Thomas F. Edgar
of the
University of Texas, Austin

AWARD LECTURE: Part 2 . . .
Computing in Engineering Education:
From There, To Here, To Where?
CARNAHAN

and . . .
Ideas About Curriculum
WOODS
Moments With Mathematica
BINOUS, McCoy
ChE Design: Problem-Solving Strategy
TURTON, BAILIE
Computer Control of a Distillation Experiment
LIRA
More Applied Math Problems on Vessel Draining
SOMMERFELD
Introducing High School Students and Science Teachers to ChE
BAYLES, AGUIRRE
Education in Process Synthesis: Application to Inorganic Processes
GUTIERREZ, GIMENEZ, AGUADO
Introducing Water-Treatment Subjects into ChE Education
CÁCERES, BRUTTNER, MONARDES, CONTRERAS, GÓMEZ-SILVA

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Winter, 1992
THOMAS F. EDGAR
of the
University of Texas at Austin

When Tom Edgar first joined the faculty at UT-Austin in 1971, he was given an excerpt from a 1966 speech by John McKetta, then Dean of Engineering, which summarized the expectations of a faculty member:

_He/she should expect to write proposals for research, equipment, and special projects; to publish articles, reports, papers, and books; to keep up-to-date in his/her profession field; to serve on councils, boards, and committees; to maintain the best possible relations with alumni, legislators, and the business and industry of the region—in short, to be a responsible member of the community and to participate in many of its activities. But we all know that these many activities must never overshadow our greatest concern—the student. If our responsibilities to, and concern for, the student ever become secondary, we will be violating the trust we accepted when we joined the faculty._

In his twenty years as a faculty member, Tom Edgar has pursued this creed, excelling in teaching, research, administration, and professional service.

The influences that shaped Tom's career began when he was a young boy growing up in Bartlesville, Oklahoma (which at that time probably had the highest number of chemical engineers per capita in the U.S.). His academic instincts were honed in the eighth grade when he won the Oklahoma Spelling Bee and received an all-expense paid trip to the National Spelling Bee in Washington, D.C. (this was his first national meeting!).

Then, when Sputnik was launched in 1959, thrusting America into the space race, the resulting heightened consciousness of science led Tom to begin dabbling in various technical fields. Encouraged by his father (a metallurgical engineer), his mother (a teacher and a housewife), and an older brother (an electrical engineer), he undertook several science-fair projects (including one on fuel cells) which whetted his appetite for science and engineering. As a high-school senior he won the Bartlesville Science Fair and a trip to the National Science Fair.

Becky, Jeff, Donna, and Tom on their favorite type of family vacation.
During his senior year, Tom's parents became concerned about his choice of a career, so he took a
battery of special aptitude tests. He scored high on
memorization and vocabulary (the spelling-bee in­
fluence!), but low on spatial reasoning—which indi­
cated he should not become an engineer. Perhaps
organic chemistry would be a good field....

But Tom ignored the aptitude-test results, and in
1963 he enrolled in chemical engineering at the
University of Kansas. He was influenced to con­
sider a research career in his second semester when
his audition for a part-time job to become a radio
announcer for a classical music station was un­
successful. Tom mentioned the audition to J.O.
Maloney, who promptly arranged for a lab-assistant
job with Russ Mesler making high-speed movies of
nucleate boiling.

At KU, Tom's only "B" was in transport phenom­
ena (darn that Bob Bird!); it is ironic that transport
was the first course he was assigned to teach at Texas. He became heavily involved in campus activi­
ties while at KU, which presaged the future level of
his professional service. Also of benefit were a num­
ber of summer jobs in industry and an NSF under­
graduate research project in process control.

Tom has fond memories of his first experience
with computer programming. The students in his
material and energy balance course were told to
write a computer program for flash vaporization (it­
erative calculation) within a two-week period of
time, and it was suggested that they could learn how
to write the computer program on their own. This
effectively forced Tom to learn how to use the com­
puter! The result was that computer decks took up
more than their share of his desk space during the
next ten years.

With this background, it was only natural for
Tom to study for the PhD under Leon Lapidus at
Princeton, who was probably the leading authority
on numerical analysis and optimal control at that
time. Since Tom had a NSF fellowship, Leon left him
alone to "do his thing," so in his free time Tom
became involved in several athletic clubs and eventu­
ally started as prop for the Princeton rugby team
for two years.

Tom's PhD dissertation dealt with the "minimum
time" control problem, which is consistent with his
mother's comment that he always wanted to be first
to finish any activity (unusual for a second child). He
managed to finish his PhD in the "minimum
time" (less than three years) even though he was
balancing child-care responsibilities (his wife Donna
was pursuing a Master's degree at Rutgers), athletic
pursuits, and research activities.

STARTING A CAREER

One of the worst times to graduate was in 1971—
there were probably only three or four academic
jobs available that year, and industry was not hir­
ing. As a college freshman, Tom had decided he
wanted to be a professor, so he was delighted when
the University of Texas offered him a faculty posi­
tion with a princely start-up package of $10,000. At
that time there was limited government research
funding (especially in control), few PhD students,
and a teaching load of four courses per year. Tom set
about to identify fundable projects where new mod­
eling and control techniques were needed to solve
the problems.

During the early 1970s, Tom decided to broaden
his background by exploring energy technology. He
was influenced by having an office next to John
McKetta, who was at the time gaining great atten­
tion for his views on the energy crisis. When Tom
came across an obscure reference to underground
coal gasification (UCG), he became interested in pur­
suing research on the problem. As he recalls, the
brief article stated that UCG was an economically
attractive synfuel alternative, especially for deeper
coal seams—but that a major difficulty existed in
that the process could not be controlled and was not
well understood. "A perfect application for modeling
and control," he thought. Since the State of Texas
was blessed with large reserves of deep lignite and
was accustomed to drilling for energy, Tom put to­
gether an interdisciplinary research project involv­
ing chemical, petroleum, and environmental engi­
neering, in addition to geology, which was funded by
NSF, DOE, and a ten-company consortium.

Tom's research in coal gasification and combus­
tion focused on developing fundamentally based
mathematical models in a field noted for empirical
approaches.

Tom's research in coal gasification and combus­
tion focused on developing fundamentally based
mathematical models in a field noted for empirical
approaches.
coal deposit for UCG. Mathematical models were verified in small-scale reactors, combustion tubes, and at the field scale. These techniques were used by several oil companies and by government laboratories and included computer models and experimental correlations for channel growth/sweep efficiency, product gas composition, gas-solid reaction characteristics, drying and mechanical properties, sulfur reactions, combustion tube tests, block gasification, flow characteristics, environmental impact, and technical and economic evaluation.

Many of these results, presented in some forty papers, have also been applied to conventional gasification and combustion processes. Of his papers on UCG, a 1978 *AIChE Journal* review article and a book chapter in *Chemistry of Coal Utilization* (1981), stand as key chemical engineering references in the field. Tom's research efforts were recognized by the AIChE Colburn Award in 1980; it was probably the only time this award has been given for "coal-burning."

While the UCG work focused heavily on modeling, Tom did not leave the control field during this period. His interests in multivariable control broadened to include adaptive control in the 1970s. In 1977, he received one of two best-paper awards at the Joint Automatic Control Conference. His 1981 work with a PhD student, Ernie Vogel, on an adaptive dead-time compensator solved a long-standing problem inherent in many chemical processes, and has been cited or used by a large number of subsequent investigators.

**PROFESSIONAL INVOLVEMENT**

Tom's leadership in professional activities began when he and another engineering faculty member founded the minority engineering program at UT-Austin in 1974. At that time there were few minorities in engineering and no engineering scholarships for economically disadvantaged students at Texas. Tom helped get the recruitment program started, established a tutoring program, raised $60,000 for scholarships from industry (a large sum in 1975!), and served as director for two years. After a successful start, the Equal Opportunity in Engineering Program now has the fifth largest number of minority students in engineering in the U.S.

Having learned how to balance a variety of outside activities with a heavy research and teaching load, Tom became active in a number of groups, including the CACHe Corporation, the AIChe CAST Division, and the American Automatic Control Council. He was selected by CACHe to edit the AICHEMI Modular Instruction Series in Process Control and an issue of *Computers and Chemical Engineering* on the "Application of Computer Graphics in Chemical Engineering." These modules are still being distributed by AIChE and have been important supplements to the standard textbooks for process control. Tom also worked with Duncan Mellichamp to develop the eight-volume CACHe Monograph Series in Real-Time Computing. His success in leading a variety of CACHe projects led the other CACHe trustees to elect him as Vice-President of CACHe in 1980 and as President from 1981-84, solidifying CACHe's financial base so the non-profit educational group could grow in influence during the 1980s.

Since 1981, Tom has served in a variety of positions in the AICHe CAST Division, and he thus provided important leadership as the division grew to the second largest division in AICHe. These offices included Director, Vice-Chairman, and Chairman (in 1986). For the past three years he has been the AICHe Council Liaison to the CAST Division, having been elected a Director of AICHe in 1988.

Since 1974, Tom has attended the interdiscipli-
Tom’s leadership in professional activities began when he and another engineering faculty member founded the minority engineering program at UT-Austin in 1974. At that time there were few minorities in engineering and no engineering scholarships for economically disadvantaged students at Texas.

nary American Control Conference every year and has seen it become the premier automatic control conference in the world during that time. His service activities in that organization include Arrangements Chairman (1974), Finance Chairman (1982), Program Chairman (1979), and General Chairman (1987). He was selected as Director (AIChE representative) of the American Automatic Control Council (AACC) in 1982 and in 1988 was elected by representatives of the six other sponsoring societies as Vice-President. He is just now finishing up a two-year term as President and is leaving AACC in excellent shape for the future.

Tom has also been a driving force behind the CPC (Chemical Process Control) series of conferences and co-chaired (with Dale Seborg) the second conference in 1981. He served on the organizing committee and as session chair in 1986 and 1991 and was also the 1991 conference manager for CACH (held at South Padre Island). Perhaps Tom is best remembered for his role as awards co-chairman in 1986 and 1991; CPC awards are like Harvard Lampoon awards and rely on a highly developed sense of humor.

During the 1980s, Tom also took on a variety of editorial board activities. He and other colleagues founded a new journal on subsurface processing in 1978 (In Situ, published by Marcel Dekker), and he served as General Editor until 1988. In addition, he has served on a variety of journal editorial boards including AIChE Journal, Computers and Chemical Engineering, Chemical Engineering Reviews, Journal of Process Control, and most recently as process-control editor of Chemical Engineering Education. He serves on the advisory board to the chemical engineering editor of John Wiley and Sons, and is also highly sought after as a program evaluator (Utah and Arizona State) and on departmental advisory committees (Kansas, MIT, and Maryland).

BOOK-WRITING

The decade of the 1980s also resulted in a flurry of books by Tom and his colleagues. In 1982 he had three book projects in progress. His first book, a professionally-oriented book on Coal Processing and Pollution Control, (Gulf Publishing, 1984), brought together a wide array of information on all aspects of coal utilization, covering extraction, conversion, and pollution control.

Tom taught an undergraduate elective course on optimization since 1972, and as a result joined with David Himmelblau to write Optimization of Chemical Processes (McGraw-Hill, 1988). This book continued the important role that UT-Austin has played in this area of chemical engineering, beginning with Beveridge and Schechter’s successful book (Optimization: Theory and Practice) in 1966. The recent textbook shows how the optimization field has matured in the past twenty years; its focus is on problem formulation (modeling) and it emphasizes only those optimization methods proven to be the best ones, while extensive coverage on various applications of optimization is also provided. Optimization of Chemical Processes is highly student-oriented in its presentation and sold nearly two thousand copies in its first year of publication.

Perhaps Tom’s best known book is Process Dynamics and Control, written with Dale Seborg and Duncan Mellichamp. This book had its origins in a five-day short course that Tom, Dale, and Duncan first gave at the University of California, Santa Barbara, in 1978. It had a very long gestation period due to extensive class-testing at ten universities (at various times) changes in process control technology, geographical separation, extensive revisions by each of the three authors, UCSB faculty governance assignments, building a house, etc (the excuses and accusations are endless). In the California "spirit," Dale’s philosophy was to "sell no wine before its time." Tom wrote most of the first drafts for the twenty-eight chapters, and Dale and Duncan then tore them to shreds (Tom’s version). In any event, the book (published by Wiley in 1989) has received excellent reviews and is now the number-one textbook on process control. It won the ASEE Meriam-Wiley Distinguished Author Award as the top new engineering textbook in 1990.

RECENT RESEARCH ACTIVITIES

In spite of his many outside activities and responsibilities as Chairman at Texas since 1985, Tom has managed to continue his strong research efforts
and is currently investigating modeling and control applied to such diverse areas as chemical reactors, distillation columns, pressure swing adsorption, and most recently, microelectronics manufacturing. While he was a "lone wolf" in his previous research efforts, alliances with his UT colleagues Jim Rawlings, Ike Trachtenberg, and David Himmelblau have permitted him to continue supervising a large number of graduate students. Tom still does much of the proposal and publication writing, and his students have learned to expect many corrections on their writing efforts. During his twenty-year career at Texas he has supervised forty-one MS and thirty-seven PhD students, which is due in part to his many good ideas and effective salesmanship techniques.

Tom's laboratories contain a wide array of highly instrumented equipment, always connected to some computer (PCs, workstations, commercial distributed control systems). Asked about recent technical achievements, Tom lists several examples:

- demonstrating high sensitivity of some nonlinear control schemes (with Chuck Alsop)
- developing theoretically-based criteria for measurement selection in distillation columns (with Wayne Bequette)
- developing a new computationally efficient scheme for using nonlinear programming to compute model-predictive controllers and demonstrating it on a packed distillation column and packed-bed chemical reactor (with Jim Rawlings, Ashu Patwardhan, John Eaton, and Glenn Wright)
- validating a fundamental reaction-transport model for a commercial multiwafer low pressure chemical vapor deposition reactor, the first highly documented modeling study on polysilicon in the industry (with Tom Badgwell and Ike Trachtenberg)

Over half of his current research group is focusing on the modeling and control of microelectronics processes, with support from NSF, the State of Texas, Sematech, Semiconductor Research Corporation, and Texas Instruments. Tom says the state of control technology in the microelectronics industry today is the same as it was for the chemical industry in 1970 and thus presents many opportunities to have an impact. His goal is to see model-based feedback control schemes (with Chuck Alsop)
- demonstrating high sensitivity of some nonlinear control schemes (with Chuck Alsop)
- developing theoretically-based criteria for measurement selection in distillation columns (with Wayne Bequette)
- developing a new computationally efficient scheme for using nonlinear programming to compute model-predictive controllers and demonstrating it on a packed distillation column and packed-bed chemical reactor (with Jim Rawlings, Ashu Patwardhan, John Eaton, and Glenn Wright)
- validating a fundamental reaction-transport model for a commercial multiwafer low pressure chemical vapor deposition reactor, the first highly documented modeling study on polysilicon in the industry (with Tom Badgwell and Ike Trachtenberg)

Tom also places a high priority on alumni relations and interactions with industrial supporters.

Consistent with his personal juggling act, Tom recognizes that the Department must have an atmosphere where good teaching and good research are valued, and where the students will receive a quality education. Evidence of this at Texas are the engineering teaching awards won by Presidential Young Investigators and the Outstanding AICHE Student Chapter Award in 1990 (the last time they won was when Tom was student chapter counselor in 1974). Tom also places a high priority on alumni relations and interactions with industrial supporters.

As Chairman, Tom spends a good part of his time in setting new directions for the department and in young faculty development. Adam Heller (who came to Austin in 1988 from Bell Labs) states, "Tom Edgar's leadership has allowed the Department to expand beyond its previous national strengths in polymers, separations, and process control into two new areas—microelectronics and biotechnology." Jeff Hubbell comments, "Tom Edgar spends considerable time so that young faculty have the opportunity to become successful."

His friend Bob Seader (at Utah) sums up Tom's impact on chemical engineering as follows: "Tom is one of the best known and most well-respected young engineering educators in the United States. During a period of twenty years, he seems to have had one major goal: to do everything he can do to advance his profession and to help others to best utilize these advancements. He is a tireless worker of almost unlimited energy, an inspiration to his many colleagues, and a servant to his profession."
EQUILIBRIUM THERMODYNAMICS—REVISITED

Dear Editor:

I am pleased that Williams and Glasser have outlined the course in thermodynamics that I introduced at the University of the Witwatersrand in 1982 and lectured there until the end of 1984. There are, however, a few points that I feel need clarification.

One reason for the difficulties students often encounter in thermodynamics is the confusion over variables and functions. One encounters references in the same context to $H$, $H(T,P)$, and $H(T,V)$, for example, in which the single symbol $H$ means at least three different things: e.g., a variable and two distinct functions.

An important objective of my approach is to attempt to overcome the confusion to which this symbolism gives rise. The symbol for any function is always constructed so that it explicitly displays the independent variables (as superscripts) and the dependent variable. Thus the function from T and P to H is written $H_{TP}$. On the other hand, the value of the function at T and P is written $H_{TP}(T,P)$. One can write

$$H = H_{TP}(T,P)$$

but not

$$H = H_{TP}$$

(at least for the present).

Williams and Glasser explain the symbolism and write statements like Eq. (1). However, they then apparently break the rules in a number of ways: a variable is equated to a function and not its value (e.g., $S = SV$ in their Eq. 19); the same symbol is used for a variable and a function (e.g., $V = V(S)$); they talk of "a new function $A = U - TS$"; etc. Having warned the reader of the importance of not confusing functions and values of functions, they do just that throughout both papers.

From the outset it is necessary to confine the use of the term function to things that are functions. A function always takes the form $H_{TP}$:

$$H_{TP}: T,P \rightarrow H$$

Then $A$ may be a variable, but it is certainly not a function. The term state function is not used—parameter or property is better.

If one has particular values for the independent variables, then one can write

$$H = H_{TP}(T_1,P_1)$$

for example. Very often one does not, in which case the presence of $T$ and $P$ twice in Eq. (1) may appear unnecessary. When the students have become familiar with the notation, and confident in its use, I draw attention to this apparent redundancy (if the students have not already done so). I then say that if the context makes clear that the value of the function is meant, we can agree, from now on, to an abbreviated notation: we may write $H_{TP}$ for $H_{TP}(T,P)$. The convention is that $H_{TP}$ always means the function unless the context shows that it must mean the value of the function. In the latter case, the $(T,P)$ is to be understood even though it is not explicitly displayed. Wherever there is any chance of confusion or doubt, $(T,P)$ is not to be omitted. Now, and only now, does it become legal to write such equations as Eq. (2) above and Eq. (19) of the paper by Williams and Glasser. I found it necessary to resort to the sort of fuss and circumspection resorted to here.

If we are taking care to distinguish functions and their values, we need to do so with derived functions or derivatives as well. Thus

$$\frac{\partial U_{SV}}{\partial S} \quad \text{or} \quad U_{SV}$$

is a derived function and

$$\frac{\partial U_{SV}}{\partial S} (S,V) \quad \text{or} \quad U_{SV} (S,V)$$

its value (the above convention still applying). It now becomes possible to agree with Eq. (18) of Williams and Glasser

$$T = U_{SV} = TSV$$

The context implies an abbreviation for

$$T = U_{SV} (S,V) = TS_{SV}$$

(5)

Williams and Glasser write (their Eq. 25)

$$\frac{\partial}{\partial S} \left( \frac{\partial U_{SV}}{\partial V} \right)$$

(6)

This violates the rules of notation just as much as

$$\frac{\partial P}{\partial S}$$

does. One needs to write

$$\frac{\partial}{\partial S} \left( \frac{\partial U_{SV}}{\partial V} \right)$$

(7)

Otherwise one has no means of distinguishing the expression from

$$\frac{\partial}{\partial S} \left( \frac{\partial U_{SV}}{\partial V} \right)$$

(8)

for example. While the order may normally be reversed with impunity in Eq. (7) (that is, when the superscripts repeat), it cannot in Eq. (8) (that is, when they do not). On the other hand

$$\frac{\partial^2 U_{SV}}{\partial S \partial V}$$

is unambiguous. There are hidden traps in Eq. (6) out of which I have rescued more than one student. Students easily obtain cross-differentiation identities that are simply not true.

My equation

$$\left. \frac{dH}{dT} \right|_{p=0} = \frac{\partial H_{TP}}{\partial T}$$

(9)

(Eq. 9 of Williams and Glasser) I have preferred since

Continued on page 29.
Mexico has been trying to improve her scientific programs and her industrial productivity ever since the heavy economic problems that were experienced in the 1980s. Industry presently faces an important transitional period from simple technology users to one in which indigenous resources must be used more intelligently and local processes must be more fully developed. To meet this challenge, Mexico needs qualified engineers.

The Instituto Tecnológico de Celaya, founded in 1958, is one of sixty technological institutes in Mexico, all part of a National System of Technological Institutes. The size of each institute has been kept under 3000 students. Celaya is a province of the state of Guanajuato and is located in the center of Mexico, about 150 miles northwest of the capital, Mexico City. The chemical engineering department in Celaya has been recognized as one of Mexico's most dynamic departments in recent years.

