the modeling and solution of several classes of problems in process engineering, and he observed that training in these approaches will better prepare chemical engineers to cope with the demands and changes of the industrial environment. From his personal experience in teaching a course on AI, he feels that the proper way to educate students about AI is to teach it from a process engineering perspective. Students were taught the interdisciplinary area of AI and process engineering by using examples and exercises from process engineering. He feels that this approach is more appropriate and meaningful than learning from a computer science point of view. The lack of a suitable text will be remedied in the future by a series of monographs on AI in process engineer-

ing to be published by CACHE Corporation, an affiliate of the AIChE.

*Colloids and Interfaces:* R. Rajagopalan (University of Houston) presented an elective course in colloids and interfaces. He asked for integrating basic concepts of colloid and interface science into the core courses and listed several topics that could be included in material and energy balances, transport phenomena, thermodynamics, and separation processes. Although many examples from high technology were cited as motivation for the topics discussed, Professor Rajagopalan echoed the warnings of others that "high-tech" is not a panacea, stating that advances in high technology often cannot wait for systematic research while at the same time academic research and education cannot afford to keep switching directions based purely on the forces of the market.

### The Chemical Engineering Laboratory

M. M. Sharma (Bombay University) began with the observation that the conventional chemical engineering laboratory course does not realize its stated objectives. He discussed various remedial measures to correct this situation, including the use of large-size equipment, open-ended experiments, demonstration experiments, and equipment study experiments. He emphasized open-ended experiments and suggested a regular turn-over from a "bank" of experiments. He proposed the inclusion of an experimental design project in which the student would be required to suggest an aim, the equipment required, and the measurements to be made for achieving the aim. He also proposed demonstration experiments chosen to satisfy well-defined criteria.

### DISCUSSIONS AND RECOMMENDATIONS

Each presentation was followed by a discussion period in which all delegates participated, and committees were formed to discuss the various components of the chemical engineering curriculum. The chairmen of the individual committees then presented the committee recommendations to the entire group of delegates. An article by Watters, Laukhuf, and Plank (University of Louisville) has examined the committee recommendations in light of ABET requirements and has concluded that implementation is possible. Generally, the organizers feel that accreditation requirements must be softened to accommodate future curricular needs.

In addressing curricular changes, the diversity of existing curricula makes a universal formula impossible. The seminar was designed as an intellectual dis-

course on curricular changes in the light of emerging technologies, with the hope of evolving some general guidelines. The following sections outline those guidelines.

*Science Courses:* The science group, headed by Professor Davis, felt that the science core should be taught by scientists and that the chemical engineering faculty must persuade physical chemists and material scientists to include concepts and examples related to emerging technologies in the core courses. More specifically, examples must include solids, polymers, catalysts, interfaces, colloids, bioreactions, *etc.* They further recommended a course on computational methods after the completion of the core math courses, and that chemical engineering students be allowed to substitute one life science course for one core chemistry course (the most logical option being the second organic chemistry course). No changes were recommended for the physics courses.

*Engineering Core Courses:* This group, led by Professor Gandhi, outlined the topics to be dealt with in thermodynamics and transport processes. Although their outline showed no changes in the list of topics currently covered in chemical engineering curricula, they suggested that a special effort be made to include new examples from the emerging technologies. Another recommendation was to include discussion of the solid state with respect to deformation, transport of energy and mass, and chemical reaction, with examples of applications to the newer technologies of materials and microelectronic devices.

*Chemical Engineering Courses:* Arvind Varma (Notre Dame) headed the group which presented observations and recommendations on chemical engineering courses such as chemical reaction engineering, separations, design, control, and laboratory. The group stressed fundamentals with inclusion of examples from both traditional and emerging technologies. Since textbooks on the newer technologies are not yet available, they recommended that examples be commissioned and circulated to chemical engineering departments in a package. They encouraged the use of realistic problems, with liberal use of computer software focusing away from numerical methods. They also recommended that in addition to the two-semester laboratory course, demonstration experiments and video tapes should be used to firm up concepts and even to introduce new course material.

*Electives:* This group, headed by J. M. Caruthers (Purdue University), classified electives in the new technology areas as microelectronics, biochemical, interfacial, AI, and polymers, and in the traditional technology areas as environmental, petroleum, pro-

cess metallurgy, and food. A third category was termed "Advanced Core" and included transport, thermodynamics, optimization, and control. The group felt that electives in the new technologies should not eliminate electives in either the traditional technologies or the advanced core. They observed that it is not necessary for each department to offer a complete package in every area.