Traditionally, few universities in Mexico have had faculties with a complete or nearly complete staff of professors holding PhD degrees, due in part to a lack of available professionals at that level. In 1980 only one faculty member in Celaya held a PhD degree. Today, however, our faculty has expanded to include seven members with PhD degrees (see Table 1). The average age of the faculty is only thirty-seven, and their backgrounds include visiting appointments...
at places such as the Universities of Wisconsin, Texas at Austin, California at Davis, Texas A&M University, and CSIRO in Australia. We hope to establish a solid faculty by sending our professors abroad for further graduate studies in the future, and possibly by adding new members to the staff. Eight faculty members are currently involved in PhD studies (see Table 2), and our eventual goal is to have a staff of fifteen professors with PhD degrees by the mid-point of this decade.

THE UNDERGRADUATE PROGRAM

The undergraduate program began in 1961 and has grown to a current figure of 300 enrolled students (see Figure 1). Female students have been enrolling at higher rates in recent years; from six percent in 1980 to twenty-nine percent in 1989. About forty chemical engineers graduate each year from our program.

The undergraduate curricula comprise typical chemical engineering courses together with additional courses emphasizing industrial engineering. We try to give our students good exposure to laboratory activities, with the result that chemical engineering laboratory is used in three courses on unit operations in addition to one in kinetics and reactor design. The laboratory includes several units on a pilot-plant scale for operations such as distillation, absorption, extraction, evaporation, and drying. There are also sections for chemical reaction, solids treatment, and transport phenomena, and students must take two courses on analytical chemical analysis. Recently, we have also incorporated computer-aided techniques more significantly into our teaching.

THE GRADUATE PROGRAM

Our graduate program (one of the youngest in Mexico) began in 1980 and offered an MS degree in chemical engineering. Initially the MS program consisted of nine courses and a thesis project. There was a set of core courses on thermodynamics, applied mathematics, transport phenomena, reactor design, and separation processes. Elective courses included process design, process control, design of experiments,

---

**TABLE 1**

1991 ChE Faculty, Instituto Tecnológico de Celaya

- Rafael Chávez (PhD, University of Utah)
- Alejandro Gómez (PhD, University of Utah)
- Arturo Jiménez (PhD, University of Wisconsin)
- Gustavo Iglesias (PhD, Texas A&M University)
- Alberto Ochoa (PhD, University of California, Davis)
- Pedro Quintana (PhD, University of Texas, Austin)
- Antonio Rocha (PhD, University of Texas, Austin)
- María-Guadalupe Almanza (MS, Tecnológico de Celaya)
- Carlos Cárdenas (MS, Tecnológico de Celaya)
- Eleazar Escamilla (MS, Universidad de México)
- Teresa del Carmen Flores (MS, University of California)
- Irma-Concepción Galindo (MS, University of North Texas)
- Salvador León (MS, Portland State University)
- David Trigueros (MS, Tecnológico de Celaya)
- Ma. de los Angeles Vázquez (MS, Tecnológico de Monterrey)
- Angel Vázquez (MS, Tecnológico de Monterrey)
- Juan Ledesma (MS, Universidad de Guanajuato)
- Emma Torres (MS, Universidad de Guanajuato)

---

**TABLE 2**

ChE Faculty Currently Pursuing Ph.D. Degrees

<table>
<thead>
<tr>
<th>Professor</th>
<th>University</th>
<th>Year of Termination</th>
</tr>
</thead>
<tbody>
<tr>
<td>Francisco Javier Alvarado</td>
<td>Texas A &amp; M University</td>
<td>1992</td>
</tr>
<tr>
<td>Cristina Coronado</td>
<td>Universidad de Barcelona</td>
<td>1992</td>
</tr>
<tr>
<td>Guillermo González</td>
<td>University de Salamanca</td>
<td>1993</td>
</tr>
<tr>
<td>Gloria María Martínez</td>
<td>Universidad Autónoma Metropolitana</td>
<td>1992</td>
</tr>
<tr>
<td>Ramiro Rico</td>
<td>Princeton University</td>
<td>1993</td>
</tr>
<tr>
<td>Julio Rocha</td>
<td>Imperial College</td>
<td>1993</td>
</tr>
<tr>
<td>Fernando Tiscareño</td>
<td>University of Wisconsin</td>
<td>1992</td>
</tr>
<tr>
<td>Rodolfo Trejo</td>
<td>Universidad Autónoma Metropolitana</td>
<td>1992</td>
</tr>
</tbody>
</table>

**FIGURE 1. Students enrolled in B.S. program.**
An interesting and vital challenge for us is to offer a solid PhD program that emphasizes research activities of interest to Mexico while at the same time keeping the solid technical basis that characterizes many of the graduate programs in the first-world universities.

Operation of a double-effect evaporation system

and selected topics on thermodynamics and transport phenomena.

We revised our program in 1985, giving more emphasis to research by reducing the academic load by two elective courses. This change yielded positive results. It shows the history of admissions and graduating students for the Master's program and demonstrates that our graduating efficiency has improved significantly in the past few years. The low graduation rate noted in earlier years was not unique to our graduate program, but in fact has been a problem of major concern to most Mexican universities offering graduate programs in chemical engineering.

One system we have implemented for supervising our students' research progress is to assign a committee (in addition to the major advisor) from the beginning of the thesis project. At the end of each semester, the student must present a seminar before the committee, and based on the progress reported, a grade for the research work is assigned by the committee. The student also benefits from committee feedback at each step.

We have also made special efforts to recruit top students for our graduate program, and this fact accounts in part for our recent good results. Some of our MS graduates have gone for further PhD work at universities such as the University of Wisconsin, University of Texas at Austin, Texas A&M University, and Princeton University.

In Mexico, graduate programs offering PhD degrees are new and at present there are only three universities where one can be obtained. The Autonomous Metropolitan University (since 1984), the National Autonomous University of Mexico (since 1988), both located in Mexico City, and just recently, the Technological Institute of Celaya. It was not until 1991 that the first PhD degree was granted by the Autonomous Metropolitan University.

An interesting and vital challenge for us is to offer a solid PhD program that emphasizes research activities of interest to Mexico while at the same time keeping the solid technical basis that characterizes many of the graduate programs in the first-world universities. For this challenge to be successfully met, we must build a proper infrastructure for research activities.

RESEARCH ACTIVITIES

As a natural consequence of our pioneering efforts to establish a solid graduate program in Mexico, part of the job has been devoted to obtaining financial support for research activities, a task that has been complicated by the economic situation in our country. We have, however, made significant progress.

Until 1982, federal support for research activities was weak, but in spite of our economic problems the situation has improved steadily since then. For instance, CONACYT (the National Council for Science and Technology) initiated a special program (Programa de Apoyo al Posgrado) that offers support for improving the infrastructure at selected universities. Celaya has received support through this program since 1984, and as a result our computing and laboratory facilities have expanded significantly. Support for individual research projects has also been received from COSNET (the Council of the National System of Technological Education). The support from these two agencies has particularly influenced our growth.

Our research programs have centered on computer-aided design, experimental work on separation processes, process control, and production of specialty chemicals. The computing facilities in the department are based on a MicroVax II system, which is also used as a network server for twenty PCs. Some process simulators and software for process
control studies are available. To support experimental work, we have some of the newer analytical equipment such as GCs, atomic absorption, TGA, etc., along with the more conventional equipment.

Some major results of experimental work concerned two projects for the production of ferrous fumarate and oxalic acid. The work was undertaken due to an interest expressed by industry, and as a result there are now industrial plants for the production of these two specialty chemicals. The economic benefit for our institution and for the research team, however, has been marginal (a fact that has produced strong criticism from our politicians!). The experience has been part of a learning process for us.

These two projects are indicative of our efforts to bridge the traditional gap between academia and industry in our country. We have also provided services to industry in the form of instrumental analysis and other specific research projects. In addition (and taking into account our previous experience), we are exploring routes for the manufacture of specialty chemicals that are currently being imported by Mexico, and a multi-purpose pilot plant is nearing completion.

Celanese Mexicana has recently given additional scholarships for four graduate students who will develop their research projects on topics of general interest to the company.

OTHER ASPECTS AND OUTLOOK

Professor J.M. Smith (University of California, Davis) was associated with our graduate program between 1984 and 1987. He twice taught a graduate course on reactor design and helped conduct a research project on the thermodynamics of three-phase reactor systems. In our effort to stimulate excellence in the department, in 1984 we instituted the J.M. Smith award, given each year to the graduate student with the highest GPA. Seven students have received the award and four of them are presently pursuing the PhD degree.

A similar award, given in honor of Professor José Martínez-Avellá, one of the first lecturers in our institute, was instituted in 1989. The recipient of that award is the student graduating from our undergraduate program with the highest GPA.

In order to stimulate research activities, in 1984 the Mexican government established a National System of Investigators. Eleven professors from the Celaya department have been inducted into the system, the highest representation of any of the technical institutes in Mexico.

Each week a lecturer is invited to address the faculty and graduate students on some topic of interest. On occasion the speaker will be one of our own graduate students talking about his or her research project. These seminars have been held since 1980.

Each year for the past eleven years, we have organized a week of chemical engineering, the Seminario Anual de Ingeniería Química, an event that has now become a tradition in Mexico. The main part of the event is a series of courses given by recognized professionals from both Mexico and abroad to an audience of national professors, graduate students, and practitioner engineers. Among the past participants in this Seminario have been J. M. Smith, Octave Levenspiel, Charles Hill, Brice Carnahan, J. D. Seader, James Fair, Warren Stewart, Edwin Lightfoot, Carlos Smith, Richard Felder, Charles Holland, and George Stephanopoulos.

We also attempt to share nonacademic activities with our students. Thus, activities such as our "Thank God It's Friday" basketball games have become traditional events enjoyed by everyone.

Recent developments in Mexico seem to indicate that those who are in government positions are acquiring a better awareness of the importance of academic and research activities. Industry, too, is showing more interest in academia. Scholarship programs, such as CONACYT, are essential for providing greater numbers of qualified professionals who will be capable of meeting the challenges of the future.

Consolidating a modern chemical engineering program in Mexico will not be an easy task, but those of us at Celaya hope to take a leadership role in effecting the needed changes. □
MOMENTS WITH MATHEMATICA*

H. BINOUS, B.J. McCOY
University of California
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Mathematica, an interactive software system that does computer algebra and other mathematical computations, is a valuable tool for solving large problems involving symbol manipulation. Mathematica symbolically performs algebraic and calculus operations such as factorization, substitution, linear algebra, solution of polynomial equations, limits, and evaluation of integrals and derivatives. Numerical computations and visualization of advanced functions by two- or three-dimensional contour plots are also attractive features of the system. Although more efficient packages (e.g., Matlab) are available for large-scale numerical tasks such as matrix inversion, Mathematica can algebraically perform manipulations of this type. Many potential applications of computer algebra systems in chemical engineering research and education are possible to imagine, and in this article we discuss some examples.

The developer of Mathematica, Stephen Wolfram, is the author of a helpful manual called Mathematica: A System for Doing Mathematics by Computer (Addison-Wesley Publishing Company, 1988). The book is readable and readily understood by those with a general familiarity of mathematics and computers. Our experience is that studying the manual with the software at hand to work the numerous illustrations is helpful in learning the system. Operations with Mathematica can also be programmed (e.g., do-loops for iterative computations); see, for example, Programming in Mathematica.[1]

Several computer algebra systems are available on the market and promise to automate mathematical computations. Mathematica is particularly attractive because it can be installed in a desktop computer, although speed is compromised. In its workstation configuration, however, Mathematica is fast and user-friendly. Computer algebra systems probably will radically change problem solving in applied mathematics; tedious mathematical computations will be much less important than the fundamental problem formulation.

Opportunities are plentiful in chemical engineering research and teaching for the application of computerized symbolic manipulation. As an example of its use, we have applied Mathematica to the computation of moment expressions for several problems in separations and chemical reaction engineering.

MOMENTS IN CHEMICAL ENGINEERING

The computation of moments is useful for (1) interpreting experimental concentration profiles, (2) determining mass transport parameters from experimental data, (3) predicting concentration histories, and (4) designing and scaling-up separation processes.

The temporal moments are given by

\[ m_n(z) = (-1)^n \lim_{s \to 0} \frac{d^n}{ds^n} \int_0^\infty c(t, z) dt \]

(1)

where the Laplace transform of the concentration is defined by

\[ c(s, z) = \int_0^\infty c(t, z) e^{-st} dt \]

(2)

Numerical or analytical integration provides values or expressions for the moments when \( c(t, z) \) is known or when \( c(s, z) \) can be derived from a model of the concentration.

---

* Mathematica is a Trademark name owned by Wolfram Research Inc., PO Box 6059, Champaign, IL 61821-9902

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Housam Binous, born in Tunis in 1964, received a general engineering degree (with biotechnology electives) from the Ecole Nationale Superieure des Mines de Paris in 1988. He recently received his MS degree in chemical engineering from UC Davis. His research interests are in separation science and application of computer systems in engineering.

Ben McCoy received his BS in chemical engineering from the Illinois Institute of Technology (1963) and his MS and PhD from the University of Minnesota (1964, 1967). He has been at UC Davis since 1967, serving as Department Chair from 1980-88. He is currently Associate Dean for Research in the College of Engineering. His research interests are in chemical reaction engineering and separation processes.

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Chemical Engineering Education
process. Thus, we avoid inverting $\bar{c}$, a task that often is not feasible. The algebraic manipulations to obtain the moments from a mathematical model are:

1. solution of differential equations to determine $\bar{c}$
2. derivatives with respect to the Laplace transform parameter $s$
3. limits as $s \to 0$

The development of $\bar{c}$ in a series provides an easy way to find the lower-order moments. Expanding $e^{-x^2}$ in Eq. (2) leads to

$$c(s,z) = \sum_{n=0}^{\infty} s^n (-1)^n m_n(z) / n!$$  

(3)

The reduced moments are defined as

$$\mu'_n(z) = m_n / m_0$$  

(4)

and the central moments are given by

$$\mu_n(z) = \left(1 / m_0\right) \int_0^{\infty} (t - \mu'_1)^n c(t,z) \, dt$$  

(5)

The binomial expansion of Eq. (5), written in terms of the binomial coefficients, yields

$$\mu_n(z) = \left(1 / m_0\right) \sum_{i=0}^{n} \binom{n}{i} m_{n-i} (-\mu'_1)^i$$  

(6)

The first four moments have an important physical significance. The zeroth moment, $m_0$, is the area under the concentration plot $c(t)$ and is proportional to the mass of the species. The mass balance ensures that $m_n(z) = m_n(z=0)$ for species that do not react. The first reduced moment $\mu'_1$, is the position of the peak and gives the average position of the species. The second reduced central moment, $\mu'_2$, measures the spread of the peak. The third reduced central moment, $\mu'_3$, is a measure of the skewness of the peak.

For many cases, mathematical models provide the moment expressions in terms of mass transport parameters and geometric properties. From experimental methods, we obtain the concentration $c(t)$. Then the moments can be obtained by numerical integration using Eq. (1). Equating the experimentally determined moments to the moment expressions based on a model of the process represents a method for obtaining equations where the mass transport parameters are the unknowns. Schneider and Smith obtained estimates for the intraparticle diffusion, axial dispersion, and adsorption coefficients using this method. Mitchell used probabilistic arguments to obtain the spatial distribution, mean position, and variance about the mean of macromolecules moving in an external field and undergoing reversible isomerization. By comparing these results to experiments, the author was able to provide values for the forward and backward switching rates. The same problem was treated by Killalea and McCoy, who derived expressions of spatial moments.

The concentration profiles can be constructed using the moments in a Gram-Charlier expansion, i.e.,

$$c(t,z) = m_0 e^{-x^2} \sum_{n=0}^{\infty} a_n H_n(x)$$  

(7)

where

$$x = (t - \mu'_1) / \sqrt{2\mu_2}$$

Expressions of $a_0, a_1, a_2, a_3, \text{and } a_4$ are depicted in Table 1. The coefficients of the series, $a_n$, depend on the reduced central moments and are obtained using the orthogonality condition satisfied by the Hermite polynomials, $H_n$,

$$\int_{-\infty}^{+\infty} H_n(x) H_m(x) e^{-x^2} \, dx = 2^n n! \sqrt{\pi} \delta_{nm}$$  

(8)

where $e^{-x^2}$ is the weighting function. The first five Hermite polynomials are given in Table 1. This procedure is useful for predicting concentration profiles when values of the model parameters are known. Breakthrough curves for fixed-bed adsorbers and reactors can be represented using moments of the impulse response. As an alternative to Hermite polynomials, the Laguerre polynomials

<table>
<thead>
<tr>
<th>TABLE 1</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Hermite Polynomials and Coefficients of Gram-Charlier Expansion, Eq. (12)</strong></td>
</tr>
<tr>
<td>$H_0(x) = 1$</td>
</tr>
<tr>
<td>$H_1(x) = 2x$</td>
</tr>
<tr>
<td>$H_2(x) = 4x^2 - 2$</td>
</tr>
<tr>
<td>$H_3(x) = 8x^3 - 12x$</td>
</tr>
<tr>
<td>$H_4(x) = 16x^4 - 48x^2 + 12$</td>
</tr>
<tr>
<td>$a_0 = \sqrt{2\pi\mu_2}$</td>
</tr>
<tr>
<td>$a_1 = 0$</td>
</tr>
<tr>
<td>$a_2 = 0$</td>
</tr>
<tr>
<td>$a_3 = \mu_3 / (3!2\sqrt{2\pi\mu_2})$</td>
</tr>
<tr>
<td>$a_4 = \left(\mu_4 / \mu_2^2 - 3\right) / (4!4\sqrt{2\pi\mu_2})$</td>
</tr>
<tr>
<td>Winter, 1992</td>
</tr>
</tbody>
</table>

For many cases, mathematical models provide the moment expressions in terms of mass transport parameters and geometric properties. From experimental methods, we obtain the concentration $c(t)$. Then the moments can be obtained by numerical integration...
are frequently used.\(^7\)

Mehta, et al.,\(^8\) were able to obtain agreement between experimental elution curves and Hermite polynomial series representation. In addition, fitting the two results provided a criterion for the trimming of tails and leading edges. Thus, it is possible to account for phenomena such as end effects. Elution curves in chromatographic columns are nearly Gaussian when dispersion is small relative to convection. For such cases, the first term in the series, the Gaussian approximation, will provide an accurate representation of the pulse.

Chromatography, a widely used separation process, utilizes differences in species behavior, e.g., solid-fluid adsorption, to effect the separation. Reliable ways that make use of the moment theory to analyze and optimize chromatographic separations have been developed. For two solutes A and B, separation is usually satisfactory when

\[
R_{s} = \left| \mu_{1A}^2 - \mu_{1B}^2 \right| / \left( \sqrt{\mu_{2A}^2 + \mu_{2B}^2} \right) > 2
\]  

(9)

The resolution, \(R_s\), provides a criterion for separation of two species when narrow pulses are injected. We can define the Height Equivalent to a Theoretical Plate concept by

\[
\text{HETP} = \frac{L}{\mu_{2}^2 / \mu_{1}^2}
\]  

(10)

Contrary to \(R_s\), HETP depends only on one input sample size and is an important characteristic for evaluating chromatographic processes.

**EXAMPLE PROBLEMS**

To illustrate how Mathematica can be used to assist in finding moment expressions for problems of interest to chemical engineers, we discuss three examples. A list of essential commands to solve these problems is available from the authors.

### Fluid-Solid Adsorption and Reaction in a CSTR

We consider a continuous-flow stirred tank reactor (CSTR) fed with an input pulse of adsorbable species. As a representation of a catalytic reaction, the adsorbed molecules undergo a reaction that is assumed first-order in the adsorbate concentration. The Laplace transform of \(c(t)\), \(\tilde{c}(s)\), is readily found from the governing equations listed below.

- **Mass balance in the fluid**
  \[
  \varepsilon \frac{\partial \tilde{c}}{\partial t} = \theta (c_0 - c) - A_p k_p \left( c - c_i(R) \right)
  \]  
  (11)

- **Mass balance on an individual particle**
  \[
  \frac{\partial \tilde{c}_i}{\partial t} = \left( D_i / r^2 \right) \frac{\partial^2 \tilde{c}_i}{\partial r^2} - r \frac{k_{ads} c_i + k_d c_a}{D_i}
  \]  
  (12)

- **Reversible adsorption with first-order surface reaction**
  \[
  \frac{\partial c_a}{\partial t} = k_{ads} c_i - k_{d} c_a - k_{r} c_a
  \]  
  (13)

  - **Initial conditions**
    \( c = c_i = c_a = 0 \) for \( t = 0 \)
    (14)

  - **Boundary conditions**
    \( (\partial c_i / \partial r)_{r=0} = 0 \) and \( D_i (\partial c_i / \partial r)_{r=R} = k_{r} (c - c_i)_{r=R} \)
    (15)

- **The inlet concentration is considered an impulse**

### Table 2

The Laplace Transform and Temporal Moments for Fluid-Solid Adsorption and Reaction in a CSTR

\[
\begin{align*}
\tilde{c}(s) &= \frac{c_0}{\varepsilon s + \theta + A_p k_p - R A_p k_p^2 / \left( D_i [b R \coth(b R) + k_p R / D_i - 1] \right)} \\
b &= \frac{8 s + k_{ads} - k_{d} k_d}{D_i} \\
m_0 &= \frac{\theta c_0}{\psi} \\
v &= b R \coth(b R) + k_p R / D_i - 1 \\
\psi &= \theta + A_p k_p - R A_p k_p^2 / (D_i \nu) \\
m_0 &= \frac{c + R A_p k_p R \coth(b R) + R^2 \xi^2 \left( 1 - \coth^2(b R) \right)}{2 D_i b_0} / (D_i \nu^2) \\
\xi &= \beta + k_{ads} k_d / \left( k_r + k_d \right)^2 \\
m_1 &= \frac{20 \xi c_0}{\psi^3} \left( \varepsilon + R A_p k_p \frac{R \xi \coth(b R) + R^2 \xi^2 \left( 1 - \coth^2(b R) \right)}{2 D_i b_0} / \left( b_0 \nu^2 \right) \right) / \left( D_i \nu^2 \right) \\
\nu &= \frac{4 \theta c_0}{\psi^2 D_i \nu^2} \left( \xi \coth(b R) + R \xi \left( 1 - \coth^2(b R) \right) \right) / \left( 4 D_i^2 b_0 \right) \\
&= \frac{6 \xi c_0 R A_p k_p}{\psi^2 D_i \nu^2} \left( \frac{R \xi \coth(b R) + R^2 \xi^2 \left( 1 - \coth^2(b R) \right)}{2 D_i b_0} / \left( D_i \nu^2 \right) \right) / \left( D_i \nu^2 \right) \\
&= \frac{6 \xi c_0 R A_p k_p}{\psi^2 D_i \nu^2} \left( \frac{R \xi \coth(b R) + R^2 \xi^2 \left( 1 - \coth^2(b R) \right)}{4 D_i^2 b_0} / \left( D_i \nu^2 \right) \right)
\end{align*}
\]  

(2-1)

(2-2)

(2-3)

(2-4)

(2-5)

(2-6)

(2-7)

(2-8)

(2-9)
The complex nature of the expression for \( c(s) \), determined from the Laplace transformed solution of Eqs. (11) to (16), makes using Mathematica to compute \( m_0 \), \( \mu'_1 \), and \( \mu_2 \) very attractive. We provide expressions for \( c(s) \), and for \( m_0 \), \( m_1 \), and \( m_2 \) in Table 2.

### Chromatographic Separation Based on Fluid-Solid Adsorption

Let us consider separation processes based on fluid-solid adsorption such as the adsorption of hydrocarbons on silica gel in a chromatographic column.\(^{12}\) The concentration of adsorbing gas, \( c(z,t) \), is the solution of the following equations:

- **Mass balance of adsorbable component in the gas phase**
  \[
  (E_{A}/\alpha)\frac{\partial^2 c}{\partial z^2} - \nu \frac{\partial c}{\partial z} - \frac{\partial c}{\partial t} - 3D_1 (1-\alpha)/(R\alpha \left( \frac{\partial c}{\partial t} \right)_{r=R}) = 0
  \]  
  \[(17)\]

- **Mass balance of adsorbable component in the particle**
  \[
  \left( \frac{D}{\beta} \right) \left( \frac{\partial^2 c}{\partial r^2} + \frac{2r}{\beta} \frac{\partial c}{\partial r} - \frac{\partial c}{\partial t} - \left( \frac{\beta_p}{\beta} \right) \frac{\partial c_{ads}}{\partial t} \right) = 0
  \]  
  \[(18)\]

- **Linear rate of adsorption**
  \[
  \frac{\partial c_{ads}}{\partial t} = k_{ads} (c_i - c_{ads})/K_A
  \]  
  \[(19)\]

- **Boundary conditions**

<table>
<thead>
<tr>
<th>TABLE 3</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>The Laplace Transform and Temporal Moments for Chromatographic Separation Based on Fluid-Solid Adsorption</strong></td>
</tr>
<tr>
<td>( c(s,z) = (c_0 /\alpha) \left( 1 - e^{-s\theta_0A} \right) e^{-\gamma s} )</td>
</tr>
<tr>
<td>( \gamma = -\left( \nu \alpha /2E_A \right) + \left( \nu \alpha /2E_A \right)^2 + (s\alpha /E_A)(1+h(s)) )</td>
</tr>
<tr>
<td>( h(s) = (3k_f /R)\left( (1-\alpha)/\alpha \right) \left[ \left( (sD_1/k_f) \right)^1 \tan \left( R \lambda \right) + s(1-D_1 /k_f) \right] )</td>
</tr>
<tr>
<td>( \lambda = (s\beta /D) \left( (1+P_F K_A k_{nds}) / (\beta K_A s + K_P k_{nds}) \right) )</td>
</tr>
<tr>
<td>( m_{00} = m_0(z=0) )</td>
</tr>
<tr>
<td>( \mu'_1(z=0) + \mu'_2(z=0) )</td>
</tr>
<tr>
<td>( \mu_2 = (2s\nu /\beta) \delta_0 + (E_{A} /\alpha)(1+\delta_0)^2 / (1+\nu^2) + \mu_2(z=0) )</td>
</tr>
<tr>
<td>( \delta_0 = \left( (1-\alpha)h /\alpha \right) \left[ \left( K_A P_f /\beta \right) \right] )</td>
</tr>
<tr>
<td>( \delta_1 = \left( (1-\alpha)h /\alpha \right) \left[ \left( R \beta^2 /15 \right) \left( 1+P_F K_A /\beta \right)^2 \right] )</td>
</tr>
</tbody>
</table>

When \( c_0(t=0) = c_0 \) for \( 0 \leq t \leq t_0A \), we have the following results:

| \( m_{00} = c_0 t_0A \) |
| \( \mu'_1(z=0) = t_0A /2 \) |
| \( \mu_2(z=0) = t_0A^2 /12 \) |

Finally, we are able to compute the derivatives of \( c(s,z) \) and obtain \( \mu'_1 \), and \( \mu_2 \). Unfortunately, rearranging the result into a neat form requires human judgement and is not convenient with Mathematica. However, this task is readily performed by hand.

### Spatial Moments of Moving and Interchanging Isomers

We are interested in finding the spatial moments of two isomers \( A_i \) and \( A_i' \), which are moving, and switching back and forth between the two isometric states as a first-order reaction. This system describes electrophoresis, gel filtration, or sedimentation if the species are moving respectively in an electrostatic, velocity, or centrifugal field. The system is a type of chromatographic reactor.

The governing equations of the concentration are...
\[
\begin{align*}
\frac{\partial c_1}{\partial t} &= D_1 \frac{\partial^2 c_1}{\partial x^2} - v_1 \frac{\partial c_1}{\partial x} - k_1 c_1 + k_2 c_2 \\
\frac{\partial c_2}{\partial t} &= D_2 \frac{\partial^2 c_2}{\partial x^2} - v_2 \frac{\partial c_2}{\partial x} - k_2 c_2 + k_1 c_1
\end{align*}
\] (24)

where \(D_1\) is the diffusion of axial dispersion coefficient, \(v_i\) is the species velocity, and \(k_i\) is the rate constant for isomerization.

- The boundary conditions are \(c_j(t, x = \pm \infty) = 0\) for \(j=1\) and 2 (25)
- The initial conditions are infinitesimally narrow distributions \(c_j(t = 0, x) = \delta(x)\) for \(j=1\) and 2 (26) with the total initial concentration given by \(f_1 + f_2 = 1\).

Mathematica provides (a) the Fourier transform of \(c_j(x, t)\) defined by
\[
\tilde{c}_j(k, t) = \int_{-\infty}^{\infty} c_j(x, t) e^{-ikx} \, dx
\] (27)

and (b) the limits of the successive derivatives of \(\tilde{c}_j\).

In terms of \(c(x, t)\) and \(\tilde{c}_j(k, t)\), the \(n^{th}\) spatial moment of species \(A_j\) is given by
\[
m_{n,j}(t) = \int_{-\infty}^{+\infty} c_j(x, t) x^n \, dx = (i)^n \lim_{k \to 0} \frac{\partial^n \tilde{c}_j(k, t)}{\partial k^n}
\] (28)

Thus we are able to compute expressions for \(m_{01}, m_{11}\), and \(m_{22}\) (see Table 4). Similar results were presented by Killalea and McCoy \(41\) and can be used to construct the concentration profiles as explained in section 1.3. Mathematica can handle readily such algebraic calculations.

**Isomerization in a Countercurrent Chromatographic Reactor**

Based on the movement in opposite directions of a sorbent and a fluid, a countercurrent chromatographic reactor can carry out separation and reaction simultaneously. This can push to completion a reaction limited by equilibrium. Thus, such a device can enhance the conversion of the product in reversible reactions of type \(A_1 \rightleftharpoons A_2\). Experimental investigation of such a system was provided by Takeuchi, \textit{et al.}, \(11\) who studied xylene isomerization.

The governing equations are given by a special form of Eq. (24)
\[
\begin{align*}
-u_1 \frac{dc_1}{dx} - k_1 c_1 + k_2 c_2 &= 0 \\
u_2 \frac{dc_2}{dx} + k_1 c_1 - k_2 c_2 &= 0
\end{align*}
\] (29)

where \(u_1 = u - v_1 K_1\) and \(u_2 = u - v_2 K_2\).

We have made the following assumptions: (1) steady state, (2) adsorption equilibrium, (3) no axial dispersion, (4) linear adsorption isotherm, (5) isothermal operation, (6) first-order reversible reactions, and (7) constant linear velocities.

The solid adsorbent, moving countercurrently to the fluid at velocity \(u_1\), carries the adsorbates \(A_1\) and \(A_2\), which have adsorption equilibrium \(K_1\) and \(K_2\). We select the feed, sorbent, and species velocities in such a way that (1) \(A_1\) is continuously fed at the bottom of the reactor, (2) sorbent is supplied at the top of the reactor, (3) \(A_1\) is less strongly adsorbed than \(A_2\), (4) \(A_1\) is moving upward with the fluid and \(A_2\) is transported downward by the sorbent, and (5) \(A_1\) is completely converted in the reactor and the exiting stream is free of \(A_2\). Thus, the boundary conditions are
The concentrations present discontinuities at the inlet and outlet of the reactor. The flux conservation equations provide values for these jumps.

\[
\begin{aligned}
    c_1(L^+) &= c_{10} \\
    c_2(L^-) &= 0 \\
    c_1(L^+) &= c_1(L^-)u_1/u \\
    c_2(0^-) &= -c_2(0^+)u_2/u_s
\end{aligned}
\]  

(31)

Expressions for the concentrations \( c_1 \) and \( c_2 \) are depicted in Table 5. With Mathematica, one can first find these expressions, then perform numerical simulations, and finally plot the results.

**CONCLUSIONS**

We have described the computation of expressions of moments using Mathematica for chemical reaction or separation processes. These computations are exceedingly tedious to perform and to confirm when done by hand. Mathematica is an interesting tool for solving problems with algebraic manipulations because it is user-friendly, powerful, and fast. This is particularly true when the software is run on a Unix machine rather than a smaller, slower personal computer. It should be clear that Mathematica has limitations, some of which can be overcome by skillful organizing of the computational steps. The numerical, graphic, and programming capabilities of Mathematica are exciting potentials that can be applied in multiple areas of chemical engineering.

**NOMENCLATURE**

- \( \alpha \) = interparticle void fraction in the adsorbent bed
- \( A_p = 3 n_p / \rho_p \)
- \( \beta \) = interparticle void fraction (internal porosity) of the adsorbent
- \( c \) = concentration of the adsorbable fluid in the adsorbent
- \( c_0 \) = input concentration of the adsorbable fluid
- \( c_1, c_2 \) = concentration of species \( A_1, A_2 \)
- \( c_{ads} \) = concentration of the adsorbed fluid
- \( \delta_0, \delta_1 \) = defined by Eqs. (3-8) and (3-9)
- \( D_{1,2} \) = diffusion or axial dispersion coefficient of species \( A_1, A_2 \)
- \( D_i \) = effective intraparticle diffusion coefficient
- \( \varepsilon = 1 - n/\rho_p \)
- \( E_A \) = effective axial dispersion coefficient
- \( f_1, f_2 \) = rate constant of species \( A_1, A_2 \)
- \( \gamma \) = defined by Eq. (3-2)
- \( h(p) \) = function given by Eq. (3-3)
- \( K_1, K_2 \) = adsorption equilibrium constant
- \( k_1, k_2 \) = rate constant of species \( A_1, A_2 \)
- \( K_a \) = adsorption equilibrium constant
- \( k_{ads} \) = adsorption rate constant
- \( k_d \) = desorption rate parameter
- \( k_r \) = mass transfer coefficient in column
- \( k_p \) = mass transfer coefficient in the CSTR
- \( L \) = length of chromatographic reactor
- \( \lambda \) = defined by Eq. (3-4)
- \( m_n \) = \( n^{th} \) moment
- \( m_{nj} \) = \( n^{th} \) moment of species \( A_j \) where \( j = 1 \) or \( 2 \)
- \( n_p \) = number of particles (grams/vol. of reactor)
- \( \rho \) = ratio of volumetric flow rate to CSTR volume
- \( R \) = radius of the spherical particle of adsorbent
- \( \rho_p \) = apparent particle density
- \( s \) = variable in the Laplace transformation
- \( t \) = time
- \( t_{0A} \) = time of duration of the injection of adsorbate
- \( u \) = superficial fluid velocity
- \( u_1, u_2 \) = velocities of species \( A_1, A_2 \) in the countercurrent column
- \( u_s \) = superficial solid velocity
- \( v \) = linear velocity of the carrier gas in the interparticle space
- \( v_1, v_2 \) = velocities of species \( A_1, A_2 \)
- \( x \) = axial coordinate in the countercurrent column
- \( z \) = length coordinate of the bed of adsorbent

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HOW ABOUT A QUICK ONE?

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Of all instructional methods, lecturing is the most common, the easiest, and the least effective. Unless the instructor is a real spellbinder, most students cannot stay focused throughout a lecture: after about ten minutes their attention begins to drift, first for brief moments and then for longer intervals; they find it increasingly hard to catch up on what they missed while their minds were wandering; and eventually they switch the lecture off altogether like a bad TV show. McKeachie cites a study indicating that immediately after a lecture students recalled 70% of the information presented in the first ten minutes and only 20% of that from the last ten minutes.

There are better ways. Actively involving students in learning instead of simply lecturing to them leads to improved attendance, deeper questioning, higher grades, and greater lasting interest in the subject. A problem with active instructional methods, however, is that they sound time-consuming. Whenever I describe in workshops and seminars the proven effectiveness of in-class problem-solving, problem-formulation, trouble-shooting, or brainstorming exercises, I can always count on someone in the third row asking—usually sincerely, sometimes beligerently—"If I do all that, how am I supposed to get through the syllabus?"

I have a variety of answers I trot out on such occasions, depending on my mood and the tone of my questioner, but they mostly amount to "So what if you don't?" Syllabi are usually made up from the standpoint of "What do I want to cover?" rather than the much more pertinent "What do I want the students to be able to do?": when the latter approach is adopted, it often turns out that large chunks of the syllabus serve little educational purpose and can be excised with no great loss to anyone. But never mind: let's accept—for the remainder of this column, at least—the principle that it is critically important to get through the syllabus. Can I (asks my friend in the third row) use any of those allegedly powerful teaching techniques and still cover it all?

Yes (I reply), you can. Here are two techniques for doing it.

In-Class Group Problem-Solving

As you lecture on a body of material or go through a problem solution, instead of just posing questions to the class as a whole and enduring the subsequent embarrassing and time-wasting silences, occasionally assign a task and give the class one or two minutes to work on it in groups of three to five at their seats. For example:

- Sketch and label a flow chart (schematic, force diagram, differential control volume) for this system.
- Sketch a plot of what the problem solution should look like.
- Give several reasons why you might need or want to know the solution.
- What's the next step?
- What variations of this problem might I put on the next test? (This and the last one are particularly instructive.)

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You don’t have to spend a great deal of time on such exercises; one or two lasting no more than five minutes in a fifty-minute session can provide enough stimulation to keep the class with you for the entire period. The syllabus is safe!

Warning, however. The first time you assign group work, the introverts in the class will hang back and try to avoid participating. Don’t be surprised or discouraged—it’s a natural response. Just get their attention—walk over to them if necessary—and remind them good-naturedly that they’re supposed to be working together. When they find out that you can see them* they’ll do it, and by the time you’ve done three or four such exercises most of the class will need no extra prodding. Granted, there may be a few who continue to hold out, but look at it this way: in the usual lecture approach, 5% of the students (if that many) are actively involved and 95% are not. If you can do something that reverses those percentages or comes close to it, you’ve got a winner.

**In-Class Reflection and Question Generation**

The one-minute paper is an in-class assignment in which students nominate the most important and/or the most confusing points in the lecture just concluded.[3,4] Variations of this device can be used to powerful effect. About two minutes from the end of a class, ask the students—working individually or in small groups—to write down and turn in anonymous responses to one or two of the following questions:

- **What are the two most important points brought out in class today (this week, in the chapter we just finished covering)?** Examination of the responses will let you know immediately whether the students are getting the essential points. Also, when the students know beforehand that this question is coming, they will tend to watch for the main points as the class unfolds, with obvious pedagogical benefits.

- **What were the two muddiest points in today’s class (this week’s classes, this section of the course)?** Rank the responses in order of their frequency of occurrence and in the next class go over the ones that came up most often.

The responses to this question will surprise you. What you would have guessed to be the most difficult concepts may not show up on many papers, if they show up at all; what will appear are concepts you take for granted, which you skimmed over in your lecture but which are unfamiliar and baffling to the students.

- **What would make this material clearer to you?** You also never know what you’ll get in response to this one—perhaps requests for worked-out examples of solution procedures or concrete applications of abstract material, or pleas for you to write more clearly on the board, speak more slowly, or stop some annoying mannerism that you weren’t aware you were doing. Responses to this question can provide valuable clues about what you could do to make your teaching more effective.

- **Make up a question about an everyday phenomenon that could be answered using material presented in class today (this week).** (Optional:) One or two of your questions will show up on the next test.

I used the last exercise—including the zinger about the next test—at the end of a course segment on convective heat transfer and got back a wonderful series of questions about such things as why you feel much colder in 20°C water than in 20°C air; why you feel a draft when you stand in front of a closed window on a cold day; why a fan cools you on a hot day and why a higher fan speed cools you even more; why a car windshield fogs up during the winter and how a defogger works; and why you don’t get burned when you (a) move your hand right next to (but not quite touching) a pot of boiling water; (b) touch a very hot object very quickly; (c) walk across hot coals. I typed up the questions (sneaking a few additional ones onto the list) and posted them outside my office—and in the days preceding the test I had a great time watching the students thinking through all the questions and speculating on which one I would put on the test. (I used the one about the fan.)

There are other short, easy, and effective instructional methods, but these should do for starters. Check them out and let me know how they work for you. If I collect some good testimonials (positive or negative) I’ll report them in a future column.

**REFERENCES**

INTRODUCING WATER-TREATMENT SUBJECTS INTO CHEMICAL ENGINEERING EDUCATION

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Traditionally, water-treatment subjects are covered extensively only in civil engineering, even though several aspects can be analyzed without difficulty under the light of current chemical engineering theoretical tools. Severe damage to the environment caused by discarded wastewater, alternatives for treatment, and theoretical considerations can all be efficiently introduced in courses such as the introduction to chemical engineering, transport phenomena, reactor design, and unit operations.

Including water subjects in engineering education is particularly important in arid regions of the world where water is a limiting factor for industrial and urban development. In Northern Chile, a region of extreme aridity, every industrial activity is affected by a limited supply of water, and chemical engineers are often faced with industrial processes susceptible to be upgraded, e.g., water recycling. Also, the trend of ever-increasing environmental regulations in industry justifies the need for introducing wastewater treatment subjects into the chemical engineering curriculum.