## CONCLUSIONS

The broad conclusions which can be drawn from this four-day seminar are:

1. Chemical engineering must retain its traditional interests, but at the same time must expand its fundamental base to include applications in the new areas of technology. In particular, background in states of matter other than the bulk fluid state (such as solids, thin films, interfaces, microstructured materials, *etc.*) was emphasized.

2. In view of the interdisciplinary nature of the newer areas and the essentially transient nature of technological developments, a fundamental background is necessary to provide a healthy appreciation of the issues involved in the new fields. Thus, chemical engineering expertise on process systems design in such areas must function within the framework of a collaborating team of scientists and engineers of various backgrounds.

3. Curricular modifications must entertain two elements. First, fundamental information must go into the science and engineering core courses, with examples to illustrate the new applications, and chemical engineering courses must be oriented similarly wherever possible (*e.g.*, chemical reaction engineering, separations, control). Second, more detailed involvement with the newer areas of technology must be accomplished through elective courses. □

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## REVIEW: Buoyancy

Continued from page 181.

neering science point of view. They focus on the formulation of appropriate forms of the transport equations in the boundary region and on the development of similarity or perturbation solutions. Hence, their book complements the book by Joseph (*Stability of Fluid Motions*) where more mathematical aspects of buoyancy-induced convection are discussed.

This book is clearly written and the material is presented in an orderly fashion. The book should serve as a valuable and comprehensive reference source for anyone interested in the engineering aspects of natural convection. Engineers and scientists doing research in this field will certainly want to own a copy of this book. □

## A CHEMICAL PLANT SAFETY AND HAZARD ANALYSIS COURSE

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- ***In January 1966, there was a major fire in LPG storage in Feyzin, France, that killed 17 people, injured 80, and caused extensive damage.***
- ***In June 1974, there was a major fire in the handling of cyclohexane at Flexborough that killed 28 people, injured 89, and caused extensive damage.***
- ***In July 1976, there was a massive release of extremely toxic dioxin produced in a runaway highly exothermic reaction that contaminated an area of 17.1 sq. km. and acquired global notoriety. (Dioxin did not directly kill any human being, but a chemist working near the reactor died due to falling masonry caused by the explosion.)***

If the impact of the above three (and other major) accidents of the 1960s and the 1970s had been what it *should* have been on public opinion, mass media, educators, the executive, legislative, and judiciary branches of governments worldwide, then the following probably would not have happened (or, so one wishes):

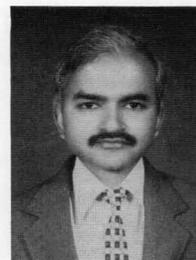
- ***In November 1984, there was a massive fire in LPG storage in Mexico City that killed over 500 people, injured 7231, and caused incalculable losses.***
- ***In December 1984, there was a tragic release of highly toxic methylisocyanate in Bhopal that killed at least 2500, injured over 200,000, and caused unimaginable human suffering for most of the survivors.***

(This is a very small listing of the process industry accidents taken from Marshall [1], which can be consulted for details of these and other major accidents.)

Everyone concerned has been aroused. The process industry can now be separated into two eras: Pre-

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Bhopal and Post-Bhopal. A strong case can now be made for teaching chemical engineering students about chemical plant safety and hazards in order to ensure that future engineers are aware of the importance of making safety a year-round practice in all spheres of their activities. With some variations, such courses should also be taught to students in other branches of engineering and the sciences.

While this article was under first review, two related articles appeared in *CEE* [17, 18]. This speaks volumes about the importance of this area.

### STARTING BLUES

Since it is a new area of study, most teachers did not have formal exposure to it during their own studies. Also, research activity in this area has been confined to a limited number of centers. Hence, initiating a safety course requires more than mere curiosity on the part of the instructor. It requires a deeply ingrained commitment. The small number of available texts, the lack of mathematical treatment starting with the fundamentals, the necessity of working with questionable probabilities of equipment failure and human error, the interplay of physical, medical, social, and political sciences, are enough to thwart any enthusiasm for the project. However, perseverance brings its own rewards. Unifying all the disciplines noted above in a manner never before possible in any course makes the effort worth-while (see Table 1).

A question that should be answered right at the

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beginning is: Should the safety and hazards aspects (1) be included as part of all the chemical engineering courses, or (2) be taught as a separate full course? The final choice depends upon the teaching philosophy of each department, but the following points should be considered.