Most educators agree that environmental-related issues need to be incorporated into the chemical engineering curriculum, but there is no agreement on the procedure for doing so. To achieve this, some U.S. universities have considered the following options:

- including some environmental-related issues in the capstone senior design course
- consideration of elective courses containing environmental-related issues
- coordinating environmental-related-issue training through examples and homework problems in the core chemical engineering courses

The chemical engineering department at the Universidad de Antofagasta has recently incorporated environmental-related water issues into the curriculum with good results and without a significant increase in the students' academic load. The aim of this activity is: 1) to promote a working knowledge of both the basic indexes used in the description of water quality and water treatment technologies, 2) to advance an understanding of the need to rid the water of microorganisms and chemicals, and 3) to enhance the students' perception of water and its relationship to environmental issues. Our approach exposes the students to exercises with incompatible or incomplete sets of data in order to encourage discussion and creativity. This non-traditional approach is a well-recognized practice that has the effect of improving the student's insight into chemical engineering processes. We also introduce key water-treatment concepts through exercises and dis-
cussions, and we emphasize both water contamination problems and water reclamation during routine visits to local mines and factories.

Water recycling and wastewater reclamation are two environmental-related issues discussed in classes at the Universidad de Antofagasta, and they are described in detail below.

**EXAMPLE 1**

**Water Recycling in a Copper Concentrating Plant**

During the course Introduction to Chemical Engineering, a once-a-year visit to the nearby Mantos Blancos mine is planned. Figure 1 shows the recycling water system used there. Chemical engineering students are asked to determine all the information necessary to complete Table 1 by interviewing supervisors and operators at the plant. Both the table and the figure are given to the student in advance of the plant trip. They must also inquire about the details of the process strategies which minimize water content in the band filter cake.

The final field report should contain a discussion on

- Data Compatibility: in order to find out how well-connected all the information collected during the field trip is, a mass balance and the corresponding degree of freedom analysis must be performed[6]
- Water recycling: From the analysis above and given the fresh-water cost, the importance of maximum cake dewaterability in the filter band must be deduced.

**TABLE 1**

<table>
<thead>
<tr>
<th>Equipment</th>
<th>Purpose</th>
<th>Inflow(s) and % solids*</th>
<th>Effluent(s) and % solids*</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrocyclone</td>
<td>Fast slurry classification into fine and coarse fractions</td>
<td>WW = 1</td>
<td>FF=</td>
<td>Particle size distribution in WW can be partially modified, if necessary</td>
</tr>
<tr>
<td>Thickener</td>
<td>Separation of settleable particles</td>
<td>FF=</td>
<td>S=</td>
<td></td>
</tr>
<tr>
<td>Mixing tank</td>
<td>Mixing thickener and hydrocyclone underflows</td>
<td>S=</td>
<td>M=</td>
<td></td>
</tr>
<tr>
<td>Filter band</td>
<td>Solid separation by filtration as to obtain cake with high solid content</td>
<td>M=</td>
<td>BF=</td>
<td></td>
</tr>
</tbody>
</table>

* Blank spaces must be filled in by students.

At this point students should "translate" the information given by the plant personnel, i.e., the use of percentage solid index, over or under 200 mesh, when standards for cake dewaterability are established. Thus, compounding elements of mass balance, integral process control, and concern for water are all involved in this example. Some field reports contain interesting suggestions on the processes studied, e.g., experimental measurements of cake dewaterability under different particle size distribution.

Water recycling is also partially reviewed in courses such as unit operations, where bench scale filtration tests are computed.

**EXAMPLE 2**

**Water Treatment in Stabilization Ponds**

Theoretical aspects of water treatment can be discussed in a single exercise in the reactor design course.

Wastewater stabilization ponds are open lagoons where aerobic bacterial and microalgal growth and metabolism transform organic matter into stable compounds and pathogenic microorganisms are gradually eliminated.21 Water can then be safely reused, either for agriculture or industrial applications, e.g.,
ore leaching. Therefore, municipal wastewater can be treated by this relatively inexpensive method in places where both low cost land and high solar irradiation are available.\(^8\)

Since continuous reactors and stabilization ponds operate similarly, the latter are also known as bioreactors. Thus, the same efficiency concept and equations studied during the reactor design course can be applied to bioreactors.

Organic matter in raw wastewater is a complex mixture of different chemicals and microorganisms. Therefore, it is necessary to find a single variable or index in order to use a single kinetic expression properly, either for total biodegradable organic matter or microorganisms population. Examples of these indexes are Total Coliform Bacteria per 100 ml of water (TCB) and Biochemical Oxygen Demand (BOD). The latter indicates the total amount of oxygen required for the biological breakdown of carbon- and nitrogen-containing material, i.e., the amount of oxygen required to sustain biological activity in an aerobic pond.\(^9\)

To better expose the students to wastewater treatment through wastewater stabilization ponds, the following topics are emphasized:

a. Due to the complexity of the process, a realistic model must consider that organic matter bioconversion and microorganism deaths are both linearly dependent on sunlight intensity, and also that the kinetics of the process can be expressed as 
\[
\frac{dA}{dt} = k * A * I,
\]
where \(A\) represents BOD or TCB, \(I\) is sunlight intensity, and \(k\) is the temperature-dependent kinetic constant.

b. Since solar energy is absorbed by water, a vertical temperature profile is reached in the pond. Therefore, there should be a discussion on how BOD or TCB is affected by such a temperature profile (assuming that \(k\) has an Arrhenius-type temperature dependency) but the kinetic expression is not affected by sunlight intensity.

c. An analysis should be made on the assumptions necessary for obtaining a single \(k\) value at any place in the wastewater stabilization pond.

d. If Fick's equation, with analytical solution, is to be used to account for the overall efficiency, the implicit assumptions involved in Fick's equation must be explained. Also, the student should try to answer the question of what happens with Fick's equation when a completely mixed or plug reactor is considered.

e. Finally, the class discusses the beneficial uses of water reclamation in Northern Chile.

Temperature, pH, and absorbance measurements at different depths and times of the day demonstrate the complexity of the biological processes occurring in a wastewater stabilization pond, and therefore its modeling. If time and depth are not considered during the measurements, a simpler model can be reached.

In topics a and b above, the discussion is centered on the need to work out mass and heat transfer equations simultaneously, including velocity terms and using the assumptions required. Furthermore, the proposed analytical form for \(\frac{dA}{dt}\) can be questioned since organic matter can also be degraded by anaerobic bacterial activity and TCB can also decrease by changes in pH. A discussion on the classical dispersion model for a non-ideal reactor is involved in topics c and d, but using the wastewater-stabilization-pond terminology.

As a result of these exercises and discussions, the students achieve a straightforward understanding of the basic operating principles of wastewater stabilization ponds. In addition, they are able to practice key kinetic reactor concepts with a minimum additional academic load. Example 2 is complemented by a field trip to the Universidad de Antofagasta's wastewater stabilization pond pilot plant. Finally, a similar discussion can be carried out on activated sludge as an alternative process where oxygen concentration replaces sunlight intensity in the analysis.

**CONCLUSION**

Water treatment subjects can be successfully introduced in the core chemical engineering courses as practical examples of standard concepts. It requires a coordinated effort in several courses in order to discuss similar wastewater aspects through various approaches.

The students can obtain a critical view of water treatment processes for recycling purposes through field trips, where real processes are seen in action.

Introducing wastewater treatment subjects in the chemical engineering curriculum provides direct access to biotechnological and ethical issues. The students are exposed to environmentally related issues and treatment alternatives which require an interdisciplinary approach in both industrial and academic research.

**ACKNOWLEDGEMENT**

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ChE letter to the editor

LANGMUIR'S ISOTHERM: Kinetics or Thermodynamics?

Dear Sir:

The Langmuir isotherm for adsorption equilibrium of m solutes is of the form

\[ q_j = \frac{a_j c_j}{1 + \sum_{i=1}^{m} b_i c_i} \quad (j=1, \ldots, m) \tag{1} \]

where the \( q_j \) and \( c_j \) are the concentrations of the solutes \( i \) on the adsorbent and in the fluid phase, respectively, and the \( a_j \) and \( b_i \) are constant coefficients. Langmuir\(^{[1]}\) derived his equation in 1916 with a kinetic argument: that the rates of adsorption and desorption must be equal at equilibrium.

To this day almost every textbook follows his reasoning, even though it does not stand up too well to close scrutiny. It postulates the adsorption rate to be proportional to the concentration of the solute in the fluid phase and the unoccupied surface area; and the desorption rate to the amount adsorbed.

While this is plausible, there is no proof. Also, in reality, adsorption and desorption rates often are controlled by mass transfer and so may obey different laws. The derivation should therefore retreat to declaring its rates as only those of attachment to and detachment from the surface,\(^{[2]}\) and even then the rate law may differ if attachment and detachment were to involve more than a single step.

More seriously, where Langmuir's equation is not obeyed, do we really believe the deviation is caused by a kinetic anomaly? Lastly, have we not warned our students on other occasions that intermingling kinetic and equilibrium arguments is fraught with pitfalls?

Although its original derivation is shaky, the Langmuir isotherm has proved to be more successful than any other of comparable simplicity. So why not show our students a derivation that is more convincing and free of merely plausible assumptions?

The isotherm describes adsorption equilibrium, and the finest tool we have for equilibria is thermodynamics. We used thermodynamics to derive the mass-action law. To recapitulate: The Gibbs free energy of a (closed) system is a function only of temperature, pressure, and conversion and is at its minimum at equilibrium; with \( m \) participants, stoichiometric coefficients \( v_i \), and at constant temperature and pressure

\[ \frac{dG}{dn_i} = 0 \tag{2} \]

at equilibrium, where \( n_i \) is the number of moles of species \( i \). Introducing the chemical potential \( \mu_i \) and its concentration dependence

\[ \frac{dG}{dn_i} = \mu_i = \mu_i^0 + RT \ln c_i \]

provided the system is ideal (activities equal concentrations). The reaction stoichiometry requires

\[ dn_i = v_i \]

so that

\[ \sum_{i=1}^{m} v_i \mu_i = \sum_{i=1}^{m} v_i \mu_i^0 + RT \sum_{i=1}^{m} (v_i \ln c_i) = 0 \]

at equilibrium. Since the term involving the standard potential, \( \mu_i^0 \), is constant

\[ \prod_{i=1}^{m} c_i^{v_i} = K = \text{const.} \tag{3} \]

at equilibrium. This is the mass-action law, with \( K \) as the equilibrium constant.

Nowhere in this derivation was it necessary to assume chemical bonds to be formed or broken, or even to identify the participants as molecules or chemical species. The derivation covers any kind of process in which something is changed into something thermodynamically distinguishable. Its result can therefore be applied to adsorption as well, and it yields the Langmuir isotherm.

An easy way of showing the long-known mathematical equivalence of the mass-action law and Langmuir isotherm is as follows. For the reversible "reaction" of a solute molecule \( j \) with free adsorbent surface to form occupied surface, the mass-action law gives

\[ \frac{\theta_j}{\theta_j^0} = \frac{c_j}{c_j^0} = K_j = \text{const.} \tag{4} \]

where the free and occupied surface are expressed as fractions \( \theta \) of total surface. Also

\[ \theta_j = 1 - \sum_{i=1}^{m} \theta_i \tag{5} \]

From Eq. (4)

\[ \frac{\theta_j}{\theta_j^0} = \frac{K_j c_j}{c_j^0} \tag{6} \]

Continued on page 51.
INTRODUCING HIGH SCHOOL STUDENTS AND SCIENCE TEACHERS TO CHEMICAL ENGINEERING

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Engineers and scientists will be key professionals in the future development and implementation of new technology programs that will serve to keep our country in its leadership role. Recent enrollment trends in engineering programs show a decrease in the number of high school students who are interested in technical careers, and many who are interested do not have an adequate background for completion of an engineering program because they do not take advanced science and math courses while in high school.

Following the national trend, the Mackay School of Mines and the Chemical and Metallurgical Engineering Department at the University of Nevada, Reno, have also experienced significant enrollment reductions for the past few years. Figure 1 depicts the number of freshmen and total enrollment for the last ten years. After reaching a low of one freshman in 1986 and a total of twenty-four in 1987, we began an active recruiting program which involved visiting high schools and telling students about careers in chemical engineering. We visited high schools in Reno, Las Vegas, northern Nevada, and neighboring counties in California. These visits proved to be very useful, with the result that students are now more aware of careers in engineering and that teachers are now better informed and prepared to advise students who have technical interests.

As a complement to the active recruiting program, a "Summer Institute" was developed. Again, the primary purpose was to introduce high school students and teachers to chemical engineering. The approach here, however, was through hands-on experimentation and exercises which were conducted with the help of university students, a more involved step than the recruiting seminars.

Active participation was the vehicle through which students could discover the challenges, the usefulness, and even the fun that is associated with this scientific discipline. The students also acquired a better feel for what types of preparatory math and
science courses they would need to pursue an education in chemical engineering.

The program which was developed for this summer instituted included an introduction to chemical engineering, a description of typical chemical engineering jobs, and general instruction in material balances, fluid mechanics, heat transfer, mass transfer, and process control. Of course, these topics could only be covered superficially in such a short time, but it was enough to provide some insight into the problems that chemical engineers solve and the corresponding scientific background and preparation that is required.

The main goal of the program was to increase enrollment in engineering and to encourage women and minority groups to increase their representation in the engineering workforce.

**STUDENT SELECTION**

The science teachers in several local high schools (within a 75-mile radius of Reno) were invited to attend the summer institute, and each of the teachers was asked to select three or four of their better students who had an interest in math and science to also attend the institute. They were also asked to encourage females and minorities to participate.

Five high schools responded to the invitation, with a total of five teachers and nineteen students participating. The student group consisted of nine women and ten men, with four of them classified as minorities. Eleven of the students had just completed the freshman year, seven had just completed the sophomore year, and one had completed the junior year. Therefore, most of the students had two remaining years of high school in which to prepare themselves in math and science in the event they wished to pursue an engineering degree.

**PROGRAM ORGANIZATION AND SCHEDULE**

The Summer Institute in Chemical Engineering was one week in duration, with sessions lasting from 9:00 a.m. until 4:00 p.m. each day. The overall schedule of activities for the week is presented in Table 1. The program began on Monday morning with a general introduction and slide presentation about chemical engineering, attended by all students. For the remainder of the Monday session, the group of twenty-four students was divided into three groups of eight students each.

For the remaining days (Tuesday through Friday) the students were divided into two groups, "A" and "B," each of which was divided into two sub-

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**TABLE 1**

General Schedule for Summer Institute

<table>
<thead>
<tr>
<th>DAY</th>
<th>TOPIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monday</td>
<td>Introduction</td>
</tr>
<tr>
<td></td>
<td>Careers in chemical engineering (videotapes and personal experiences)</td>
</tr>
<tr>
<td></td>
<td>Material balances (lecture, problems, and computer exercises)</td>
</tr>
<tr>
<td>Tuesday</td>
<td>Fluid mechanics session: Group A</td>
</tr>
<tr>
<td></td>
<td>Mass transfer session: Group B</td>
</tr>
<tr>
<td>Wednesday</td>
<td>Mass transfer session: Group A</td>
</tr>
<tr>
<td></td>
<td>Fluid mechanics session: Group B</td>
</tr>
<tr>
<td>Thursday</td>
<td>Heat transfer session: Group A</td>
</tr>
<tr>
<td></td>
<td>Process control session: Group B</td>
</tr>
<tr>
<td>Friday</td>
<td>Process control session: Group A</td>
</tr>
<tr>
<td></td>
<td>Heat transfer session: Group B</td>
</tr>
</tbody>
</table>

---

groups of five to seven students each. Dividing the students into smaller groups provided for a more personal level of participation and understanding by all students involved, which fulfilled the course criteria of active participation in experiments rather than simply listening to a lecture or watching a demonstration.

Each group of approximately twelve students (groups A and B) had a common one-hour lecture in their first morning session. This was necessary in order to provide background information and to introduce the students to the subject. Some of the activities and experiments scheduled for the day were also discussed in this session, and explanations about the phenomena they would be observing or measuring were provided.

After the morning lecture the groups separated and participated in activities such as laboratory experiments, calculations to analyze experimental data, and computer exercises. Each of the laboratory sessions was directed by a teaching assistant, who provided guidance to the students. A rotation procedure was developed so that each of the smaller groups had an opportunity to participate in all laboratory sessions. A list of activities for each daily session (fluid mechanics, heat transfer, mass transfer, and
process control) is presented in Table 2.

Lunch and refreshments were provided for all participants. These periods provided a more informal atmosphere in which the students could interact with the instructors and the teaching assistants, as well as make friends with each other.

A comprehensive notebook was prepared and distributed to each of the student participants. It contained all of the lecture notes, a description and explanation of all the experiments and demonstrations, and worksheets for performing calculations and other exercises. This material enabled the students to follow along more easily, and hopefully it will serve as a reference for them in the future. It should also be a useful guide for science teachers who might later integrate some of the material into their teaching.

The Summer Institute was taught by two professors of chemical engineering (the authors) with the help of four teaching assistants who were seniors or graduate students in the Chemical and Metallurgical Engineering department.

DESCRIPTION OF TOPICS

A list of the topics covered in the Summer Institute, with a brief description of their content, follows.

**Introductory Topics**

**Material Balances** This topic introduced the students to chemical engineering. They learned how to formulate and solve material balance problems which are the basis in the design of process plants. The topic was covered in three different sessions: introductory lecture, solution of problems, and demonstration of applications using a microcomputer. In this last session the students used the CAAPS (Computer Aided Analysis for Process Systems) software which is a linked system of menu-driven, compiled BASIC programs for the elementary steady-state analysis of chemical processes. The software was demonstrated for balancing chemical reactions, converting units, and performing some simple steady-state material balances.

**Biotechnology** A ten-minute videotape which explores the variety of careers open to chemical engineers in the field of biotechnology was shown.

**Advanced Materials** A fifteen-minute videotape which explores the variety of careers open to chemical engineers in the field of advanced materials was shown.

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| List of Activities |

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**Environmental Protection** A twenty-five-minute videotape exploring the variety of careers open to chemical engineers in this field was shown. It described many of the current environmental problems and the role chemical engineers have in their solution.

**Chemical Engineering Job Experience** A description of typical job assignments given to chemical engineers was presented. The two instructors have had prior work experience in the petroleum refining and steel industries, and therefore a presentation of each of those industries was made, including a description of the petroleum refining process and the steelmaking and cokemaking processes. In addition, each instructor presented examples of his/her own job assignments while employed in those industries.
Fluid Mechanics Topics

Reynold's Number Experiment  Visual observations of various types of flow (laminar, turbulent, and transition) were made by allowing water to flow through various sized and shaped conduits, and injecting a small stream of dye. These visual observations were compared to predicted values via calculation of the Reynold's number.

Pressure Drop in Pipes and Fittings  Laboratory experiments were performed to measure the frictional losses of water flowing through various sized pipes, valves, and fittings. These frictional losses were compared to theoretically-predicted pressure drops.

Computer Design of Slurry Pipelines  Personal computers were used to demonstrate a program that is used for designing slurry pipelines. Use of the computer enabled students to investigate problems associated with slurry pipeline design through some specific design problems.

Heat Transfer Topics

Double-Pipe Heat Exchanger  Three steam-jacketed, copper, circular tubes of different diameters were used to demonstrate the operation of double-pipe heat exchangers. Water was passed through the inner tube, and steam was passed through the annular space. The heat transfer coefficients, both as a function of flow rate and tube diameter, were determined for comparison with literature values.

Temperature Profiles in Solid Rods  Three cylindrical rods of varying diameters and construction materials were heated at one end. The temperatures along the rods were measured to determine the temperature distribution of each rod. These results were then compared to theoretical predictions. The use of a thermocouple as a temperature-measuring device was also demonstrated.

NASA Space Shuttle Tile Demonstration  An actual NASA space-shuttle tile was used to demonstrate the thermal insulating power of modern ceramic materials. The tile was heated to 900°C in a furnace, and then, due to the thermal conductivity of the material, the students found they were able to hold it without burning their hand.

Mass Transfer Topics

Diffusion Experiment  The diffusion coefficient of acetone in air was determined at various temperatures. Acetone was placed in a graduated cylinder and maintained at a constant temperature while air was blown through the top. The rate of diffusion was determined by measuring the change in acetone liquid level as a function of time. The experimental results were compared to theoretical predictions.

Distillation Column Operation  A pilot-plant size distillation column was operated to demonstrate the principles underlying separation of two liquid components in solution. Liquid samples and temperature measurements were taken during steady-state operation while separating an acetone-water solution. The students were taught how to plot equilibrium data and to calculate the number of stages required for a given separation by using the McCabe-Thiele method. They used this information to compare with their experimental measurements and to calculate the overall efficiency of the distillation column.

Flotation Demonstration  A Denver laboratory cell was used to demonstrate the underlying principles of flotation. This process uses differences in the surface properties of particles in an aqueous pulp to affect a separation. Hydrophobic particles are floated to the surface by finely dispersed air bubbles and are collected as froth concentrate. Hydrophilic particles do not adhere to the air bubbles, but remain in suspension in the pulp and are carried off as underflow.

Process Control Topics

Valve Characterization  The valve-sizing coefficient of a miniature control valve was determined as a function of valve-diaphragm pressure. The students also determined whether the control valve had linear or equal percentage inherent characteristics. The procedures used for specifying control valves in practical applications were also discussed.