The first approach has an advantage in that it can be coordinated with the rest of the course material. However, it would probably require deleting some other topics in order to accommodate several lectures (one or two lectures won't do), and since instructors are already hard-pressed for time, unwelcome compromises may have to be made. It would also necessitate that instructors self-learn the topic, and some instructors may only do lipservice. This would leave the students in even worse shape, erroneously thinking that they knew about safety and hazard analysis in all branches of chemical engineering (a tall order even for an expert). Inevitably, several important topics related to the transportation of hazardous materials, inspection and maintenance of plants, medical and toxicological aspects of dangerous chemicals, legal and social responsibility of plant managers, *etc.*, would not even be mentioned.

In the second alternative, teaching a separate full course, the above disadvantages would disappear, the course would be more coherent, and topics could be better coordinated. The lectures could be supplemented by specialists in specific disciplines, by case studies, films on safety aspects, *etc.*, and students could be encouraged to do term papers and to visit nearby industries to learn first-hand the steps taken by diverse industries for safe operation. At the end of the course, they would have had a finite exposure to safety and hazard analysis in the process industries that would not only make them better design engineers but would also improve their job and promotional avenues. Also, students from other disciplines such as mechanical engineering, industrial engineering, management, *etc.*, could enroll in the course. Hence, the second alternative appears to be better.

It should be realized at the very outset that the teaching of safety and hazard is different from teaching any other course. The students' ingrained attitudes, their thinking, and their approach to safety all need to be changed; human inertia has to be overcome; the viewpoint of "it has not happened thus far so it will never happen" has to be discarded. It takes as long to unlearn a wrong attitude as it does to learn a new one. Students should be taught that minor incidents are usually precursors of a major one. (There were several leaks of MIC at Bhopal which had adversely affected some of the workers, but which were ignored by the

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. . . research activity in this area has been confined to a limited number of centers. Hence, initiating a safety course requires more than mere curiosity on the part of the instructor. It requires a deeply ingrained commitment.

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**TABLE 1**  
**Disciplines Involved in**  
**Chemical Plant Safety and Hazard Analysis**

- **Physical Sciences (and Engineering)** • Chemical Kinetics; Thermodynamics; Chemistry; Equipment Design; Fabrication; Operation; Maintenance; Dispersion and Diffusion of Gases; Shock Waves; Combustion; Radiation; Corrosion; Fracture Mechanics; Transportation of Hazardous Materials; Environmental Pollution; Pressure Relief Devices; Instrumentation; Failure; Statistical Analysis; Hazard Analysis; Reliability and Failure Analysis; Personal Safety; Operator Training; *etc.*
- **Medical Sciences** • Effects of High Temperature Radiation on Human Body; Burn Treatment; Toxicity; Ingestion Through Skin; Lethal Doses; Industrial Hygiene; First Aid and Emergency Aid; *etc.*
- **Social Sciences** • Public Perception and Social Acceptance of Risk; Hazards *vs.* Industrial Progress (or Profits *vs.* Public Safety); Professional Ethics; Information Dissemination to Workers and Public; Legal Aspects; Tort Law; Emergency/Disaster Management Planning; Coordination with Civic Authorities; Educating Management; Risk Calculation; Insurance Premiums; Attitude to Safety; Human Error; Operator Reliability; Stress Factors; *etc.*

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plant authorities, local administration, and the national press.)

#### **COURSE DETAILS**

Our list of course topics is similar to that in both references [17, 18]. We also include a lot of case studies, and fortunately, the available literature is vast [2-6]. Students are assigned case studies to read at home, and then they must make brief presentations of the cases to the class. The causes and effects are discussed, and conclusions are drawn. This takes up the first eight to ten minutes of each lecture. Advantages of this approach are several:

- While reading one case, the student generally ends up reading several others from the related books and journals.
- Since the student has to present the material to the class, he tries to better understand it, and the chances of his learning more are increased. (All teachers already know this to be true.)
- The students get into a spirited (but guided) discussion about the causes, effects, and precautions to take, and this builds a receptive mood for the remaining forty-five minutes of the lecture hour.

Students are also encouraged to look for unsafe

situations in the home, the dormitory, on the road, in railway stations, hospitals, kitchens, laboratories, etc. These may be related to stair height, sharp corners on furniture, slippery floors, blind turns, identification of fire hazards, as well as insufficient light, escape routes, and/or first-aid facilities. Local industries such as urea manufacturers, LPG and industrial gas cylinder filling stations, tanning industries, and textile, woolen, and foot-wear mills are visited to see firsthand the safety measures, the procedures for hazard identification when making any changes in the process or piping, the emergency preparedness plans, and their liaison with the civic authorities. The city fire chief is invited to talk about the city's fire-fighting capabilities in case of a major fire in any industry.