Automatic Control of Liquid Level  An analog controller was used to maintain the liquid level in a tank at a desired value. The principles of automatic process control were described, and the student was exposed to the actual instrumentation used in the field. Performance of the level controller was evaluated for various operating conditions. The problems which can arise by improper design or through selection of the wrong settings was also demonstrated.

Computer Simulation of Level Control  A computer program that simulates the operation of three non-interacting tanks in series was used to demonstrate some of the principles of process control. The program runs on a microcomputer and graphically displays the level of one of the tanks.
This level can be monitored on-line as the user changes various controller parameters. The program runs interactively and the student can become the plant operator who has the capability of making changes to the process. The student can open or close the control valve, select manual or automatic operation, change the setpoint, or change controller settings. As a result, he or she can observe the results of any given change immediately on the screen.

COURSE EVALUATION

At the end of the week the students were asked to complete a course evaluation to help us improve the course in future years. The questions included in the form are shown in Table 3.

The response to the Summer Institute was very favorable; many of the students and teachers indicated that they would be interested in attending the next session also. The students selected the computer sessions and the laboratory experiments (which involved more participation) as their favorites. The videotapes and some of the calculation sessions seemed to be less attractive. However, in response to the question about the session they liked the least, the answer that students repeated the most was "none." Several students indicated that they would include "all" sessions as those they liked the most, and one student wrote, "I liked almost all of them the same. They put into perspective the thoughts installed into our brains in the morning." The difficulty level of the material covered was considered appropriate by 74% of the students, while the remaining 26% thought it was somewhat high. One student commented, "A few early-morning sessions were hard to understand at first but were cleared up by the afternoon. Having daily periods build on each other was very effective."

The majority of the students (62%) indicated that the time spent on lectures should remain the same, and 33% of them would like this time reduced. The opposite occurred for the time spent in the laboratory doing experiments or computer work: 62% suggested an increase and 33% no change. More mixed results were obtained for the time spent doing calculations: 52% suggested no change, 38% indicated that the time should be decreased, and 10% suggested an increase. The notebook that was prepared received very favorable comments, as did the instructors and teaching assistants. One student said about the notebook, "It was nice to have notes completed so we could look back and read what we missed. It will be nice to keep and look back at." Another student wrote, "I plan to study this book and use it for future reference."

The students made several suggestions on how to improve the course. Their suggestions ranged from making the course and/or days shorter to making it a four-week course. Even though the course emphasized hands-on laboratory experimentation by the students, they would like to see more experiments in a variety of areas. One general suggestion was that students should have had a course in chemistry before attending the institute since some of those who had not been exposed to chemistry had trouble understanding the material.

In summary, the Summer Institute in Chemical Engineering proved to be a very enjoyable and useful experience for everyone involved.

ACKNOWLEDGEMENT

The financial support of the University of Nevada System Chancellor's Office and Nevada Mining Association is gratefully acknowledged. We would also like to thank Thomas Lugaski and the teaching assistants Timothy Burchett, David Castillo, Bainian Liu, and Carl Nesbitt, for their help.

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Chemical Engineering Education
LETTER: Equilibrium Thermodynamics  
Continued from page 7.

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Q = \int TdS  
(19)

are justifiable in this context only as abbreviations for integrals like those above.

In their treatment of my approach to conservation of energy, Williams and Glasser employ what I think is a little unnecessary circularity. They use the concept "well-insulated enclosure" to discover the concept commonly called "heat." But it is not clear what a "well-insulated enclosure" means when one has yet to meet "heat." My approach is to argue that experiments are found to fall into two classes: those for which

\[ \Delta U = w \]  
(20)

holds, and those for which it does not. The former are called anything we like—say, adiabatic (but it could as well be well-insulated for that matter)—or are said to be surrounded by an adiabatic wall; the latter, non-adiabatic, or surrounded by a diathermal wall. At this stage of the argument these terms mean nothing except that Eq. (20) is or is not obeyed. (It is easy to add terms on the left where necessary to account for kinetic and potential energy.) Now one is ready to invent a new quantity which can be given the symbol q; it is merely the quantity that allows Eq. (20) to be modified so that it always holds. The modified equation (and definition of q) is

\[ \Delta U = q + w \]  
(21)

The confused thinking one encounters elsewhere over "work" and "heat" is quite remarkable. Suggestions that the gerunds "working" and "heating" be used instead do not seem helpful. I use "mechanical" and "thermal transfer of energy." I also quote Callen's analogy of the pond and the modes of transfer to it of water by rain and by stream which, when I encountered it, gave me just the sort of aha!-insight into thermodynamics that I had badly needed.

I borrowed (and modified) the postulates from Callen that now appear in the latter half of Williams and Glasser. Much of what follows there is also based on Callen. But there are other sources and influences; for example, the early ideas of researchers such as Georgian with whom I had corresponded about the units of temperature and the "universal gas constant" R.

Williams and Glasser describe what Callen calls the basic problem of thermodynamics and use his method of solving it when the internal adiabatic constraint is removed: one maximizes entropy over all constrained states. At the end of Part 2 they suggest that the student try three ostensibly similar problems in which other internal constraints are removed. Their first problem requires removal of an internal rigidity constraint and no other. It turns out, however, that the method does not work in this case (as it is not difficult to show). Solution by maximization of entropy always assumes removal of the adiabatic constraint at least. Earlier in Part 2, Williams and Glasser raise the practical difficulty of how to relax the permeability constraint without relaxing the adiabatic constraint as well. The answer is that one does not.

Continued on page 37.
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 and which elucidate difficult concepts. Please submit them to Professors James O. Wilkes and Mark A. Burns, Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

MORE APPLIED MATH PROBLEMS ON VESSEL DRAINING

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Processing and storage vessels in the chemical and allied industries come in a large variety of shapes. There are almost as many reasons for this variability as there are shapes; these reasons can include convenience, insulation requirements, land and material costs, safety considerations, tradition, etc. Drainage of such vessels through an orifice-type hole at the bottom of the vessel represents a class of non-linear, ordinary, first-order differential equations, amenable to analytical solution. Thus, from an academic standpoint, this category of practical applications provides engineering educators with a wide variety of useful problems in the area of applied mathematics.

Solutions to these drainage problems have appeared for many of the geometrical configurations that typically occur in practice. These solutions normally appear in trade journals or similar outlets. For example, in one of the earlier such articles on this subject, formulas were summarized to compute the time requirements for emptying vessels of four different shapes: vertical cylinder, cone, horizontal cylinder (with flat ends), and sphere. Later articles gave similar formulas for draining elliptical vessel heads at the bottom of vertical cylinders,\[^{[2]}\] elliptical saturator troughs (horizontal elliptical cylinders with flat ends),\[^{[3]}\] and horizontal cylinders with elliptical dished heads or end.\[^{[4]}\]

One can conceive of a number of other geometrical shapes for vessels or tanks. Admittedly, they might not occur often in the real world, but such configurations may be of some use for academic purposes, e.g., examination or homework problems. Thus (and also in the interest of completeness) this brief article presents tank-drainage formulas for five new configurations: parallelepiped (or box), vertical elliptical cylinder, regular tetrahedron, pyramid (inverted), and paraboloid.

GENERAL CONSIDERATIONS

There are two fundamental engineering equations which must be invoked in the solution to any of these tank drainage problems. The first of these is a dynamic material balance for the liquid in the tank, which in this rather simple case merely reduces to the rate of accumulation being equal to the negative of the output rate

\[
\frac{dV}{dt} = -q
\]  

or, more specifically

\[
A \frac{dz}{dt} = -A_{v2}v_{2}
\]  

For the simpler geometric configurations (e.g., vertical cylinders [circular or elliptical] and box), the

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cross-sectional area (A) of the liquid surface in the tank is a constant quantity and not a function of the variable liquid level (z). This results in a very tractable, non-linear differential equation.

The effluent liquid velocity \( v_2 \) through the drain hole or orifice is determined from a mechanical energy balance, specifically between elevation points 1 and 2 in Figure 1. This results in the classical Bernoulli equation

\[
P_1 + \frac{g}{2} v_1^2 + Z_1 = P_2 + \frac{g}{2} v_2^2 + Z_2 + h_e \tag{3}
\]

Two assumptions are conventionally made at this point. The first of these assumes that the vessel is 1) vented to, and 2) drains to, the atmosphere, and thus \( P_1 = P_2 \). The second assumption asserts that the rate of change of the liquid level in the vessel \((v_x)\) is negligible at all times in comparison with the liquid velocity through the drain hole \((v_2)\). After replacing the variable elevation difference, \(Z_1 - Z_2\), with the liquid level \((z)\) in the tank, we have

\[
v_2^2 = 2g(z - h_e) \tag{4}
\]

When the orifice discharge equation is used, the fluid head loss \((h_e)\) due to friction is not explicitly calculated. Rather, an orifice discharge coefficient \((C,\) generally less than unity) is introduced to attenuate the fluid head and compensate for this head loss

\[
v_2 = C_0 \sqrt{2gz} \tag{5}
\]

As shown in most unit operations and fluid flow textbooks, this quantity \(C_o\) is a function of the fluid velocity (as incorporated in the Reynolds number) and the downstream (orifice)/upstream diameter ratio, although a constant value is generally assumed for a given application. Typical values of \(C_o\) are between 0.60 and 1.0. Indeed, a value of 0.75 for this coefficient is reported in a recent article describing an undergraduate experiment on efflux times through a drain hole at the bottom of a horizontal cylinder with flat ends. By way of information, civil engineers[5] know Eq. (5) (with \(C_o = 1\)) as the Torricelli theorem. Insertion of this latter expression into Eq. (2) then yields

\[
\frac{A}{dt} = -C_0A_o \sqrt{2gz} \tag{6}
\]

as the non-linear differential equation to be integrated.

**SPECIFIC CASES**

The general integrated form of Eq. (6) can be written as

\[
t = \frac{1}{C_0A_o \sqrt{2g}} \int_{0}^{h} \frac{A}{\sqrt{z}} \, dz \tag{7}
\]

It should be emphasized at this point that the integral in the above expression cannot be replaced by the total volume \((V)\) to be drained divided by the square root of the average fluid head over the total height \((h)\) to be drained. That is

\[
\int_{0}^{h} \frac{A}{\sqrt{z}} \, dz \neq \frac{V}{\sqrt{\frac{h}{3}}} \tag{8}
\]

where the denominator represents the average fluid head. When \(A = \text{const}\), the integration of Eq. (7) yields

\[
t = \frac{2A \sqrt{h}}{C_0A_o \sqrt{2g}} \tag{9}
\]

as the general equation for the efflux time to completely drain a tank whose cross-sectional area is not a function of height.
Parallelepipeds

This first simple case will employ Eq. (9). We consider a rectangular parallelepiped with a length and width (both in the horizontal plane) of a and b units, respectively. In this case, \( A = ab \), and the efflux time from Eq. (9) is

\[
t = \frac{2ab\sqrt{h}}{C_o A_o \sqrt{2g}}
\]

Clearly, in the case of a square \((a = b)\) parallelepiped, one merely replaces the product \(ab\) in Eq. (10) with \(a^2\).

Vertical Elliptical Cylinder

This is another case wherein the surface area \(A\) formed by the liquid level is a constant, namely \(\pi ab\), where \(a\) and \(b\) are the lengths of the major and minor axes (again both in the horizontal plane), respectively, of the elliptical cross-section. Equation (9) in this case then becomes

\[
t = \frac{2\pi ab\sqrt{h}}{C_o A_o \sqrt{2g}}
\]

and in the special case of a vertical circular cylinder \((a = b = D/2)\), Eq. (11) reduces to the equation presented earlier by Foster.11

Regular Tetrahedron

We consider here only the case of a regular tetrahedron with four equilateral triangular surfaces and with the drain hole located at a bottom vertex opposite the top triangle in the horizontal plane. The length of any edge of this figure is denoted by \(a\). By application of the Pythagorean theorem, the height of any one of these triangles is equal to \(a\sqrt{3}/2\). The total height of this figure is determined to be \(a\sqrt{2}/3\) from a second application of this theorem, and then, from similar triangles, the cross-sectional area \(A\) of the liquid surface at any level \(z\) is given as \((3\sqrt{3}/8)z^2\). Lastly, insertion of this result into Eq. (7), followed by integration, then yields for the efflux time

\[
t = \frac{3\sqrt{3} h^{5/2}}{20 C_o A_o \sqrt{2g}}
\]

Power of 5/2 in the integrated expression of Eq. (12), which is consistent with Foster's result11 for a conical tank.

Inverted Pyramid

This case of an inverted pyramid, like the tetrahedron above, is also similar to the case of an inverted cone. The drain hole is at the bottom vertex of the inverted pyramid, the total height of which is equal to \(c\). A rectangular cross-section is assumed for generality. Thus, let \(a\) and \(b\) (both in the horizontal plane) represent the length and depth, respectively, of the pyramid at its top. Two successive applications of similar triangles yield \((ab/c^2)z^2\) as the expression for the area \(A\) of the liquid level at any elevation \(z\). Integration of Eq. (7) with this expression for the area then gives

\[
t = \frac{2abh^{5/2}}{5c^2 C_o A_o \sqrt{2g}}
\]
as the expression for the time for complete drainage. We note again the appearance of \(h\) to the power of 5/2 in Eq. (13), as in the preceding case. The product \(ab\) in this equation is merely replaced by \(a^2\) in the case of a regular pyramid with a square side length of \(a\).

Paraboloid

This last case examines an elliptical (again for generality) paraboloid of total height \(c\). As with the vertical elliptical cylinder, \(a\) and \(b\) here represent the lengths of the major and minor axes, respectively, of the ellipse in the horizontal cross-section at the top of the paraboloid. The equation for this figure then becomes

\[
\frac{x^2}{a^2} + \frac{y^2}{b^2} = \frac{z}{c}
\]

It should be noted that in many mathematical handbooks and textbooks the right-hand side of the above equation is written as \(cz\) or \(2cz\), in which case \(c\) would have the units of reciprocal length. In any event, any horizontal cross-section of this figure is elliptical, and from Eq. (14) it follows that the lengths of the major and minor axes of any such intermediate ellipse at an elevation of \(z\) are equal to

\[
a\sqrt{z/c} \quad \text{and} \quad b\sqrt{z/c}
\]

respectively. Thus, the area of this ellipse becomes \(\pi abz/c\), and the resulting efflux time formula is

\[
t = \frac{2\pi abh^{3/2}}{3c C_o A_o \sqrt{2g}}
\]
Finally, Eq. (15) becomes

$$t = \frac{\pi D^2 h^{3/2}}{6 cC_0 A_0 \sqrt{2g}}$$

(16)

as the expression for the efflux time in the special case of a circular \((a = b = D/2)\) paraboloid.

**NOMENCLATURE**

- \(A\) cross-sectional area of the liquid level in a tank at any time, \(L^2\)
- \(A_0\) cross-sectional area of the drain hole or orifice, \(L^2\)
- \(a\) length of a rectangle, edge of a regular tetrahedron, or major axis of an ellipse, \(L\)
- \(b\) width of a rectangle or minor axis of an ellipse, \(L\)
- \(C_0\) orifice discharge coefficient
- \(g\) acceleration due to gravity, \(L/T^2\)
- \(g_c\) conversion factor, \(M/L^3\)
- \(h\) initial height of liquid in a tank, \(L\)
- \(h_f\) fluid head loss due to friction, \(L\)
- \(L\) length unit
- \(M\) mass unit
- \(P\) pressure, \(F/L^2\)
- \(q\) liquid volumetric flow rate out of a tank, \(L^3/T\)
- \(T\) time unit
- \(t\) time, \(T\)

**Greek Letters**

- \(\pi\) number \(\pi\) (3.14159...)
- \(\rho\) liquid density, \(M/L^3\)

**Subscripts**

1. liquid surface in the tank at any time
2. bottom of tank (at drain hole)

**REFERENCES**

IDEAS ABOUT CURRICULUM

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What a challenge it is to develop a curriculum that will prepare our students for the years 2020 to 2040! Should we focus on breadth, or depth? Produce a generalist, or a specialist? Besides subject knowledge, how much explicit training should be included to develop problem-solving skills, communication skills, interpersonal and team skills, and the ability to learn-how-to-learn? What is the role of projects?

Our department at McMaster is relatively small and does not have expertise in some of the "emerging technologies." We feel that the design project is the capstone course, that synthesis activities should be spread over the whole curriculum, and that computer skills should be well developed. In this context, what should our curriculum be and how should we go about developing it?

GOALS AND ANALYSIS OF OPTIONS

To address the issues of curriculum design subject to our unique constraints, we examined and defined our goals, and consulted with many others during our two years of deliberations. As a department, we set goals so that our graduates

- would be technically sophisticated, with an emphasis on the fundamentals
- would not only be computer literate, but also be able to program effectively and efficiently and would be familiar with a wide range of computer executive programs such as FLOWTRAN, PROCESS, HYSIM, and various spreadsheets
- could learn on their own
- would have good communication, problem-solving, interpersonal, and group skills
- would know how to create hypotheses, perform experiments, and draw valid conclusions
- would have enriched experience through senior electives drawn from our research expertise

Acceptance of these goals immediately highlighted some directions: depth of the core fundamentals, generalist with electives available in our areas of expertise. Because the students cannot learn in class all that they will need to know in their career, we will have explicit activities to develop the student's confidence in their own how-to-learn ability.

We held a number of faculty retreats for identifying and streamlining the core concepts in chemical engineering and removing the overlaps and the inconsistencies. Concurrently, a team of students performed the same tasks from their perspective. Special workshops were held on such topics as the laboratory (led by O.M. Fuller) and on the results of our four-year research project to discover methods of improving the development of problem-solving and interpersonal skills.

We discovered, among other things, that using open-ended problems and modeling how we solved problems did not develop the student's problem-solving skills, just as giving them good trouble-shooting problems did not improve their trouble-shooting ability. If they entered the activity with the ability to think of several causes (whereas we hoped they would be able to think of, say, ten), they left the activity still able to think of only several.

To develop the student's ability to learn-how-to-learn, we chose as a model the problem-based, small-group, self-assessed, self-directed learning model used by McMaster Medical School. However, we did not have the advantage of its admission policies (that eliminated students who did not have well-developed problem-solving and group skills), the timetable flexibility, or the resources to provide a faculty tutor for small groups of five students each. So we had to rephrase the problem to "how can we adapt their approach to our constrained system?" and chose...
We discovered, among other things, that using open-ended problems and modeling how we solved problems did not develop the student's problem-solving skills, just as giving them good trouble-shooting problems did not improve their trouble-shooting ability.

to use a thread of courses throughout the curriculum which would develop problem-solving and interpersonal skills and small-group learning skills. The development of problem-solving and interpersonal skills was an important goal in its own right as well as an important component needed for the design project.

Another issue was the integration of previous courses with the capstone design course so that the team-approach project course could focus on synthesis. Our approach was that the principles of engineering economics, ethics, professionalism, process improvement, and process design would be handled in a separate "course" and to have industrial clients with real projects. Teams of about ten students and two faculty would tackle a problem. For example, a recent project was with Esso/Texaco on assessing an industrial wastewater-treatment facility. Difficulties arose since the students entered the project without sufficient experience with computer executive programs and without having had some of the core courses (such as reaction kinetics and reactor design, mass transfer and process control).

In rethinking the approach for the new curriculum we were not trying to replace the design experience—we wanted to enrich it. Four important changes pertaining to the design course were:

1. Introducing computer programming (especially the executive programs PROCESS and HYSIM) in the sophomore and junior years so that the students would enter the project with this expertise already in place.
2. Providing all of the basic fundamentals before the end of the junior year.
3. Shifting the course load in the design course so that it was two tutorials per week in both semesters.
4. Providing explicit training ahead of time on how to work effectively in groups and how to be a team leader.

Thus, in addition to a "stream" of core fundamentals that would be completed by the end of the junior year, we envisioned a series of learning activities

- on computer programming, numerical analysis, and executive programs
- on "how to experiment"
- to develop communication skills
- to develop problem-solving and interpersonal skills

These activities would culminate in and be integrated through the capstone design course. The skill of learning-how-to-learn would be acquired through problem-based, small-group, self-directed learning in the course "engineering economics."

CURRICULUM

For the core fundamentals the former senior-level courses were altered as follows:

- the topics of reaction kinetics and reactor design, stagewise operations, diffusional transport phenomena, and separations were split into two phases, with the junior level offering the basics and a senior level offering enrichment. This actually increased the amount of coverage of this material
- process control was shifted to the junior year.

Thus, by the end of the junior year the students had the core fundamentals in all areas.

To provide expertise in the computer executive programs that would be needed for the design project course, a string of three courses in the sophomore-junior years focused on computer programming, numerical methods and modeling, and the use of executive packages. For example, PROCESS or HYSIM was introduced in the sophomore course, was used to enrich other courses in the sophomore-junior years, and was used explicitly in a computer-simulation course in the junior year that considered a relatively well-structured problem on a small section of a process. Since the content in this string of courses is not ambitious, we decided to combine the problem-solving/interpersonal skills development activities with each of these three courses. In principle this would provide a ready-made "problem" and "group activity" where the problem-solving skills could be applied. Thus, the problem-solving activities would not be developed in a vacuum. Rather, they would be embedded and bridged into the computer programming, model building, and process simulation activities. An example of the latter is given by Woods, Wood, and Gallinger.