Some term paper topics are listed in Table 2. Each topic is assigned to more than one student to work independently. This results in a little competition and

ensures deeper study. Students are also invited to suggest topics based upon their own experiences. They are required to present it to the class using overhead transparencies.

## CONCLUSIONS

The time has come when chemical plant safety and hazard analysis should be taught in classrooms. These topics have become too important to be left only to those who have learned it on the job or have taken some specialized training obtainable only at select places. The course proposed in this paper is but one step in the direction that academics should take. The author will be glad to provide a more detailed listing of the topics in Table 2 (some of which may also be included as lecture topics) and a longer list of references to anyone interested in starting a course and/or bringing their library up-to-date in these areas.

## ACKNOWLEDGEMENT

Thanks are due to Prof. Stuart W. Churchill, University of Pennsylvania, for his detailed review of the first draft of this paper from which this article has been adopted.

## REFERENCES

(The following is only a representative listing of important references. For a more complete list, write to the author.)

- | TABLE 2<br>Some Topics for Term Papers  |  |
|---|--|
| • Hazards in teaching labs (Unit Operations, Controls) and research labs in the department  |  |
| • Calculation of safe distance between two storage tanks taking into account the flammability and contents, size of storage tank, radiation intensity, ignition temperature, etc. |  |
| • Inventory of hazardous material in a distillation column depending on the type of trays used, and its effect on column sizing   |  |
| • Effect of shock or blast wave on columns, horizontal tanks, and their support structures  |  |
| • Comparison of safety and reliability in nuclear power plants vs. chemical process plants.   |  |
| • Computer program for HAZOP study of small set-ups   |  |
| • Computer program to calculate insurance premiums of plants allowing for penalties and reductions depending upon the actual plant layout vs. standard requirements               |  |
| • Accidents in transport of hazardous materials: types of accidents, causes, consequences, probability, emergency measures  |  |
| • Pressure relief devices: types, sizing, calibration, testing, reliability, detection of failure   |  |
| • Construction and location of control room, installation of instrument panels and alarms for easy visibility and access  |  |
| • Alarm systems: design, testing, reliability   |  |
| • Dispersion of toxic gases lighter/heavier than air and emergency procedures to tackle the situation   |  |
| • Automatic explosion suppression, flame arrestors: types, working principles, installation, reliability  |  |
| • Personal protection items under different hazardous situations  |  |
| • Classification and safe handling of combustible/flammable gases, liquids, and solids  |  |
| • Toxic effects on human body of various chemicals and dusts inhaled or ingested or received by skin contact  |  |

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# ***AUTHOR GUIDELINES***

This guide is offered to aid authors in preparing manuscripts for *Chemical Engineering Education (CEE)*, a quarterly journal published by the Chemical Engineering Division of the American Society for Engineering Education (ASEE).

*CEE* publishes papers in the broad field of chemical engineering education. Papers generally describe a course, a laboratory, a ChE department, a ChE educator, a ChE curriculum, research program, machine computation, special instructional programs, or give views and opinions on various topics of interest to the profession.

## *Specific suggestions on preparing papers.*

**TITLE** • Use specific and informative titles. They should be as brief as possible, consistent with the need for defining the subject area covered by the paper.

**AUTHORSHIP** • Be consistent in authorship designation. Use first name, second initial, and surname. Give complete mailing address of place where work was conducted. If current address is different, include it in a footnote on title page.

**TEXT** • Manuscripts of less than twelve double-spaced typewritten pages in length will be given priority over longer ones. Consult recent issues for general style. Assume your reader is not a novice in the field. Include only as much history as is needed to provide background for the particular material covered in your paper. Sectionalize the article and insert brief appropriate headings.

**TABLES** • Avoid tables and graphs which involve duplication or superfluous data. If you can use a graph, do not include a table. If the reader needs the table, omit the graph. Substitute a few typical results for lengthy tables when practical. Avoid computer printouts.

**NOMENCLATURE** • Follow nomenclature style of *Chemical Abstracts*; avoid trivial names. If trade names are used, define at point of first use. Trade names should carry an initial capital only, with no accompanying footnote. Use consistent units of measurement and give dimensions for all terms. Write all equations and formulas clearly, and number important equations consecutively.

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