The problem solving/interpersonal skills/self-directed learning components were dovetailed into the three team-taught computer programming courses described above and into a senior-level course on process economics and synthesis. In addition, the first sophomore course has as a co-requisite the mass and energy balances course. In this way we hoped to ensure that we had sufficient variety and opportunity to apply the problem-solving skills in solving
homework problems. Details of this approach are available.\textsuperscript{[10]}

A revised series of activities for the laboratories and on experimentation were added. In the sophomore year the emphasis was on familiarity with the hardware\textsuperscript{[11]} and on measurement techniques. In the junior year the emphasis was on doing a series of medium-size, medium-duration experiments to illustrate principles. In the senior year, the students do several in-depth experimental projects. A lecture component is included with the laboratories to consider activities on data treatment, hypothesis testing, and providing individual feedback about the written reports.

Another stream of experience focused on communications skills. The Faculty of Engineering has a policy that before students are admitted to the sophomore year, they must pass a Test of Writing Competence. So the students in our sophomore course on communication (see Woods and Feuerstein\textsuperscript{[12]}) had the necessary basic fluency in English. We then formally reinforced this skill with private reviews and feedback on the laboratory reports in the junior and senior years and in the presentation of the design project.

Many of our introductory, graduate-level courses were modified so that, although the lecture component was common, a graduate and undergraduate offering of the course would be presented in areas of our research expertise: biomedical, polymer engineering, process control, statistics, environmental engineering, particle processing, and surface phenomena. Senior students could elect to take three of these courses.

Figure 1 shows the resulting new curriculum. The freshman year is common to all branches of engineering, so we had no direct control over the content in that year. Accreditation requirements dictate the eighteen credits of English and humanities (in the freshman, sophomore, and senior years). Faculty requirements dictate the engineering courses in mechanics/structures and electricity/magnetism.

- design project: senior year, 4 credits
- enrichment chemical engineering electives: senior year (compared with general technical electives), 9 credits
- computer/simulation stream: introduction, freshman year, 4 credits; sophomore year, 1 credit; junior year, 1.5 and 2 credits
- communication stream: sophomore year, 1.5 credits; part of 2-credit lab in both junior and senior years and part of the design project
- problem solving/interpersonal skills/self-directed learning: sophomore year, 2 credits; junior year, 1.5

HOW WELL HAS IT WORKED?

In two words—extremely well. Employers comment very positively on the quality of our entry-level graduate. Alumni are enthusiastic about the curriculum and the preparation they have received. The most unique innovation has been in the problem-solving/interpersonal skills/self-directed learning components. For this reason, we have conducted a variety of pre- and post-tests as well as control-group assessments. They have shown a statistically significant increase in performance in the main-stream chemical engineering courses and a 1 to 2 standard deviation shift in confidence that they now possess skill in problem solving. The self-directed
learning has been more difficult to quantify. Anecdotal evidence abounds as to the student’s preference for this mode of learning and to instructors who feel that the students learned more and performed as well, if not better, on written exams than did students who previously "learned" the material via traditional lectures.\[5,6\]

We are changing some components since they did not work out as we had hoped. In particular, the blend of problem solving with computer programming in the sophomore year did not provide the synergy we anticipated. The students viewed them as two separate parts. So we have integrated computer programming into the mass and energy balances course and maintained a separate 2-credit course on problem solving that applies the skills in the required co-requisite mass and energy balances course. This latter bridge has worked extremely well.

The extra course in reactor design in the senior year, likewise, has not lived up to its expectations. So we combined the non-ideal behavior with the junior course (now 4 credits) and created a richer, elective course in reactor design. Also, the students found that the sophomore fluid mechanics course was very challenging, so we have now switched this to the junior year.

The design project is much more effective in the new format. We have shifted from PROCESS to HYSIM as the computer executive program of choice.

These changes have been minor. All in all, we feel that this new format offers a very viable curriculum model for the year 2000.

ACKNOWLEDGEMENT

I am pleased to acknowledge the efforts and input of my colleagues. To Bob Moore, Leslie Eubanks, Cam Crowe, Terry Hoffman, Joe Wright, Andy Hrymak, Phil Wood, Paul Taylor, Bob Marshall, and Ian Doig for nurturing the problem-solving courses; to Derek Ryder, Steve Kelly, Joe Laricchia, Craig McDougall, Bret Cousins, and Sandra Allen; to Bob Anderson, Les Shemilt, John MacGregor, Irwin Feuerstein, Malcolm Baird, Marios Tsezos, Andy Benedek, Keith Murphy, Archie Hamielec, John Brash, John Vlachopoulos, and Jim Dickson. The Ontario Universities Program for Instructional Development and McMaster University funded the four-year program to understand and develop the problem solving/interpersonal skills components. In particular, I thank Alvin Lee, Vice-President Academic, and Les King and Alan Blizzard, Instructional Development Center, for ongoing support.

REFERENCES


LETTER: Equilibrium Thermodynamics

Continued from page 29.

The adiabatic constraint is removed in their second and third problems, which should, therefore, cause the student no difficulties.

(Many of the points discussed here I raised in the literature a decade ago or more.\[6,11\])

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REFERENCES


Winter, 1992
COMPUTER CONTROL OF A DISTILLATION EXPERIMENT

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Using the GENESIS environment, software has been developed for computer control of a 10-tray column in the chemical engineering department at Michigan State University. The software permits sequenced start-up of the column, transition to steady-state cascade control, and data acquisition. During runtime, process data are displayed on an equipment schematic or a graphical trend window. The GENESIS software is a powerful authoring system for writing control and data acquisition programs and requires minimal background in computer control.

EQUIPMENT AND INSTRUMENTATION

Our department developed the control program to help introduce industrial-style computer control to undergraduate students. The system has two different columns which may be used independently and a single reboiler, condenser, and tank system.

Flows through the desired column are obtained by moving blind flanges just above the reboiler and just below the reflux splitter. The columns are Pyrex, which permits the students to observe upsets in the columns as well as normal tray operation. The six-inch diameter columns have ten trays. One column consists of five valve trays and five bubble cap trays. The other column consists of sieve trays. The trays are constructed from stainless steel and Teflon. (Further reference to the system will refer to "the column" since only one column is used at a given time.)

A schematic of the equipment is shown in Figure 1. The input and output signals are summarized in Table 1. All of the wiring from the column passes through conduit to a wall panel box. An identical panel box is installed on the back of the computer cart. BNC and computer cables are used to connect the two panels. This provides flexibility in computer location as well as in use of the computer with other experiments.

INTERFACE HARDWARE

An IBM AT is used for computer control. We purchased interface hardware from Analog Devices Inc. We use both RT1815 and RT1817 boards in the computer. These boards require signal conditioning which must be performed with additional boards.

The combination of boards and configuration are dependent on the large number of signals which were interfaced in our system, and details will be supplied upon request.

SELECTION OF SOFTWARE

Several different commercial programs are available which could equivalently fulfill the objectives of this project. GENESIS was selected because of the following capabilities:

1. A user-friendly interface which requires minimal expertise in hardware/software interfacing and data input
2. Graphic display of the process flowsheet and process variables
TABLE 1
Summary of Computer I/O

<table>
<thead>
<tr>
<th>Device</th>
<th>Signal Type</th>
<th># of Signals</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermocouple</td>
<td>Analog (V)</td>
<td>13</td>
</tr>
<tr>
<td>DP cell</td>
<td>Analog (mA)</td>
<td>2</td>
</tr>
<tr>
<td>Float Level</td>
<td>Digital (V)</td>
<td>8</td>
</tr>
<tr>
<td>Pressure</td>
<td>Analog (mA)</td>
<td>1</td>
</tr>
<tr>
<td>Feed Flow</td>
<td>Analog (mA)</td>
<td>1</td>
</tr>
<tr>
<td>Valve Position</td>
<td>Digital (V)</td>
<td>6</td>
</tr>
</tbody>
</table>

Computer Outputs

<table>
<thead>
<tr>
<th>Device</th>
<th>Signal Type</th>
<th># of Signals</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reflux Splitter</td>
<td>Digital (V)</td>
<td>1</td>
</tr>
<tr>
<td>bottoms Overflow</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Solenoid Valve</td>
<td>Digital (V)</td>
<td>1</td>
</tr>
<tr>
<td>Steam Control Valves</td>
<td>Analog (mA)</td>
<td>1</td>
</tr>
<tr>
<td>Valve Position</td>
<td>Digital (V)</td>
<td>6</td>
</tr>
</tbody>
</table>

3. Graphic-based control-loop strategy to provide easy editing and visualization of the control loop
4. Sequencing to permit stepwise start-up of the column
5. Security to limit the control parameters and setpoints the students can change
6. Capability of "on-the-fly" alteration of control parameters.

In addition to the above advantages, MSU had previously purchased the interface hardware and therefore did not need a hardware/software combination. We also knew that GENESIS software had received favorable reviews.11,21

PROGRAMMING WITH GENESIS

There are two main components of GENESIS—the strategy builder and the runtime system. The strategy builder is used to "write" the control program. Actually, no code needs to be written since the control loops are entered graphically on the screen. As part of the strategy builder, GENESIS provides a powerful graphics program (the graphics builder) to construct schematics of the process which are to be viewed during process control.

An example of a simple strategy is shown in Figure 2. The strategy is constructed using a mouse to select icons from pictorial menus. By clicking on an icon, the algorithm blocks are selected and may be placed on the screen, dragged, and sized with the mouse.

Each of the algorithm blocks is labeled with an acronym which identifies the type of block. In Figure 2, DEV represents the interface board (hardware device). AIN, AOUT, and DOUT are analog inputs, analog outputs, and digital outputs, respectively. DGAP and PID represent a gap controller and PID controller. Many other blocks may be used, including an F(x) block which may contain up to five lines of calculations using several inputs and registers.

Each algorithm block is given a tag name to make the block unique and easily identifiable. In this example, temperature input blocks are indicated by PLATE1 and PLATE7. The DGAP controller and PID controllers are used to control the reboiler level and steam flow. Specification of details of a block is achieved by selecting the block with the mouse and entering information in parameter win-
dows which pop up on the screen. The actual control loop is more complex than Figure 2 because it is desirable to use direct manipulation of the steam flow setpoint while keeping the temperature controller disabled during start-up of the column or for manual override of cascade during operation, as shown in Figure 3.

An example of our control screen designed with the graphics builder is shown in Figure 4. As the students step through the start-up procedure, different control screens are displayed. For each of our screens, the equipment schematic remains the same, but the control panel in the upper left contains different instructions. Figure 4 is the cascade control screen. The control screen is displayed using colors which are not reproduced here. During runtime, the graphics screens provide instructions and data display. Depending on how the graphics are designed, process data may be displayed numerically, graphically, or pictorially using a change in the size or color of an object. In our schematic the valves are displayed in brown when closed and bright green when opened.

On the control screen, all process data are numerically displayed near the sensing device in the schematic and are updated each second. The security of cursor positions and the range of valid entries is controlled. The only valid cursor locations are the data-entry positions in the control panel in the upper left of the screen. Alarm messages in the boxes on the right side of Figure 4 are displayed only if triggered by a specific condition. Different alarm levels may be used to identify the severity of an event. In our application, all of the alarms are warnings except for a low reboiler level which triggers the emergency state and shuts off the steam line.

RUNTIME

Once a strategy and associated graphics display have been programmed, the process may be executed. Trend windows permit graphic display of the data during runtime to follow the controller performance and the approach to steady state. Trends may be displayed over time intervals of 1, 6, or 30 minutes only. Up to 20 variables may be trended and are displayed on the screens in groups of up to 5. The screens may be selected using the "Page Up" and "Page Down" keys. An example of a trend window is shown in Figure 5, illustrating the effect of a temperature setpoint change on the steam flow rate. The trend windows utilize colors to differentiate between variables and labels. For Figure 5, different fonts have been used to differentiate variables for
purposes of this publication. During runtime, acquired data may be written to the hard disk at time intervals ranging from $1/10^6$-second upwards.

**STUDENT USE**

The objectives of the use of the distillation equipment are:

- to expose the students to the industrial equipment
- to run the column at steady-state and collect and analyze tray samples to calculate tray efficiencies
- to expose the students to an industrial-control system.

The students are provided with a short problem statement. Typically, they are to separate an equimolar feed of ethanol and propanol to a product of 90% ethanol and bottoms of 90% propanol and to determine Murphree tray efficiencies. They must obtain literature data to construct the x-y diagram and then perform a McCabe-Thiele analysis to predict the composition on tray 7 at steady-state, which determines the setpoint temperature. Also, the appropriate reflux ratio must be calculated.

During the first 3-hour laboratory period the students familiarize themselves with the experiment by watching a video tape which illustrates the start-up procedure and use of the computer. The teaching assistant demonstrates the use of the gas chromatograph used for sample analysis. Students read through the laboratory manual which contains portions of the data sheets and documentation which the manufacturers supply with the instrumentation. Upon student request, the column is started to further illustrate correct operation.

The students submit a written project proposal twenty-four hours before the second laboratory period which summarizes their McCabe-Thiele calculations and proposed laboratory procedure. Upon approval, the students may begin the experimental work.

A six-page instruction summary in the laboratory manual provides the necessary guidance for the use of GENESIS with this experiment. Although an experienced operator can start the column without the instructions, the printed information provides useful reference regarding the steps performed at each screen during the sequence, hints on steam flow during start-up, explanation on handling alarms, and important keystroke combinations to plot trend data on the control screen.

The sequencing capability of GENESIS is utilized during the start-up to display instruction screens to the students. At each screen the students must take some action, such as verifying that the cooling water is flowing, or draining condensate from the steam line, or turning on the pump. When they are ready to proceed, a keyboard command takes them to the next sequence step.

Feed is prepared by mixing alcohols from the product and bottoms tanks. The composition is determined by gas chromatography. Usually, students use 30-45 minutes to drain the tanks and prepare the correct feed composition. Start-up of the column is achieved using the steam-flow controller only. The setpoint is entered on the screen by the students. Although the written instructions provide suggestions on the steam flowrate, the final choice is made by the student. Typically, the students will encounter some type of difficulty during start-up, such as

- flooding due to vapor flow up the downcomer of the bottom tray
- flooding on the feed tray
- reboiler level too high or too low
- slugs of vapor in the reboiler thermal siphon, causing incorrect readings in the reboiler level.

![Figure 5. Example trend window which may be viewed during experimental runs.](image)
Usually, we permit the students to encounter these difficulties because they help to illustrate the limitations of control systems. In the absence of complications, vapors reach tray 7 in about fifteen minutes and the condenser in thirty minutes.

After vapors have reached the condenser the students proceed to the cascade control screen shown in Figure 4. Two factors are important in determining the approach to steady-state. First, the temperature controller has very little integral control due to the sluggish behavior of the system. Students are encouraged to use the manual steam flow setpoint until the temperature of plate 7 is within three degrees Celsius of the desired setpoint before proceeding to cascade. The second factor is that GENESIS provides bumpless transition of the steam flow setpoint upon transfer to cascade control, which means the steam setpoint will be adjusted gradually from the value existing at transfer to cascade control. Students are encouraged to anticipate the sluggishness and adjust the steam flow setpoint up or down before transferring to cascade control. This adjustment requires them to make a judgement as to whether the system will overshoot if operating at the current settings. An overshoot of a couple of degrees will result in stabilization at setpoint taking up to fifty minutes. A well-planned transfer to cascade will result in a stabilization in about twenty minutes. The trend screen data plots are useful in watching the approach to setpoint and steady-state.

After tray 7 has reached the setpoint value, tray temperatures are monitored for at least twenty minutes to assure that temperature drifting (composition changes) are not present on any trays. The students then collect tray samples.

Shutdown of the system is also performed using GENESIS. Shutdown uses the same procedure as an emergency shutdown, so the student operator enters a "Y" in the cursor location next to the "EMERGENCY SHUTDOWN?" prompt in Figure 4. (This prompt is present on all screens.) The record of column history is printed from the hard disk following completion of the experiment and is submitted with the student's laboratory report.

Typically, students will repeat the experimental run in a third laboratory period, making slight modifications to the reflux ratio or setpoint temperature. With our current laboratory objectives, the students do not have adequate time to fully explore the wealth of control experiences feasible with GENESIS. Possible control exercises include studying the effects of sudden changes in feed flowrate or reflux ratio. Another possibility is to further explore the tuning of the controllers. Typically, the students do not fully appreciate the sluggishness of the system. An example exercise would permit them to increase the integral control to improve the rate of approach to setpoint and then observe that the change results in continuous oscillations about the setpoint value. Another possibility is to permit the students to perform the Ziegler-Nichols tuning of the controllers, or to attempt control without using cascade methodology. We do not utilize these unsteady-state exercises because, with the available laboratory time, it is not possible to restabilize the system and collect tray samples for meaningful comparison with McCabe-Thiele analysis.

CRITIQUE AND SUMMARY

Student response to the use of GENESIS is extremely positive. We have chosen to install the control system on equipment that illustrates the use of a large number of data inputs. GENESIS would also be extremely useful for a smaller scale experiment with a single control loop. The flexibility of software permits the instructor to prepare exercises and control screens which require little knowledge of controllers or which are very advanced. The capability for watching unsteady-state behavior is excellent. It would be easy to plot the integral, derivative and proportional components of a controller on the same trend window as the overall controller and loop response. The use of logged data from the spreadsheet compatible files permits the students to further manipulate their data and prepare plots. The data files are compatible with LOTUS 1-2-3 and may be manipulated further, although we do not use this feature.

We have found the application of GENESIS to provide a powerful method for design of control and data acquisition programs, especially for those without experience in computer control. Because of the graphic-based strategy builder, the programmer does not need to develop or maintain expertise in reading or writing to registers. Once an understanding of the software has been developed, it becomes easy to write new control loops. The control program does not greatly change the instructional time that must be spent with the students, but provides exposure to an important aspect of control technology.

ACKNOWLEDGEMENTS

I would like to thank Al Paulsen of Dow Chemical for his assistance in specification of instrumentation, Dow Chemical for funds for the instrumentation, and Bruce Wilkinson of the Chemical Engi-
neering Department at MSU for planning and supervising the installation of the instrumentation.

REFERENCES


APPENDIX 1: Equipment Description

The level indicators are floats which indicate only whether a tank is nearly full or empty. All of the ball valves are air actuated, with a sensor to indicate valve position. The air supply is switched to the valves using solenoid valves in an air-supply line. The feed pump is a small bellows pump. Feed rate is sensed with a Micromotion mass-flow meter. The oscillations from the reciprocating pump cause fluctuations in the flow-meter readout which are dampened by adjusting the electronic filter furnished on the flow meter. The flow-meter signal is furnished to the computer as a 4-20 mA signal. The feed enters the column after passing through a single tube in shell preheater constructed from two different sizes of stainless-steel tubing.

The steam is regulated from a supply pressure of 90 psig to 20 psig before entering the system. A steam pressure sensor is furnished to the computer as a 4-20 mA signal to the computer. Steam flow is sensed with a DP cell across an orifice plate. The DP cell provides a 4-20 mA signal on a single pair of wires using a 24V supply. Steam flow is regulated by a 4-20 mA signal from the computer. An I/P (current to pressure) converter provides the air pressure to drive the control valve. The relative placement of the orifice plate and control valve have provided satisfactory control of the steam flow is passed through the conditioning system through either the RTI815 or the RTI817.

APPENDIX 2: Interface Hardware and Software

Analog signals are isolated and converted with an Analog Device 3B signal conditioning system. Analog input signals from the thermocouples and current inputs are converted to 0-10V signals which the interface boards then converted to numerical values of 0-4096. GENESIS reads the registers and converts the register values to engineering units. The analog output for communication between blocks, using the mouse, to specify the flow of information. For example, in Figure 2 the reflux splitter is driven by a 120 VAC solenoid. The reflux splitter is driven by a 120 VAC solenoid. The computer may be used to close a relay to provide the AC power or a separate electrical/mechanical timer may also be used.

APPENDIX 3: Using the Strategy Builder

The start-up of the column is achieved using a sequencing algorithm block which is not illustrated in Figure 2. The sequencer is designed with a series of states. Eight states are used in our start-up sequence, along with an emergency state. Control events may be associated with each state. Sixteen bits are associated with each state which may also trigger events. The status of each bit may change with a given state of the sequencer. In our application, the sequencer is used to control the display of control screens which provide instructions for start-up, enable alarms and warning messages which alert the students when a step has not been completed, and provide restrictions on the type of steam-flow control for a given state.

After an algorithm block has been placed on the screen, the details regarding the block may be entered by clicking the mouse on the block. When a block is selected, a parameter window pops up on the screen. Parameter values for input ranges, output ranges, alarms, controller settings, etc., are entered in this window. All of the values entered in the blocks are in engineering units, making the programming quite simple. The instrument range and operating range may differ. For example, our thermocouple inputs provide an instrument range of 0-500 C, but the measurements are only expected in the 15-110C range. By specifying the operating range, the graphical use of the acquired data is kept on a meaningful scale. GENESIS scales all data internally for communication between blocks.

Following specification of the blocks, arrows are added between blocks, using the mouse, to specify the flow of information. For example, in Figure 2 the reboiler level (REBLVL) is obtained from the interface card (RTI815). At the time the arrow is constructed, windows pop up to facilitate specification of the input channel of the card which carries the signal. REBLVL serves to convert the raw signal to engineering units. OVERFLW provides a digital signal to OVR, which communicates with the hardware card.

TMPSET is an example of a block which does not obtain its value from the interface card. The initial value of TMPSET can be entered at the time the strategy is constructed, but the value may be changed during runtime from the computer screen. This is done by associating a particular cursor location on the control screen with TMPSET during graphical construction of the control screen. The graphics builder is used after the strategy has been developed to design the computer-control screens which display data from the strategy during runtime.

Careful design of the control loop and graphic display should precede programming to minimize modifications. Alteration of the strategy block connections or graphic display requires leaving the runtime system and reentering the strategy builder program. Our system runs on an older 286 IBM AT which was slow in loading the large strategy builder and in saving the compiled control program "code." On the other hand, most of the parameters for the algorithm blocks may be changed during runtime, eliminating the need for reentering the strategy builder if the structure of the strategy is correct. This makes controller tuning relatively simple. The revised parameters are stored on the hard disk, and by simply renaming a file after completion of the run the revised parameter file becomes the default file. The details of some of the strategy algorithm blocks are not described completely in the GENESIS documentation, but many of the capabilities exceed the needs for most applications. In general, a phone call to the company quickly resolves any confusion. GENESIS offers a training course which is helpful in learning the capabilities of the software.
CHEMICAL ENGINEERING DESIGN

Problem-Solving Strategy

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A significant fraction of our undergraduates accept industrial employment that requires dealing with problems associated with an operating system (production). These responsibilities depend on an ability to both predict problems before they occur and to diagnose problems after they occur, in addition to designing and developing new processes. Problems must be solved under the constraints imposed by physical equipment and the existing processes. Neither course work nor the typical capstone design course makes a conscious effort to develop such abilities in the student.

To address this problem, the chemical engineering department at West Virginia University has initiated a process in the senior design course that focuses on the development of the necessary skills for solving problems which production engineers may expect to confront. The program introduces a series of comprehensive problems, extracted from a single process flowsheet, into the two senior design courses. The problems are worked out individually under the same rules that apply in the AIChE student-contest problem wherein the student presents a written report and a one-hour oral report on each problem. The student is "escorted" through the transition from a detailed consideration of a single unit operation to management problems that can include several interrelated unit operations. This is accomplished by providing intensive individual and group feedback after each assignment.

Major adjustments in student attitudes are sometimes necessary. It is difficult for the student to go from solving narrow, focused, single-answer problems that involve no creativity to global, multi-answer problems that require considerable creativity. They find that the well-entrenched strategies for problem solving that worked for them in the past are no longer effective.

DISCUSSION

The general content of the comprehensive problems are summarized in Table 1. It shows the skills that are necessary for solving the problem and the area of its industrial application. The order of the problems is significant. The skills required in a previous problem must be mastered in order to solve each new problem. Each problem develops a single skill while introducing a new skill that is the basis for the following problem. For example, the first problem develops an ability to visualize—and introduces analysis. The second problem assumes the ability to visualize, develops an ability to analyze—and introduces synthesis. In terms of industrial application, the three problems will cover trouble-shooting, retrofit operations, and new process design.

The problems are introduced to the student...
through industrial "role-playing." The student (a novice engineer) joins a company and is assigned to a plant site where three assignments are given that cover the areas shown in Table 1. The student is given a packet of materials that includes a process flowsheet and flow table, a description of changes that have been made to the process, thermodynamic data, and various other items of information describing the process and the company that may be useful.

The process flowsheet is special. It represents a poor process design (it was built many years ago) under current conditions and includes several poor design areas that could be improved. Some defects have been distorted (like big ears and long noses) to make them stand out and be easy to detect. The special flowsheet represents a "caricature flowsheet" and is an aid to the early development of visualization skills. In addition to poor design, several process modifications (operating conditions) have been made in response to changes in constraints and availability of new technology.

In the process of solving problems, students 1) will identify all of the "caricature problems" and offer solutions, 2) will identify many other problems, not highlighted for identification, and offer solutions, and 3) will create new processes that improve the original process and eliminate the poor engineering of the original system. All solutions must be justified by economic considerations.

All three projects are associated with the production of the same chemical commodity. Since each successive problem requires mastery of the previous problem, it has been necessary to provide extensive individual and group feedback during the oral and after each project.

### STUDENT ASSIGNMENTS

The assignments and experiences of our 1988 class are used here as an example of how the comprehensive problems, along with the "caricature flowsheet," are used to introduce and develop skills. Figure 1 is a "caricature" flowsheet for the production of acrylic acid. It was created from a 1986 AIChE student contest problem on the production of acrylic acid via partial oxidation of propylene.

A packet of material (about twenty pages) was provided that contained information concerning the instability of the acrylic acid with temperature (even with the addition of an inhibitor, it will rapidly polymerize at above 90°C when present in large concentrations). Some additional information on current operations is also given.

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**Figure 1. Acrylic Acid Process Flowsheet**

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### EQUIPMENT LIST

- AB-1 Quench Tower
- AB-2 Off Gas Absorber
- C-1 Inlet Air Blower
- E-1 Reactor Coolant Exchanger
- E-2 Absorber Product Cooler
- E-3 Solvent Separator Condenser
- E-4 Solvent Separator Reboiler
- E-5 Waste Water Separator Condenser
- E-6 Waste Water Separator Reboiler
- E-7 Product Separator Condenser
- E-8 Product Separator Reboiler
- E-9 Incinerator Waste Heat Boiler
- H-1 Off Gas Incinerator
- M-1 Solvent-Product Mixer
- S-1 Solvent-Product Liquid Separator
- T-1 Solvent Separator
- T-2 Waste Water Separator
- T-3 Product Separator

### UTILITY LIST

- BFW Boiler Feed Water
- CW Cooling Water
- CWR Cooling Water Return
- CR Condensate Return
- DI Deionized Water
- NG Natural Gas
- STM Steam
ASSIGNMENT 1

The plant faces a serious problem. Our largest customer cancelled its order. We shipped off-spec material (a slight discoloration in the normally clear acrylic acid). It damaged their process and their product was worthless (colored). The potential loss to our company is in excess of $500,000/day, and this is the economic incentive that calls for an immediate resolution. The assignment, to be completed in one week, is 1) to identify the cause of the off-spec material, 2) to recommend action to be taken to correct the situation, 3) to present a written report, and 4) to make an oral presentation to the company president.

There are several potential explanations for the "off-spec" material. There is evidence to support some of the explanations, while others are no more than speculation. Table 2 gives a partial list of some of the explanations. They can be separated into three groups: 1) global, 2) numerical, and 3) research. An example from each group follows and possible solutions are included in Table 2.

Global problems require that the student consider items outside of the process unit for an explanation. For example, the off-spec material may have resulted from low-quality feed. There is evidence in the material packet given to the student that supports this explanation: the amount of feed has increased (feed may not be pure propylene); the amount of steam generated in the waste heat boiler increased (the non-propylene material in the feed may not react in the reactor and burns in the afterburner); the non-propylene material was colored.

This problem was intentionally set up for the student to discover. Poor feed is, in fact, the most common cause of an off-spec product. We shipped our customer tainted feed and ruined their product. This could be the same problem we have. We could have received tainted feed material. We have evidence to support this explanation. Students not only fail to make a connection between these two situations but they also are not ready to accept the explanation.

A limited number of explanations can be verified numerically (the purpose of this problem was to limit the number of necessary calculations). The refrigerated water (at 10°C) to E-7 (Figure 1) was replaced with cooling water (at 30°C). Many of the students noted this and suggested that it might have caused the temperature of the acrylic acid to reach +90°C, causing polymerization. When asked to determine this temperature, many of the students had a vague idea of how to approach the solution, but only one in twenty was able to fully analyze the problem and calculate the temperature. The level of analysis required to solve the problem is similar to that used by a plant engineer. We expect our students to understand and be able to employ such an analysis.

Figure 2 gives the temperature-duty profile for the design case (all this information was available to the student). The temperature of the cooling water is known and is plotted on the same figure. For the same recycle ratio, the condenser duty is constant.

<table>
<thead>
<tr>
<th>Possible Cause</th>
<th>Evidence</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRE-PROCESS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Feed is not pure</td>
<td>1. Increased feed rate to maintain output</td>
<td>Check feed for impurities and return to the supplier</td>
</tr>
<tr>
<td></td>
<td>2. Increased steam production in waste heat boiler</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3. New supplier</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4. Temperature and pressure of storage vessel has changed</td>
<td></td>
</tr>
<tr>
<td>PROCESS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Reactor system</td>
<td>1. Increase in feed rate and lower conversion</td>
<td>Replace spent catalyst</td>
</tr>
<tr>
<td></td>
<td>2. Lower selectivity</td>
<td></td>
</tr>
<tr>
<td>Separation systems</td>
<td>1. High temperature in purification columns</td>
<td>Change from refrigerated to cooling water in condenser E-7</td>
</tr>
<tr>
<td></td>
<td>2. Absorber malfunction</td>
<td>Increase in feed rate and steam production in waste heat boiler.</td>
</tr>
<tr>
<td>POST PROCESS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Product storage</td>
<td>Inhibitor not added to product in storage</td>
<td>Check inhibitor and injection system</td>
</tr>
<tr>
<td>Product transportation</td>
<td>Dirty tank cars or product exposed to air and sunlight</td>
<td>Check transportation company?</td>
</tr>
<tr>
<td>Customer error</td>
<td>Mishandling of material by customer</td>
<td></td>
</tr>
<tr>
<td>OTHER</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Product not discolored</td>
<td>Check analytical equipment, testing procedures, and records</td>
<td>Rerun samples in our lab</td>
</tr>
</tbody>
</table>
To achieve a constant duty, $Q = U \cdot A \cdot T_{10}$. Where $A$ is constant and $U$ is assumed constant, the value of $T_{10}$ must be constant. If the curves for the refrigerated water coolant are shifted upward until the low temperature line corresponds to cooling water, the process temperature at the top becomes 46°C. This is the equilibrium temperature for the exiting acetic acid.

Figure 3 provides the vapor pressure curve for the distillate and the bottoms that were obtained from the vapor pressures of the pure components (and Raoult’s law). From Figure 3, for a temperature of 46°C the condenser pressure is 6.2 kPa. The pressure drop in the column is largely the result of the liquid level on each plate and the number of plates. Since this remains constant (at 15.9 kPa), the bottom pressure is 22.1 kPa. From Figure 3 this corresponds to a temperature of 95°C. This is well over the 90°C limit for polymerization.

Some students elected to look for information outside of the material packet that was provided and came across the information that iron enhances polymerization. Iron may have come in with the feed and been the cause of the off-spec material.

Student performance on this assignment was poor. Unfortunately, once a single explanation was identified, most students ended their search. No consideration was given to the economic loss of $500,000/day when they made their recommendations. Recommended changes were sequential, and no thought was given to making simultaneous changes to save time and money.

**Assignment 2**

The plant was returned to the original feed material, refrigerated water was returned to condenser E-7, and the catalyst was replaced. The high product quality returned and the immediate problem was solved.

The next assignment was to improve the plant profitability. There are recent changes in the value of steam and credit for excess steam will no longer be given.

The first step was to identify the major costs under the current conditions or base case. Figure 4 shows the costs of feed materials and utilities that were calculated from information provided. It identifies the major costs and shows that the overwhelming cost is propylene. There was no information on the catalyst that had been replaced. A recommendation that serious consideration be given to the development of a new catalyst with higher conversion and selectivity is appropriate.

The next largest cost is steam. If large savings are to be realized, the purchase of steam must be curtailed. Two methods of reducing the steam costs could be reducing the use of steam or generating steam in the process. The acrylic acid reaction is exothermic, and the heat generated is removed with cooling water in E-1 (another example of the caricature nature of the problem). Replacing E-1 with a steam boiler eliminates the need to purchase steam.
Table 3 lists some of the options for using the steam produced to reduce the costs of utilities shown in Figure 4.

Student performance on this assignment improved dramatically from the first assignment. While the assignment was more difficult and the changes were subtle, the students uncovered and corrected many process changes that improved profitability. The changes were ranked by incremental return on investment.

**Assignment 3**

This assignment requires the design of a new plant based on new technology. The students are free to be as innovative as possible under the given structure. There are new catalysts that provide very high selectivity at low conversion; they are temperature sensitive and ideal for a fluid bed. The single reactor system is replaced by a two-reactor system that can operate at different temperatures and pressures. The students are provided with detailed kinetics along with a computer program that considers both the kinetics and a fluid-bed model. This program allows computation of the reactor size (given the conversion and operating conditions). It is clear that the new catalysts provide increased selectivity and, with a recycle stream, the possibility of high overall conversion.

Even though the students are provided with the computer program, they will likely fail if they proceed to obtain the optimum design by a random approach. Using the kinetic expressions or performing a few well-chosen simulations will provide a feel for the effects of operating variables. Solely from the reaction kinetics point-of-view, astounding savings are possible by increasing the recycle. However, once the cost of compressing the recycle gas is considered, the advantages rapidly diminish and a sharp optimum is reached. In the old plant without recycle, large amounts of steam were introduced into the reactor. With the recycle stream this is not necessary.

The students did well on this assignment. Figure 5 is a typical flowsheet for section -AA- of Figure 1, using new technology. It is noticeably different from the old flow diagram. The plant costs are estimated along with the predicted return on the investment.

**CONCLUSIONS**

Teaching the student about acrylic acid is not the objective of this course. It is only a vehicle to demonstrate how to approach a complex open-ended problem. While it is true that every process is different, it is equally true that the methodology of visualizing, analyzing, and synthesizing are universal and transferrable to other processes.

The goal of these problems is modest. The student is not expected to master the strategies needed to be effective in working problems of the type outlined. We only hope to introduce the student to these types of problems and to move them to the breakpoint on the learning curve where the rise becomes rapid with a little more experience. We feel that if we have accomplished this, the process has been successful. The final conclusion deals with student motivation. Motivation provides both a high driving force and a low resistance to learning, enabling the student to learn more rapidly. One student’s view of the sequence of problems is as follows:

*On September 15th, 1988, we were presented with our first in a series of design projects. It was apparent that our experience in the classroom had to be challenged by the real-world situation. Instead of performing a “cookbook”*
type problem, we were supplied with a minimal amount of information. Assumptions, answers, and suggestions for rather vague situations had to be made. The time to test our knowledge in a real world situation was suddenly upon us.

As the semester progressed, many hours of sleep were lost, many times tempers became short, and often the most docile student exhibited impatient behavior. The effort put forward was not wasted though; the increase in knowledge greatly outweighed the amount of time put forth towards the projects.

It is for the above reasons that I am pleased to present this final in a series of three design projects. The knowledge which has accumulated over the past two semesters will be of great importance in the years to come.

An expanded version of this paper and copies of the original problems are available from the authors.

ACKNOWLEDGEMENTS

The authors would like to acknowledge that the concept of these individual projects or "majors" has been in existence at WVU for almost twenty years and that many faculty have contributed to its success. Most recently, we would like to recognize the contributions of A.F. Galli and W.B. Whiting.

REFERENCES

2. Bailie, R.C., "Mining the AIChE Contest Problem for All It's Worth," Proceedings of the 1990 ASEE Annual Conference, Toronto, Canada; p. 506

REVIEW: Chemical Kinetics

Continued from page 33.

Chapter 5 with catalysis. The former is conventional in its coverage, while the latter introduces autocatalysis and oscillating reactions (a subject of much current interest in chemical engineering) in addition to homogeneous catalysis, heterogeneous catalysis, and enzyme reactions. These first five chapters, two hundred pages in length, comprise nearly half the book.

Chapter 6, a brief discussion of the transition from the macroscopic to the microscopic level, sets the stage for the remainder of the text. It introduces the description of reactive collisions in terms of collision cross sections and relates the cross section to the rate coefficient. Also introduced at this point are the quantum state description of reactions (state-to-state kinetics), microscopic reversibility and detailed balance, and a short discussion of the relationship between macroscopic and microscopic kinetics.

Chapter 7 discusses the role of the potential energy surface in governing the outcome of reactive events. Succeeding chapters take the microscopic approach to kinetics, covering the kinetics of elementary reactions, and chemical dynamics. A treatment of bimolecular collision dynamics and molecular beam scattering is followed by another chapter on experimental methods, this time for state-to-state kinetics. Chapters on transition-state theory (including variational transition-state theory) and unimolecular reactions are followed by one on dynamics in solution and at interfaces. Chapters 13 and 14 cover the advanced topics of the information-theoretic approach to dynamics, including surprisal analysis and the master equation. The book concludes with a chapter on applications: atmospheric chemistry, and hydrogen and methane combustion.

This book has been used for the past two years in a one-quarter course given to chemical engineering graduate students at the University of Minnesota. In the ten weeks of lectures it has not been possible to cover the entire book. The chapters on reactions in solution and dynamics in solution, catalysis (which is covered in another course), information theory, and the master equation have been omitted, and supplementary material on bimolecular collision dynamics, chain reactions, and the kinetics of combustion reactions has been incorporated. It has proved to be a satisfactory text, treating the subject at a level suitable for graduate students and giving more comprehensive coverage (particularly of modern developments) than many other texts.

For undergraduates, portions of the book could be employed as the basis for a series of lectures on kinetics that would introduce students to material of interest to engineers in a more modern vein than most chemical engineering kinetics texts. For example, at Minnesota juniors are given approximately six weeks of lectures on kinetics during the spring quarter. The first five chapters of this book, plus some selected material on rate theory from the chapters on collision dynamics, transition state theory, and unimolecular reactions (and perhaps atmospheric chemistry and combustion reactions), would provide good reading material to accompany the lectures. Students mastering this material would have an excellent foundation for future work in kinetics and reaction engineering.

Chemical kinetics in an enormously broad area. It is difficult to find a text that gives good treatment of the fundamentals of the subject, as well as coverage of subjects of interest to chemical engineers. This book is one that succeeds and can be recommended.

Winter, 1992
The first task in process design is selecting the raw materials and the reactions and operations needed to manufacture the desired product. Process synthesis accomplishes this task by generating different process alternatives and selecting the best ones.

Taking into account the void existing in the literature about inorganic process synthesis, this paper is an attempt to show, in a simple and summarized manner, how the principles of process synthesis can be applied to inorganic processes. These principles can also be applied in other fields of chemical engineering.

Process synthesis uses heuristics, or "rules-of-thumb" based on experience, for the generation and selection of process alternatives. Education in process synthesis implies that students will acquire, in a systematic way, the necessary experience to enable them to apply heuristics, or even to "invent" them when the situation demands it. Douglas[1,2] pronounced a systematic application of heuristics to process synthesis of organic processes and also indicated the possibility of using the procedure in chemical engineering instruction.

The application of process synthesis methods to inorganic processes requires specific considerations due to the different chemistry and properties of inorganic compounds. However, it seems possible to give heuristics which will permit the student to acquire systematic knowledge about the processes.

Raw materials are very important in inorganic processes. Natural compounds are the raw material for one (or a very reduced number) of the derived compounds of every element, and from this (or these) all the other compounds of the element are obtained. The natural raw material for an element and its derived compounds is selected according to the element concentration, ease of mineral extraction, ease of separation of the desired compounds, associated impurities, etc. The most frequent natural raw materials are sulfides, oxides and hydroxides, chlorides, carbonates, and silicates.

The next step in process synthesis of inorganic processes is the selection of the reaction path. Three types of reactions can be considered in inorganic processes: redox, displacement (exchange of ions between compounds), and change of crystal structure.

For redox reactions, the general rules are: oxidations must be made at the beginning of the process; reductions will, if possible, be the latest steps of the process; and electrochemical reactions will be the last step. The oxidant or reductor selection can be made using Ellingham's (or a similar) diagram and taking into account the price of the reactants and the ease of reaction-products separation. Air for oxidations, and H₂, C, or CO for reductions, will be considered first. Displacement reactions are closely
related with separation steps and are generally used when a precipitate or an easily separable gas is formed. When a change of crystal structure is required, the corresponding reaction will be the latest step in the process.

Following the scheme given for organic processes, the next step in process synthesis is to decide the species allocation, i.e., the route of each species through the process. Thus, quantity and reactivity of impurities permit one to decide if they are processed or not. If there are ions in the solution, every valuable product or by-product and every group of species with waste destination and similar solubility will constitute an outlet. Recirculation of the mother liquor, with a purge to avoid the build-up of impurities, can be convenient.

The general structure of the separation system depends upon the phases leaving the reactor. In every case, first separation is a phase split, and after that the stream of each phase is driven to the corresponding separation system (solid, liquid, or gas). From each separation system, streams of different phases are normally produced and driven again to the corresponding separation system.

The same heuristics as in organic processes can be applied when choosing the separation task. Crystallization and precipitation operations, followed by solid-liquid separations (sedimentation or filtration, by example) are used in many cases. In inorganic processes there are normally not a great number of separations and the sequencing problem is not difficult. In all cases, heuristics such as the removal of corrosive and dangerous species first, removal of the most abundant species, making difficult separations last, etc., can be applied.

The last step in process synthesis is the integration of operations. In the inorganic processes, the same general criteria are valid as in organic processes.

It can thus be concluded that the student's education in process synthesis can consist of transmission of the necessary experience together with heuristics or rules-of-thumb. This instruction in process synthesis can be an advantageous substitute for the exhauscive descriptions of chemical processes which is given to students in subjects such as industrial chemistry.

REFERENCES

LETTER: Langmuir's Isotherm

Continued from page 23

And from Eqs. (4) to (6)

\[
\theta_j = \frac{K_c j \theta_{free}}{1 + \sum_{i=1}^{m} (K_i c_i)}
\]

Solved for \(\theta_j\)

\[
\theta_j = \frac{K_c j \theta_{free}}{1 + \sum_{i=1}^{m} (K_i c_i)}
\]

The concentration of j on the adsorbent is proportional to the surface fraction occupied by j, so that

\[
q_j = k_j \theta_j = \frac{k_j K_c j \theta_{free}}{1 + \sum_{i=1}^{m} (K_i c_i)}
\]

where \(k_j\) is another constant. This is of the form of Eq. (1), with \(k_j K_c j\) corresponding to \(a_i\) and the \(K_i\) to the \(b_i\).

This derivation also gives the same result as Langmuir's for adsorption of a dissociating molecule, for instance, of \(H_2\) as 2 H occupying two sites.

Langmuir-type adsorption is seen to result from "ideal" thermodynamic behavior, that is, from the absence of any specific interactions that would result in activity-coefficient corrections or call for the definition of additional species. This is a more germane reason than are the adsorption and desorption rates. That adsorption equilibrium has a basis in thermodynamics will be easier for the student to accept and will convey better insight into why many adsorbents behave in this manner, and why some do not.

When I went to school, more years ago than I care to count, textbooks still derived the mass-action law for reactions with the kinetic argument of equal forward and reverse rates at equilibrium—one of them even with the reaction

\[
Cu^{2+} + 6NH_3 \leftrightarrow [Cu(NH_3)_6]^{2+}
\]

postulating a single-step mechanism with hepta-molecular formation and decay into seven fragments! Happily, we have long outgrown such nonsense and have put the mass-action law for reactions on a sounder basis. Is it not time that we accord the Langmuir isotherm the same courtesy?

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The Pennsylvania State University


Winter, 1992
COMPUTING IN ENGINEERING EDUCATION

From There, To Here, To Where?

Part 2: Education and the Future*

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What have engineering schools/colleges been doing about the remarkable computing developments chronicled in Part 1 of this lecture?*

With the arrival of the first campus computers in the mid-1950s, many faculty researchers gravitated to computing centers to solve their equation systems. The computer has been central to creation of new research disciplines (e.g., numerical fluid mechanics) and reorientation of old ones (such as process analysis and design). The availability of computing resources has caused a major shift in the way research is done.

On the other hand, it would be inaccurate to claim that undergraduate education has been radically transformed by the computer. The impact of computing on engineering education has been much less profound than research. No paradigm shift away from the traditional lecture-recitation-laboratory-tutorial format, with the textbook as principal instructional resource, has yet occurred. Nevertheless, there has been a gradual infusion of computing work into the curriculum since the early 1960s.

THE ACADEMIC COMPUTING ENVIRONMENT

The computing experience of our undergraduates has been controlled to a considerable extent by their access to computing facilities: mainframes for research only in the 1950s; mainframes accessible for instruction (initially with batch processing and later with timesharing from hard-wired terminals) in the 1960s; mainframe time-sharing from remote terminals, wide-area networks, and decentralized mini-computer facilities in the 1970s; personal computer clusters, local area networks, student-owned computers, and network-accessible supercomputers in the 1980s; workstations, heterogeneous internets, distributed services (client-server model), intensely graphical interfaces and applications, and parallel processing in the 1990s. Every engineering school now has computing facilities for all its undergraduates, though the quantity and quality of the hardware, software, and services vary widely from school to school. A pertinent statistic*: in 1989 there were more than 200,000 university-owned microcomputers in the US, and a significant fraction of them were in engineering school clusters.

EARLY DEVELOPMENTS

In 1959, Don Katz (then chairman of the Chemical Engineering Department at Michigan) foresaw the tremendous impact that computing would have on engineering practice. He convinced the Ford Foundation to support a feasibility study of broad-scale integration of computer use into undergraduate engineering curricula that would make recommendations, prepare teaching materials, and train faculty. In a three-year period, over two hundred faculty from nine engineering disciplines and sixty-five engineering schools participated in the various activities of the Michigan project. They jointly produced more than 120 completely documented computer problems/programs for classroom use that were widely distributed to other faculty.

My first contact with this project occurred in the summer of 1959 when Don offered me a full-time job with his project. My acceptance put my thesis on hold and delayed my PhD by an unconscionable number of years. But I have never regretted that decision. It provided opportunities that I would not have otherwise had and steered me toward an academic career which has brought me much pleasure.

Principal recommendations of the project:
1. Train faculty to use computers
2. Provide ("free") time-shared computing services to all students
3. Require a computer-programming course
4. Teach numerical and optimization methods
5. Integrate computing assignments into all engineering, science, and design courses
6. Stress design-like (now called "open-ended") problems throughout the curriculum

Some of these recommendations are a bit dated, but most are still on the mark.

WHAT SHOULD STUDENTS KNOW?

According to ABET guidelines, our current engineering students must have access to computing facilities, use computers for technical calculations, problem solving, data acquisition and processing, process control, and design, and be able to apply digital computing techniques to specific problems in a disciplinary program. In addition, chemical engineering students must be able to program in a high-level language, use software packages for analysis and design, use computing facilities such as editors, and simulate engineering problems.

My own view is that students should be able to formulate algorithms, be familiar with a procedural computer language, and be able to understand and write simple programs in that language.

In addition, I believe that graduating engineers should have competence in workstation-centered activities having little to do with traditional program writing—in particular

• Electronic communication
• Preparation of most written materials and reports with editing, word-processing, page layout, or desktop document preparation and publishing software
• Drawing, drafting, plotting, and CAD tools
• Spreadsheets for technical and financial analysis
• Direct access to engineering and other information resources (e.g., property and equipment data bases, engineering abstracts, library card catalogues, on-line display of journal articles and technical archives)
• Signal processing and statistical analysis of machine-acquired experimental data
• Symbolic mathematical software
• Numerical methods and mathematical software
• Powerful analysis simulation and synthesis packages for solution of complex discipline-oriented engineering problems
• Interpretation of computer-generated visual images as important aids to understanding computed results, physical phenomena, and engineering systems
• Group project work in which the computer is a major factor in effective collaboration
• Computer-assisted instruction/training (multi-media)

Are faculty implementing such recommendations so that our students graduate with computing skills essential for successful careers? A recent (unpublished) CACHE survey of three large petroleum/chemical companies suggests that industry views recent graduates as having acceptable-to-good computing knowledge and abilities. My own view is that while our students do graduate with significant computing skills, we are closer to implementing the letter than the spirit of even the ABET requirements, particularly when it comes to integrating computing work into our core engineering science courses.

BUILDING A NETWORKED INFRASTRUCTURE

I believe that a college- or university-wide networked computing infrastructure is an essential ingredient if we are to be successful. Departmental resources alone will be inadequate for the job that needs to be done. Since both our college and departmental administrations at Michigan are committed to "computing" as a vehicle for significantly improving the quality of instruction, I would like to relate some of what we have been, and are now, doing to make this happen. The impetus came first in 1983 when our dean (now President of the University) brought a group of faculty (myself included) together to plan the "complete" integration of "computing" into the life of the college (target date, 1993). After lengthy argument and discussion, our principal conclusion was:

The personal computer/workstation, connected to the rest of the world through a hierarchical, heterogeneous multi-vendor network, will be central to the engineering computing paradigm well before the turn of the century.

We decided that a networked personal computer/workstation infrastructure was the first prerequisite for effective implementation of the broad goal of "computing in the curriculum."

In 1984, the college began to implement the plan by

• Starting to build a college network connected to, but otherwise independent of, the university's central mainframe computing facilities.
• Creating a college network management structure that would foster personal, academic, and research use of the new facilities. This included a full-time network staff and an Executive Committee representing the faculty. An "Applications Sector" concept for supporting general-purpose commercial productivity and discipline-oriented professional software (e.g., CAD, design, control) was also put into place.
• Putting a networked personal computer on the desk of every faculty member in the college. The dean sent out the word that electronic mail should be the principal means of communication for the faculty and staff.
• Putting in place a long-range financial plan. The college made a firm commitment to maintain state-of-the-art facilities, replacing outdated equipment and software with the current "best" affordable.

Since 1984 our network has grown to a size and complexity that even we did not envision at the outset. Here are some facts and figures on its current status:

1. 100 mbps FDDI optical-fiber token ring backbone
2. Two IBM Token Ring Lans interfaced to the backbone
3. Over thirty Ethereans (at least one in each engineering building) interfaced to the backbone
4. Three bridged Apollo workstation 15 mbps optical-fiber token rings gatewayed through Ethernets to the FDDI backbone
5. Subsidiary LANS (e.g., office Apple Talk networks) gatewayed to building Ethernets
6. About 2000 attached machines distributed as follows:
   - 650 in 18 open (24 hours a day) computing clusters, principally for undergraduates
   - 700 in departmental teaching laboratories and in research laboratories (principally for graduate student and faculty research)
   - 650 on faculty and professional staff desks, and for college and departmental administrative and clerical staffs.

The public workstations directly available to our undergraduate students include the following mix:

<table>
<thead>
<tr>
<th>Machine Type</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>IBM PS/2 (386DX and 386SX)</td>
<td>125</td>
</tr>
<tr>
<td>Macintosh II (various models)</td>
<td>250</td>
</tr>
<tr>
<td>Apollo workstations</td>
<td>140</td>
</tr>
<tr>
<td>DEC workstations</td>
<td>50</td>
</tr>
<tr>
<td>Sun workstations</td>
<td>50</td>
</tr>
<tr>
<td>Hewlett Packard workstations</td>
<td>20</td>
</tr>
<tr>
<td>IBM (RS6000) workstations</td>
<td>20</td>
</tr>
</tbody>
</table>

Because all of the high-performance workstations use variants of UNIX for their operating systems, the actual number of computing nodes available to our students from these open machines is much larger than 650. Computing tasks can be distributed over a large number of network workstation nodes (e.g., 75 RS6000s, several hundred Apollos, many high-performance computation servers) operating in client-server mode. The network also supports a state-of-the-art visualization laboratory.

**THE FIRST COMPUTING COURSE**

With the infrastructure in place, we began the transformation of our traditional programming course into a "computing" course to prepare our undergrads for immersion in our networked computing environment. Jim Wilkes and myself are responsible for the required computing course for all of our undergraduates, including those in the Computing Science Division of our Electrical and Computer Engineering Departments. Our premises for switching from the traditional programming course format were:

1. Engineering computing involves much more than traditional programming
2. The networked workstation will be central to engineering computing in the 1990s; every student and practicing engineer will have personal access to one
3. Central mainframes will function principally as information servers to networked clients
4. The predominant operating system characteristics of the future will: support multi-tasking; be multi-user and distributed; have windowed graphical user interfaces; support pointing and other non-keyboard devices.
5. Application programs will have a uniform interface across hardware platforms with: common menu appearance; common text and graphical element selection; on-line, context-sensitive help.

6. The network will support workstation access to any network file, information, computation server; there will be a common file storage format for all servers.
7. Future workstations will support rapid and natural manipulation of text, graphics, sound, video, and other media.
8. Cooperative activity will be supported for both communication and computation (e.g., group report, data-base, spreadsheet access/generation, design project work—even homework).

We decided (after substantial and continuing consultation with college faculty) to include the following topics in the first computing course:

- General computer "literacy"
- Hardware and network facilities that will be used throughout the student's academic career
- Basic productivity software that will be used later on, regardless of discipline (word processing; drawing, drafting, plotting; spreadsheeting; symbolic math; data-base manipulation; data acquisition/analysis)
- Programming in a procedure-oriented language
- Solution of problems designed to expose students to topics from different engineering disciplines
- Participation in a group activity (e.g., cooperative design and implementation of a problem solution on the computer)

To make the balance of our activities a bit clearer, the course syllabus is shown in Table 1. In truth, we have not yet been able to include the last two topics without consuming more than a fair (3 credit-hour) share of the student's time during the term. It is likely that we will eliminate some of the introductory material and include one or both of these topics in future terms, since our students are arriving with more knowledge of computers and more experience in computer programming with each passing year.

**IMPACT ON ENGINEERING COURSES**

Almost all of our faculty have taken the productivity enhancing services of the networked personal computer/workstation (mail, wordprocessing, desktop publishing, and even spreadsheeting and drawing applications) in stride, much more easily than I would have thought ten years ago. Our students have taken to network services like fish to water—especially the major productivity tools like word processing, plotting, and spreadsheeting.

But what about the impact of computing and the networked environment on engineering course content and teaching methodology? In upper-level professional design courses the computer already has had a pervasive influence. In effect, most of the college's design and control courses have become computer-aided courses. The computer has also had a significant impact in our undergraduate laboratory courses, which now emphasize experimental
design and data analysis.

Unfortunately there is still a reluctance by many faculty to truly integrate "computing" into the middle-level engineering science courses. Historically, our computing activities in these courses have been similar to those at many other colleges—hit-and-miss, with little course-to-course coordination. A few courses, such as our senior/graduate numerical methods offering depended heavily on computing assignments, while many courses ignored the computer altogether or had only an occasional computer assignment (typically the writing of a program).

Around 1986 our department adopted a policy that every core course would involve at least two "computing" problems and at least one "open-ended" problem. The computer problems started out as programming assignments for solving assigned analysis problems, but over the years, the trend has been toward use of application packages for solving more realistic (nonlinear) technical problems.

THE COMPUTER AS TEACHER

There is still a vast potential for enhancing our engineering science courses with computer simulations and computer-assisted instruction. Bob Seader[21] points the way with the following comment:

The microcomputer is the most powerful learning device since the printed textbook. If the computer is used properly, individualized interactive learning is economically possible for the first time.

Substituting "networked workstation" for "microcomputer," I agree with Bob. The networked workstation with high-quality color graphics (and in the future, CD-ROM, video and sound) and access to a variety of information servers has the potential of being the near-perfect vehicle for bringing unique "open-ended" problems to individual students who make the technical decisions while the computer generates alternative solutions and displays them in easily understandable (principally graphical) forms.

Unfortunately, the creation of good instructional software is very demanding of faculty time, student manpower, and money. There is unlikely to be any significant effort outside the university to generate such software because there is little prospect of financial return. And since the reward structure, at least at research universities, discourages such activity, there is little prospect of major faculty efforts to develop instructional software except in association with popular textbooks or when supported by outside funding.

Two of our faculty (Scott Fogler and myself) began to work on instructional modules for personal computers several years ago. Scott developed a set of several stand-alone modules for his reaction engineering course. They were well received by students and have been acquired by many schools that adopted his reaction engineering textbook. At about the same time, several students and I developed a CAI authoring package and several chemical engineering and numerical and optimization modules for stand-alone PCs.

More recently, Scott received a NSF curriculum-improvement grant and has undertaken development of several (four to six each) instructional modules for introduction to chemical engineering thermodynamics, reaction engineering, separations, and fluid mechanics. Many of these will be released to the chemical engineering community through CACHE in the next year or so.

In the meantime, I supervised development of a system-management tool called MicroMENTOR that supports networked delivery of all IBM-oriented software (including Scott's modules) used in our department. MicroMENTOR allows individual faculty to install software and other instructional materials directly on network servers without going through network administrators, to control access to the materials by their students, to automatically collect student comments/criticisms, and to gather statistics on user activity and software use. I believe that the concept of departmentally-controlled instructional software embedded in a more global environment of network services will prove to be an effective way to deliver educational software to our students.

Two other NSF-sponsored curriculum improvement grants promise to deliver very high
quality products that will be widely distributed (through CACHE) at low cost. One project (co-directed by Rex Reklaitis and Bob Squires at Purdue) is developing comprehensive simulation models of industrial processes. The simulations are very flexible, involve professionally produced videos, and could be used effectively in a simulation lab, design course, or engineering-science courses.

The second project (directed by Bruce Finlayson at the University of Washington) focuses on numerically intensive solution of general fluid mechanics, reaction, and heat and mass transfer models: its major features are extensive graphical input and high-quality color display for the visualization of computed results.

In addition, a few faculty scattered across the country are producing very useful instructionally-oriented software. I hope that the recent showcasing of some of this software at the national AIChE meeting in Los Angeles will be an annual event, giving faculty an opportunity to demonstrate their programs/lessons to a nationwide faculty audience.

THE FUTURE

What about the future? The track record for long-range predictions about computing is only fair, at best. Nevertheless, I’d like to end with some predictions about the future of computing and the impact of computing on engineering education in the short (five to ten years) term.

By 1996

1. Microprocessors will be the dominant computing technology; differences in personal computer and workstation characteristics (and probably technology) will virtually disappear. Most functions of the simpler microcomputers will be incorporated into a single chip.
2. Typical workstation memories will be 16 MBytes; typical operating speeds will be 50-100 MIPS.
3. The dominant mode of professional and academic engineering computing will be networked and distributed with mainframes functioning principally as large-scale networked information servers.
4. Character-based applications will disappear; essentially all applications will operate in graphical mode.
5. "Three-dimensional" graphical interfaces will be available (no glasses). Flat panel displays will be widely available.
6. The visualization capabilities of the newest workstations will be widely used for research and education.
7. Multimedia workstations will be both available and affordable for instruction, but only in limited numbers; high-quality multimedia instructional software will begin to appear on engineering campuses.
8. With the advent of digital high-definition television, there will be a significant merging of video and computing technology. Some campus workstations will have a camera and microphone as peripherals.
9. New authoring tools will make it much easier to create visually attractive and interesting interactive instructional modules (e.g., with animation and video). Standards will be in place for capturing and encoding audio and visual information. New image compression algorithms will reduce hardware demands for visual-image storage. Hypertext (non-sequential information representation) tools will play an important role in authoring software.
10. It will still be time-consuming and expensive for faculty to design, create, and test discipline-oriented instructional software. Some colleges will begin to recognize faculty-authoring efforts as a valued contribution at merit salary time (but not as criteria for promotion or tenure).

By 2001

1. Procedure-language programming will decrease in importance and will probably not be required of students. Object-oriented and visual-programming tools will fill the void left by the decline of algorithmic languages.
2. Interactive instructional modules will have a significant impact on the education and continuing education of engineering students and professionals.
3. Workstations operating in the 1000 MIP/100 MFLOP range will be available on the desktop (and in a briefcase) for about the price equivalent to a current high-end personal computer.
4. Students will take notes on pen-based notebook computers; in-class transponders will allow immediate storage of figures, assignments, etc., in these computers.
5. Network transmission rates will increase several fold to many gigabit/sec. Much of the paperwork (class handouts, homework assignments, collections of assignments) associated with current engineering classes will be handled electronically using network services. (So far the computer has hardly produced the paperless society—but I think this will happen anyway.)
6. A digital cellular wireless network will allow access to the international Internet from virtually anywhere in the world.
7. Many technical publications will be electronically accessible, with new mechanisms for copyright, royalties, etc., in place.
8. Spoken-language interfaces will begin to appear.
9. Parallel processors on a single chip will be common in personal workstations.
10. Microcomputers will compete effectively with supercomputers in the solution of many computational-intensive problems. Supercomputers will be able to maintain superior speeds, but only by increased parallelism. They will remain, relatively speaking, quite expensive.
11. Massively parallel machines will be available and widely used for engineering research. Many will operate at Teraflop speeds. Programming tools and application software will be slow to develop, but in place and very effective.
12. Some faculty will still not be using computers, except grudgingly (E-mail only?).

And finally, no one will remember these predictions. I will not be asked to comment on them—and a good thing too!

REFERENCES

2. Seader, J.D., “A Brief History of Computing in Chemical Engineering,” first Katz lecture, Chemical Engineering Department, University of Michigan (April 1990)

Chemical Engineering Education
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).

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